APS March Meeting 2015
San Antonio, Texas
http://www.aps.org/meetings/march/index.cfm
8:00AM A0.00001 Beyond nematicity: emergent chirality in iron-based superconductors RAFAEL M. FERNANDES, University of Minnesota, STEVEN A. KIVELSON, Stanford University, ÉREZ BERG, Weizmann Institute of Science — In most iron superconductors, the magnetically ordered state is of stripe-type, with an ordering vector \( \mathbf{Q}_1 = (\pi, 0) \) or \( \mathbf{Q}_2 = (0, \pi) \). One of its hallmarks is the emergence of an Ising-nematic symmetry, whose breaking triggers a vestigial nematic phase that lowers the tetragonal symmetry of the system to orthorhombic. Recent experiments have observed a magnetic state that remains tetragonal, which can be understood only as a double-\( Q \) configuration (i.e. simultaneous order at \( Q_1 \) and \( Q_2 \)) that is either non-uniform or non-collinear. Here we show that these magnetic states also display emergent Ising degrees of freedom that are related not to a rotational, but to a translational symmetry breaking in real space. While in the non-uniform state the Ising symmetry is related to a charge-density wave with ordering vector \( \mathbf{Q}_1 + \mathbf{Q}_2 = (\pi, \pi) \), in the non-collinear state it is related to a chiral symmetry arising from a spin-current density-wave with the same ordering vector. We show that, in the presence of a magnetic field, the former becomes a Neel-like magnetic state, while the latter is converted into a staggered charge-current pattern. We discuss the experimental manifestations of these emergent phases and their impact in the phase diagram of the iron superconductors.

8:12AM A0.00002 Nematic-driven anisotropic electronic properties of underdoped detwinned \( \text{Ba(Fe}_{1-x}\text{Co}_x\text{)}_{2}\text{As}_2 \) revealed by optical spectroscopy\(^1\), L. DEGIOIRGI, ETH Zurich — We collect optical reflectivity data as a function of temperature across the structural tetragonal-to-orthorhombic phase transition at \( T_s \) on \( \text{Ba(Fe}_{1-x}\text{Co}_x\text{)}_{2}\text{As}_2 \) for \( x = 0 \), 2.5\% and 4.5\%, with uniaxial and in-situ tunable applied pressure in order to detwin the sample and to exert on it an external symmetry breaking field. At \( T < T_s \), we discover a remarkable optical anisotropy as a function of the applied pressure at energies far away from the Fermi level and very much reminiscent of a hysteretic-like behavior. Such an anisotropy turns into a reversible linear pressure dependence at \( T \gtrsim T_s \). Moreover, the optical anisotropy gets progressively depleted with increasing Co-content in the underdoped regime, consistent with the doping dependence of the orthorhombicity but contrary to the non-monotonic behavior observed for the dc anisotropy. Our findings bear testimony for an important anisotropy of the electronic structure and thus underscore an electronic polarization upon (pressure) inducing and entering the nematic phase.

8:24AM A0.00003 Anisotropic transient reflectivity across optimal doping in the isovalent-doped superconductor \( \text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_{2} \), ERIC THEWALT, JAMES HINTON, JOSEPH ORENSTEIN, UC Berkeley, LBNL, IAN HAYES, UC Berkeley, TONI HELM, JAMES ANALYTIS, UC Berkeley, LBNL — The isovalent-doped high-\( T_c \) superconductor \( \text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_{2} \) is characterized by a rich temperature-doping phase diagram, which includes structural, antiferromagnetic, electron nematic, and superconducting phase transitions. Of particular note is the proposed existence of a quantum critical point at optimal doping. In this work, we use 1.5 eV pump-probe reflectivity measurements to study the recombination dynamics of photoexcited quasiparticles as a function of temperature, doping, and polarization. We find that the low-temperature response is strongly anisotropic across a wide range of dopings, both above and below optimal. This indicates that the anisotropy arises independently of the orthorhombic-tetragonal and antiferromagnetic phase transitions, which occur only on the underdoped side of the phase diagram.

8:36AM A0.00004 Divergent nematic susceptibility of optimally doped Fe-based superconductors. JIUN-HAW CHU, HSUEH-HUI KUO, IAN FISHER, Stanford University — By performing differential elastoresistivity measurements on a wider range of iron based superconductors, including electron doped \( \text{Ba(Fe}_{1-x}\text{Co}_x\text{)}_{2}\text{As}_2 \), hole doped \( \text{Ba}_{1-x}\text{K}_x\text{Fe}_{2}\text{As}_2 \), and chalcogenides, we show that a divergent nematic susceptibility in the \( B_{1g} \) symmetry channel appears to be a generic feature of optimally doped compositions. For the specific case of optimally “doped” \( \text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_{2} \), the nematic susceptibility can be well fitted by a Curie-Weiss temperature dependence with critical temperature close to zero, consistent with expectations of quantum critical behavior in the absence of disorder. For however all the other optimal doped iron based superconductors, the nematic susceptibility exhibits a downward deviation from Curie-Weiss behavior, suggestive of an important role played by disorder.

8:48AM A0.00005 Orbital Nematic Order and Interplay with Magnetism in the Two-Orbital Model for Iron Pnictides, ANDRIY NEVIDOMSKYY, ZHENTAO WANG, Department of Physics and Astronomy, Rice University — Motivated by recent ARPES measurements on FeSe [1] and LiFeAs [2] families of iron-based superconductors, we have studied the orbital nematic order and its interplay with magnetism within random phase approximation, as well as using a non-perturbative variational cluster approximation (VCA). We found that the electron and hole doping affect the two orders differently within the two-orbital Hubbard model. While hole doping tends to suppress both antiferromagnetism and orbital ordering, the electron doping suppresses magnetism faster, so that orbital nematicity is stabilized in the absence of long-range magnetic order for moderately high electron doping. This is reminiscent of the orbital nematic phase observed in FeSe in the absence of magnetism [1,3], as well as in overdoped \( \text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_{2} \) where ARPES finds splitting of \( d_{xz} \) and \( d_{yz} \) orbitals inside the superconducting phase [4]. This raises the possibility that at least in some cases, the observed electronic nematicity may be primarily due to orbital rather than magnetic fluctuations.

**References**


9:48AM A0.00008 New tetragonal magnetic phase in (Ba,K)Fe2As2, ANNA BÖHMER1, FRÉDÉRIC HARDY, LIRAN WANG, PETER SCHWEISS, THOMAS WOLF, CHRISTOPH MEINGAST, Institut für Festkörperphysik, Karlsruhe Institute of Technology, Germany — The recently discovered C4-symmetric magnetic phase in (Ba,Na)Fe2As2 [2] is a rare exception among iron-based superconductors, which usually display a stripe-type spin-density wave (SDW) ground state at low doping. We re-examine the phase diagram of the closely related (Ba,K)Fe2As2 in great detail, using high-quality single crystals and thermodynamic (thermal-expansion and specific-heat) measurements. We find a small region of a, previously missed, C4-symmetric phase in the ambient-pressure phase diagram, likely related to an unidentified phase transition observed under hydrostatic pressure [4]. We investigate the remarkable interplay of the new C4 phase with superconductivity and with the SDW phase by studying the electronic entropy and the effect of uniaxial pressure on the phase diagram.

1present address: Ames Laboratory/ Iowa State University, USA
2Avci et al., Nature Commun. 5, 3845 (2014)

10:00AM A0.00009 Electronic correlations in hole- and electron-doped Fe-based superconductors , FREDERICK HARDY, ANNA BOEHMER, PETER SCHWEISS, THOMAS WOLF, ROLF HEID, ROBERT EDER, IFP, Karlsruhe Institute of Technology, ROBERT A. FISHER, Lawrence Berkeley National Laboratory, CHRISTOPH MEINGAST, IFP, Karlsruhe Institute of Technology — High-temperature superconductivity in the cuprates occurs at the crossover from a highly-correlated Mott insulating state to a weaker correlated Fermi liquid as a function of hole doping. The iron pnictides were initially thought to be fairly weakly correlated. However, we have recently shown using transport and thermodynamic measurements that KFe2As2 is strongly correlated. Both the Sommerfeld coefficient and the Pauli susceptibility are strongly enhanced with respect to their bare DFT values. These correlations are even further enhanced in RFe2As2 and CsFe2As2. The temperature dependence of both the susceptibility and the magnetic field dependence of the Fe spin dynamics are significantly different from the highly correlated cuprates in the metallic regime. We now have good thermodynamic data covering both the hole and electron sides of the BaFe2As2 system and we will discuss how these correlations are modified by doping.

10:12AM A0.00010 Preformed pairing in superconducting FeSe in the BCS-BEC cross-over regime, SHIGERU KASAHARA, Y. SHIMOYAMA, R. KOBAYASHI, T. YAMASHITA, T. WATASHIGE, Y. MATSUDA, Kyoto University, T. SHIBAUCHI, The Univ. of Tokyo, T. WOLF, A. E. BÖHMER, F. HARDY, C. MEINGAST, H. V. LÖHNEYSEN, Karlsruhe Institute of Technology — The BCS-BEC cross-over bridges the two important theories of bound particles (Bardeen-Cooper-Schrieffer theory and Bose-Einstein condensation) in a unified picture with the ratio of the attractive interaction to the Fermi energy as a tuning parameter. A key issue is to understand the intermediate regime, where new states of matter may emerge. It has been shown that the Fermi energy of FeSe (Tc ~ 10 K) is extremely small, with the result that this system is located at the verge of a BCS-BEC cross-over [1]. Here we show that resistivity, Hall effect, Seebeck and Nernst coefficients all exhibit anomalies at T ~ Tc, well above the superconducting transition temperature. Moreover, our highly sensitive torque magnetometry shows a suppression of the Pauli susceptibility in the same regime. These anomalies appear to suggest a reduction of the density of states ( pseudogap) caused by the onset of pair formation. Based on these results, a new phase diagram of FeSe above Tc is proposed.


10:24AM A0.00011 Impacts of Co-doping on the superconductivity and the orbital ordering state in Fe1−xCoSe single crystal studied by the electrical transport, TAKAHIRO URATA, YOICHI TANABE, Department of Physics, Graduate School of Science, Tohoku University, SATOSHI HEGURI, WPI-Advanced Institutes of Materials Research, Tohoku University, KATSUHIKO TAMAGI, WPI-Advanced Institutes of Materials Research, Tohoku University and Department of Physics, Graduate School of Science, Tohoku University — In the FeSe with the simplest crystal structure in the Fe-based superconductor families, although both the superconductivity and the orbital ordering states are investigated, the relation between them is still unclear[1-4]. Here, we report Co doping effects on the superconductivity and the orbital ordering state in Fe1−xCoSe single crystals. The electrical transport measurements demonstrated that the superconductivity vanishes at 4% Co doping while the orbital ordering state may be robust against Co doping. Present results suggest that the orbital ordering state is not related to the emergence of the superconductivity in FeSe. [1] F. C. Hsu et al., Proc. Nat. Aca. Sci. 105, 14262 (2008). [2] K. Nakayama et al., arXiv:1404.0857v1 [3] T. Shimojima et al., Phys. Rev. B 90, 121111(R) (2014). [4] K. K. Huynh et al., Phys. Rev. B 90, 144516 (2014).

10:36AM A0.00012 Relationship between structure anisotropy and Tc and phase diagram of AFe2(As1−xP)x2 (A=Ba, Sr, Ca), TORU ADACHI, TATSUYA KOBAYASHI, SHIGEKI MIYASAKA, SETSUKO TAJIMA, MASAYOSHI HICHIKAMI, MASAKI SHIDA, Osaka Univ., REIKI KUMAI, HIRONORI NAKAO, YOUICHI MURAKAMI, KEIK PF/CMRC — We investigated how the electronic phase diagram changes when the crystal structure changes in AFe2(As1−xP)x2 where A =Ba/Sr or Sr/Ca. In this study, we synthesized the single crystals of Ba0.8Sr0.2Fe2(As1−xP)x2, Sr0.92Ca0.08Fe2(As1−xP)x2, and Sr0.8Ca0.2Fe2(As1−xP)x2, measured the resistivity and determined precise structure parameters using synchrotron X-ray, then elucidated their phase diagrams and detailed crystal structures. The phase diagram of A =Ba0.8Sr0.2,Fe2(As1−xP)x2 is similar to those for A =Ba and Sr, while for A =Sr/Ca systems the superconducting phase appears at a smaller P content than the case for A =Ba and Sr. The important finding is that the maximum Tc values are almost the same in all AFe2(As1−xP)x2 systems. From the X-ray structural analysis, it has been revealed that in the optimally doped crystals, the local structures of FeAs4 tetrahedra such as pnictogen heights or bond angles of As-Fe-As are almost the same, whereas the anisotropy of the crystal structures, c/a, systematically changes. We conclude that Tc is not affected by the anisotropy (c/a) but strongly depends on the local structure such as the pnictogen height.
10:48AM A0.00013 Electronically driven nematicity in multilayer FeSe Film on SrTiO3, WEI LI, YAN ZHANG, J.J. LEE, Stanford University, HAO DING, Tsinghua University, MING YI, Stanford University, ZHI LI, Tsinghua University, SUNG-KWAN MO, Lawrence Berkeley National Lab, MAKOTO HASHIMOTO, DONGHUI LU, R.G. MOORE, SLAC National Accelerator Laboratory, XI CHEN, QI-KUN XUE, Tsinghua University, ZHI-XUN SHEN, Stanford University; SLAC National Accelerator Laboratory — Nematicity in iron-based superconductors is an intensely investigated contemporary subject. Although it is closely connected to the structural transition, it is unclear whether the lattice degree of freedom is responsible for the nematicity. Here we combine molecular beam epitaxy, angle-resolved photoemission spectroscopy and scanning tunneling microscopy together to study the nematicity in multilayer FeSe films on SrTiO3. Our results demonstrate direct connection between electronic anisotropy in momentum space and standing waves in real space. The lifting of orbital degeneracy of dxz/dyz bands causes the unidirectional interference fringes, observed in real space as standing waves produced by scattering electrons off C2 domain walls and Se-defects. On the other hand, the formation of C2 nematic domain walls unexpectedly shows no correlation with lattice strain pattern. Our results establish a clean case that the nematicity is driven by electronic rather than lattice degrees of freedom in FeSe films.

Monday, March 2, 2015 8:00AM - 11:00AM —
Session A1 DMP: Focus Session: Graphene, Adsorbates, and Electronic Structure 001A - Jeremy Robinson, Naval Research Laboratory

8:00AM A1.00001 Electronic and Structural Properties of Vacancies and Hydrogen Adsorbates on Trilayer Graphene, MARCOS MENEZES, RODRIGO CAPAZ, Universidade Federal do Rio de Janeiro — Using ab initio calculations, we study the electronic and structural properties of vacancies and hydrogen adsorbates on trilayer graphene. Those defects are found to share similar low-energy electronic features, since they both remove a pz electron from the honeycomb lattice and induce a defect level near the Fermi energy. However, a vacancy also leaves unpaired pz electrons on the lattice, which lead to important structural differences and also contribute to magnetism. We explore both ABA and ABC stackings and compare properties such as formation energies, magnetic moments, spin density and the local density of states (LDOS) of the defect levels. These properties show a strong sensitivity to the layer in which the defect is placed and smaller sensitivities to sublattice placing and stacking type. Finally, for the ABA trilayer, we also study how these states behave in the presence of an external electrical field, which opens a tunable gap in the band structure of the non-defective system. The pz defect states show a strong hybridization with band states as the field increases, with reduction and eventually loss of magnetization, and a non-magnetic, midgap-like state is found when the defect is at the middle layer.

8:12AM A1.00002 Hidden Kekule Order of Ghost Atoms on Monolayer Graphene, CHRISTOPHER GUTIERREZ, Columbia University, LOLA BROWN, EDWARD LOCHOCKI, Cornell University, ETHAN ROSENTHAL, Columbia University, CHEOL-JOO KIM, YUI OGAWA, KYLE SHEN, JIWOONG PARK, Cornell University, ABHAY PASUPATHY, Columbia University — Various charge and spin ordered phases have been predicted to exist when the lattice symmetry is broken on the atomic scale. One such phase is the Kekule distortion, whereby the C-C bond symmetry is broken and the graphene unit cell is tripled. It has been proposed that when certain adatoms are placed on monolayer graphene, strong interactions can exist between them mediated by the graphene lattice. The graphene-adatom interaction can induce Kekule order in the graphene itself, and move the adatoms to produce a hidden Kekule ordering. In this talk I will discuss evidence from scanning tunneling microscopy, electron diffraction and angle resolved photoemission spectroscopy that shows the existence of this unique ordering in epitaxial graphene on copper. Interestingly, we find in this case that the Kekule order is induced by a dilute number of “ghost atoms” — unidentified atomic features — in the otherwise perfect copper lattice underneath monolayer graphene.

8:24AM A1.00003 Ytterbiun-driven strong enhancement of electron-phonon coupling in graphene, CHOONGYU HWANG, Pusan Natl Univ, DUCK YOUNG KIM, Carnegie Institution of Washington, DAVID A. SIEGEL, KEVIN T. CHAN, JESSE NOFFSINGER, University of California, Berkeley, ALEXEI V. FEDOROV, Lawrence Berkeley Natl Lab, MARVIN L. COHEN, University of California, Berkeley, BORJE JOHANSSON, Royal Institute of Technology, JEFFREY B. NEATON, ALESSANDRA LANZARA, University of California, Berkeley — The interactions between electrons and phonons attract practical and fundamental interests in graphene, as they can not only govern transport properties, but also realize novel phenomena, such as superconductivity. By using angle-resolved photoemission spectroscopy in conjunction with first principles calculations, we provide an experimental evidence for the strong enhancement of electron-phonon coupling in graphene. Ytterbiun adsorption leads to the enhancement of electron-phonon coupling as much as a factor of 10 with respect to as-grown graphene, resulting in the highest strength ever measured for graphene and suggesting a viable route to the realization of superconducting graphene.

8:36AM A1.00004 Molecular Bound States of Supercritical Charged Impurities on Graphene1, KIRILL VEILZIHANIN, LYUDMYLA ADAMSKA, Los Alamos National Laboratory, DMITRY SOLENOV, Saint Louis University — Functionalization of graphene by chemical groups/atoms allows one to tune its electronic, chemical and mechanical properties. For example, metallic adatoms (e.g., Li, Ca, Y) can be important in applications ranging from hydrogen storage to superconductivity. Such adatoms bind ionically to graphene and the resulting positive ions move along graphene relatively freely, so understanding the energetics of their interaction with graphene and between each other becomes critical for assessing stability of resulting materials in practical applications. It has recently been demonstrated that ions with charge greater than Z ∼ 1 induce a very peculiar non-linear electronic polarization of graphene, which is reminiscent to the Dirac vacuum reconstruction around superheavy nuclei. In our work we demonstrate that such non-linear polarization quantitatively changes not only graphene electronic structure but also the energetics of the effective graphene-mediated interaction between such ions. In my talk, I will discuss the properties of such effective interaction and its dependence on various parameters of the system. In particular, I will report on our findings that molecular bound states of supercritically charged ions can be formed on graphene at certain conditions.

1This work was performed under the NNSA of the U.S. DOE at LANL under Contract No. DE-AC52-06NA25396.

8:48AM A1.00005 Doping, adsorption, and polarity of atomic-layer materials: A predictive theory from systematic first-principles study1, SUSUMU SAITO, YOSHITAKA FUJIMOTO, Department of Physics, Tokyo Institute of Technology, TAKASHI KORETSUNE, RIKEN Center for Emergent Matter Science — Based on the extensive first-principles electronic-structure study of various doped hexagonal boron-nitride (h-BN) atomic layers as well as that of various doped graphene and carbon nanotubes, we propose a simple but predictive theory of polarity in doped atomic-layer materials. We first report the electronic structure of the pristine h-BN, h-BN layers with B and B2N vacancies which have been experimentally produced and observed frequently, and doped h-BN layers, and show that both p-type and n-type h-BN layers can be produced in a variety of ways. We next review the electronic structure of doped graphene and carbon nanotubes and the effect of the H adsorption which can even change the polarity of the system. Finally we propose a simple but predictive theory which is based on the number of valence electrons of each system, and can explain the polarities of all the h-BN, graphene, and nanotube-based systems studied so far.

1Supported by MEXT 25107005 and 25104711, JSPS 22740252 and 26390062, and MEST TIES project.
9:00AM A1.00006 Screening properties of graphene layers studied by Kelvin Probe Force Microscopy and Landau Level Spectroscopy1. JOHN VETICK, CHIH-PIN LU, MICHAEL ALTWATER, JUNXU DUAN, GUOHONG LI, EVA Y. ANDREI, Rutgers University, Department of Physics and Astronomy, 136 Frelinghuysen Road, Piscataway, NJ 08855 USA — Graphene is one of the best conductors known, but due to its two dimensional structure and the need to support it on insulating substrates, its electronic properties are often masked by substrate-induced random potential fluctuations. In order to realize graphene’s full potential for electronic application it is therefore important to understand its screening properties and to find ways to minimize substrate invasiveness. We employed Kelvin Probe Force microscopy (KPFM) to investigate the screening properties of CVD grown graphene crystals as a function of layer number and substrate material using a gated device geometry. The KPFM study was complemented by low temperature scanning tunneling microscopy and Landau level spectroscopy in similar samples and device configurations. Measurements were carried out on single layer, bilayer, trilayer and twisted bilayer samples deposited on SiO2 and hBN substrates. Our findings show that twisted graphene layers provide superior screening of charged impurities and random potentials while at the same time preserving the unique electronic band structure of single layer graphene.

3Work Supported by DOE-FG02-99ER45742 and NSF DMR 1207108.

9:12AM A1.00007 Adsorption of monovalent aluminum halides on graphene defects. SUFIAN ALNEMRAT, JOSEPH HOOPER, Naval Postgraduate School — Density functional theory is used to study the adsorption of the monovalent aluminum halide AlCl on pristine and defective graphene (GR). Recent experimental efforts have shown that monovalent aluminum halide solutions can nucleate and grow small Al nanoparticles on a graphene surface. This nucleation and growth process may also shed light on how similar monovalent AlCl and AlBr solutions assemble into ligand-stabilized metalloid clusters. In this study we examined several point-type defects on GR to determine favorable sites for cluster nucleation. We found that the AlCl weakly physisors on pure GR, Stone-Wales point defects, and N-, B- doped-GR. On the other hand, the AlCl monomer chemisorbs on monovacancies, divacancies, and pyridine-like N, B, and O doped monovacancies. The binding energy is on the order of 5.0 eV and a strong covalent bond found that the AlCl weakly physisors on pure GR, Stone-Wales point defects, and N-, B- doped-GR. On the other hand, the AlCl monomer chemisorbs on monovacancies, divacancies, and pyridine-like N, B, and O doped monovacancies. The binding energy is on the order of 5.0 eV and a strong covalent bond found that the AlCl weakly physisors on pure GR, Stone-Wales point defects, and N-, B- doped-GR. On the other hand, the AlCl monomer chemisorbs on monovacancies, divacancies, and pyridine-like N, B, and O doped monovacancies. The binding energy is on the order of 5.0 eV and a strong covalent bond found that the AlCl weakly physisors on pure GR, Stone-Wales point defects, and N-, B- doped-GR. On the other hand, the AlCl monomer chemisorbs on monovacancies, divacancies, and pyridine-like N, B, and O doped monovacancies. The binding energy is on the order of 5.0 eV and a strong covalent bond found that the AlCl weakly physisors on pure GR, Stone-Wales point defects, and N-, B- doped-GR. On the other hand, the AlCl monomer chemisorbs on monovacancies, divacancies, and pyridine-like N, B, and O doped monovacancies. The binding energy is on the order of 5.0 eV and a strong covalent bond found that the AlCl weakly physisors on pure GR, Stone-Wales point defects, and N-, B- doped-GR. On the other hand, the AlCl monomer chemisorbs on monovacancies, divacancies, and pyridine-like N, B, and O doped monovacancies. The binding energy is on the order of 5.0 eV and a strong covalent bond found that the AlCl weakly physisors on pure GR, Stone-Wales point defects, and N-, B- doped-GR. On the other hand, the AlCl monomer chemisorbs on monovacancies, divacancies, and pyridine-like N, B, and O doped monovacancies. The binding energy is on the order of 5.0 eV and a strong covalent bond found that the AlCl weakly physisors on pure GR, Stone-Wales point defects, and N-, B- doped-GR. On the other hand, the AlCl monomer chemisorbs on monovacancies, divacancies, and pyridine-like N, B, and O doped monovacancies. The binding energy is on the order of 5.0 eV and a strong covalent bond found that the AlCl weakly physisors on pure GR, Stone-Wales point defects, and N-, B- doped-GR. On the other hand, the AlCl monomer chemisorbs on monovacancies, divacancies, and pyridine-like N, B, and O doped monovacancies. The binding energy is on the order of 5.0 eV and a strong covalent bond found that the AlCl weakly physisors on pure GR, Stone-Wales point defects, and N-, B- doped-GR. On the other hand, the AlCl monomer chemisorbs on monovacancies, divacancies, and pyridine-like N, B, and O doped monovacancies. The binding energy is on the order of 5.0 eV and a strong covalent bond.

9:24AM A1.00008 Absence of a transp ort signature of spin-orbit coupling in graphene with indium adatoms. JIA ZHENZHAO, YAN BAOMING, NIU JINGJING, HAN QI, ZHU RUI, WU XIAOSONG, YU DAPENG, Peking Univ. — Enhancement of the spin-orbit coupling in graphene may lead to various topological phenomena and also find applications in spintronics. Adatom absorption has been proposed as an effective way to achieve the goal. In particular, great hope has been held for indium in strengthening the spin-orbit coupling and realizing the quantum spin Hall effect. To search for evidence of the spin-orbit coupling in graphene absorbed with indium adatoms, we carry out extensive transport measurements, i.e., weak localization magnetoresistance, quantum Hall effect and non-local spin Hall effect. No signature of the spin-orbit coupling is found. Possible explanations are discussed.

9:36AM A1.00009 Direct observation of ordered configurations of hydrogen adatoms on graphene. CHENFANG LIN, YEXIN FENG, YINGDONG XIAO, Peking Univ., MICHAEL DUERR, Justus Liebig University Giessen, XIANGQIAN HUANG, XIAOZHI XU, RUGUANG ZHAO, ENGE WANG, XIN-ZHENG LI, ZONGHAI HU, Peking Univ. — Ordered configurations of hydrogen adatoms on graphene have received great attention because they are closely tied to tuning of graphene properties including large band gap opening and formation of specific magnetic orders, both of which are highly desirable in potential applications. Many ordered structures of hydrogenated graphene have been proposed, including double sided and single sided ones, with the calculated band gap width depending on the respective H coverage. However, none of these ordered structures has been observed directly. Here we report direct imaging of several ordered configurations of H adatoms on graphene by scanning tunneling microscopy. The H atoms in the configurations exhibit apparent sublattice selectivity and tiny deviations from the exact atop-of-carbon positions. Scanning tunneling spectroscopy measurements of the configurations showed a larger than 0.6 eV gap in the local density of states. These findings can be well explained by our density functional theory simulations based on models of double sided H configurations.

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9:48AM A1.00010 Disorder induced topological transition in graphene with random adatoms1, EDUARDO CASTRO, CeFEMA, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal, MARIA LÓPEZ-SANCHO, MARÍA VOZMEDIANO, Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, E-28049 Madrid, Spain — Abstract One of the first proposals for a two-dimensional topological insulator was made for graphene, the so called Kane-Mele model, but the very low spin-orbit coupling makes this phase undetectable. It has been suggested that randomly depositing certain heavy adatoms can amplify the effect by many orders, and that a dilute concentration should be enough to open a detectable topological gap. Still lacking, however, is a precise determination of the critical density of random adatoms based in the evolution of the topological index. Based in a finite size analysis of the topological index as a function of the density of randomly distributed adatoms, and also on the localization properties of the system accessed through the Lyapunov exponent, we not only determine the critical density but also establish the nature of this peculiar topological transition.

1EC acknowledge the financial support of FCT-Portugal through grant No. EXPL/FIS-NAN/1720/2013.

10:00AM A1.00011 Electronic Structure of Iridium Clusters on Graphene1. BRADFORD A. BARKER, University of California - Berkeley, Lawrence Berkeley National Laboratory, AARON J. BRADLEY, Univ of California - Berkeley, MIGUEL M. UGEDA, University of California - Berkeley, SINISA COH, ALEX ZETTL, MICHAEL F. CROMMIE, MARVIN L. COHEN, STEVEN G. LOUIE, University of California - Berkeley, Lawrence Berkeley National Laboratory — Graphene was predicted to exhibit non-trivial Z2 topology, but its exceedingly weak spin-orbit coupling prevented this from being observed. Previous theoretical work has proposed enhancing the spin-orbit coupling strength by depositing individual adatoms adsorbed onto the surface of graphene. We show experimental evidence that the iridium adatoms cluster, with a cluster size of at least two atoms. We investigate through theoretical calculations the orientation of the iridium dimers on graphene, contrast the electronic structure of iridium dimers with iridium monomers, and compare the theoretical results with scanning tunneling spectroscopy of the experimental results determined via scanning tunneling spectroscopy.

1This was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at LBNL’s NERSC facility.
but also the lattice thermal conductance is anisotropic, making this material a promising candidate for thermoelectric applications.

Using first-principles calculations and models, we study several fundamental properties of few-layer black phosphorus. We predict the quasiparticle band gap, energy positions of these edge states. The reconstructions self-passivate most edge dangling bonds by switching the coordination number of phosphorus from 3 to 4 or 5.

Extensive density functional theory calculations show that edge reconstructions are responsible for multiple edge states located inside the 2 eV gap and below the Fermi level. To understand these edge states, we have modeled a series of 1D phosphorene and its edges [Liang et al., Nano Letters, 2014, 14, 6400]. A detailed scanning tunneling microscopy/spectroscopy (STM/S) study with first-principles calculations reveals the presence of a semiconducting 2 eV gap, the direct bandgap for phosphorene. More importantly, we were able to identify a magnetic moment. We investigate the electronic properties of graphene nanoislands grown on Ni(111), using local tunneling spectroscopy measurements performed the first-principles based Density Functional Theory (DFT) calculations to study the stability, geometrical structures, and electronic properties of a (Pd/Pt) atom adsorbed graphene to investigate the possibility of using Pd/Pt decorated graphene as energy storage materials with reference to pristine graphene. The London dispersion forces have been incorporated by the DFT-D2 levels of calculations implemented in Quantum Espresso packages. Our findings show that Pd and Pt both adsorb on graphene at Bridge site. The electronic structures of Pd(Pt) adsorbed graphene possess band gap opening due to breaking of the symmetry of graphene. Further we have studied the adsorption of molecular hydrogen ((H 2 ) n , n = 1-7) on the Pd(Pt)-graphene system. The adatom Pd(Pt) enhances the binding energy per hydrogen molecule in Pd(Pt)-graphene system in comparison to that in the pristine graphene. The binding energy per hydrogen molecule of the adatom-graphene system decreases as the number of H 2 molecules increases and finally it saturates to 0.15 eV (0.16 eV) per hydrogen molecule for Pd-graphene (P-graphene) systems respectively.
8:24AM A2.00003 Tuning the exciton energy in single and multi-layer black phosphorus by strain and electric field. FRANCOIS PEETERS, DENIZ CAKIR, Universiteit Antwerpen, Dept. Physics, B-2020 Antwerpen, ANDRE CHAVES, UFP, Fortaleza, Brazil, HASAN SAHIN, Universiteit Antwerpen, Dept. Physics, B-2020 Antwerpen, CMT COLLABORATION — The effect of strain on the electronic and optical properties of single layer black phosphorus is investigated using first principles calculations. Biaxial strain is able to tune the optical band gap from 0.38 eV (at -8% strain) to 2.07 eV (at 5.5%). The exciton binding energy is found to be 0.40 eV for compressive biaxial strain of -8% and becomes 0.83 eV for tensile strain of 4%. The stack effect in the exciton energy is obtained by direct diagonalization of the effective mass Hamiltonian. The dependence on the number of phosphorus layers and the strength of the electric field is investigated. Band anisotropy becomes evident in the direction dependent field induced polarizability of the exciton.

8:36AM A2.00004 Anisotropic polarization dependence of light scattering in black phosphorus . JAE-UNG LEE, JUNGCHEOL KIM, Department of Physics, Sogang University, JINHWAN LEE, CHANGGU LEE1, Department of Mechanical Engineering and Center for Humann Interface Nanotechnology (HINT), Sungkyunkwan University, HYEONSIK CHEONG, Department of Physics, Sogang University — We investigated anisotropic polarization dependence of light scattering in black phosphorus by optical microscopy and Raman spectroscopy. Due to a high carrier mobility (~ 300 V cm$^{-2}$s$^{-1}$) and a high on/off ratio (~ $10^3$), black phosphorus is attracting interest as a promising candidate for a field effect transistor. Black phosphorus has an anisotropic crystal structure, which leads to directional dependence of the mobility and infrared light absorption. We prepared samples on SiO$_2$/Si substrates by mechanical exfoliation. We chose a few-hundred-nanometer thick sample with well-defined edges. By using a polarized optical microscope, we found that the optical contrast depends on the crystal direction. By comparing results with TEM measurements, we can determine the crystallographic orientation of the sample. We also performed polarized Raman measurements with several excitation energies. The intensity of each mode is largely dependent on the incident polarization direction. Furthermore, these polarization dependences vary with the excitation energy. From the polarization dependence of the Raman intensity one can determine the crystallographic orientation of the sample.

1SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University

8:48AM A2.00005 Symmetry analysis of phosphorene: electronic structure with spin-orbit interaction , PENGKE LI, IAN APPELBAUM, Univ of Maryland-College Park, APPELBAUM’S GROUP TEAM — We present a symmetry analysis of electronic band structure including spin-orbit interaction close to the insulating gap edge in monolayer black phosphorus (“phosphorene”). Expressions for energy dispersion relation and spin-dependent eigenstates for electrons and holes are found via simplification of a perturbative expansion in wave vector $k$ away from the zone center using elementary group theory. Importantly, we expose the underlying symmetries giving rise to substantial anisotropy in optical absorption, charge, and spin transport properties, and reveal the mechanism responsible for valence band distortion and possible lack of a true direct gap. We discovered that, spin flip processes are decoupled by symmetry from flexural phonons, allowing us to predict a spin lifetime comparable to bulk Si, vastly greater than graphene.

9:00AM A2.00006 Tuning Electronic and magnetic properties of phosphorene by vacancies and adatoms1, POOJA SRIVASTAVA, K.P.S.S. HEMBRAM, HIROSHI MIZUSEKI, KWANG-RYEOL LEE, SANG SOO HAN, SEUNGCHUL KIM, Korea Institute of Science and Technology — In the search of novel materials, phosphorene (2D layers of black phosphorus) has been synthesized recently. Intrinsic bandgap, hydrophilicity and anisotropic electron mobility make phosphorene different from graphene and also, its hole mobility is higher than that in MoS$_2$. All these properties make it a very promising material for electronics and optoelectronics applications. As with other as-synthesized materials, phosphorene exhibits defects such as vacancies, and these defects can affect the properties of the material significantly. The present work provides a detailed understanding of various vacancy defects (mono- and di-vacancies) and their effect on the electronic and magnetic properties of phosphorene. We have also studied the effects of omnipresent non-metallic C/N/O and transition metal (TM) Fe/Co/Ni on the electronic and magnetic properties of phosphorene. We show that, for various adatom adsorbed pristine/defective phosphorene structures the magnetic moment can be tuned via the control of Fermi level. The magnetism for non-metallic adatom adsorbed pristine/defective phosphorene systems can be switch ON/OFF. TM adatoms provide extra flexibility by tuning the magnitude as well.

1We acknowledge support from KIST Institutional project (Grant No. 2E24630) and Industrial Strategic Technology Development Program (Grant No. 10041589) funded by the MOTIE, Korea

9:12AM A2.00007 Quantum Monte Carlo Studies of Bulk and Few- or Single-Layer Black Phosphorus1, LUKE SHULENBURGER, ANDREW BACZEWSKI, Sandia National Laboratories, ZHEN ZHU, JIE GUAN, DAVID TOMANEK, Michigan State University — The electronic and optical properties of phosphorus depend strongly on the structural properties of the material. Given the limited experimental information on the structure of phosphorene, it is natural to turn to electronic structure calculations to provide this information. Unfortunately, given phosphorus’ propensity to form layered structures bound by van der Waals interactions, standard density functional theory methods provide results of uncertain accuracy. Recently, it has been demonstrated that Quantum Monte Carlo (QMC) methods achieve high accuracy when applied to solids in which van der Waals forces play a significant role. In this talk, we will present QMC results from our recent calculations on black phosphorus, focusing on the structural and energetic properties of monolayers, bilayers and bulk structures.

1Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:24AM A2.00008 Atoms dictating shape: The discrete geometry of conformal two-dimensional materials, MEHRSHAD MEHBOUDI, KAINEN UTT, Univ of Arkansas-Fayetteville, HUMBERGE TERRONES, Rensselaer Polytechnic Institute, ALEJANDRO PACHECO, Universidad del Norte, EDMUND HARRISS, SALVADOR BARRAZA-LOPEZ, Univ of Arkansas-Fayetteville — The electronic, optical, thermal, mechanical and chemical behavior of two-dimensional (2D) materials depends on their shape (geometry). 2D materials are nets [1], with covalent bonds representing edges, and where atoms are vertices. Here we use a mathematical language to tell the shape of meshes and discuss the geometry of 2D materials of varied lattice structures, such as: hexagonal boron nitride, black phosphorus monolayers, low-buckled silicene, germanene, blue phosphorus, newly predicted III-V buckled 2D compounds such as AlP, conformal “thicker” layered materials such as 2D tin, “single-layer” transition metal dichalcogenides (MX$_2$’s), and a single-quintuple-layer of the topological insulator Bi$_2$Se$_3$. We characterize the geometry of each atom position without recourse to a continuum parametric model. The new framework generalizes the discrete geometry we introduced recently for graphene [2,3]. References: 1. Discrete Differential Geometry, edited by A. I. Bobenko, P. Schroder, J. M. Sullivan, and G. M. Ziegler, Oberwolfach Seminars Vol. 38 (Springer, Berlin, 2008), 1st ed. 2. Pacheco Sanjuan, A. A., Mehboudi, M., Harriss, E. O., Terrones, H., & Barraza-Lopez, S. ACS Nano 8, 1136-1146 (2014). 3. Sanjuan, A. A. P., Wang, Z., Imani, H. P., Vaneˇ ci, M., & Barraza-Lopez, S. PRB 89, 121403(R) (2014).
9:36AM A2.00009 Raman modes of exfoliated black phosphorus down to the monolayer. ANNE- LAURENCE PHANEUF-L’HEUREUX, Polytechnique Montreal, ALEXANDRE FAVRON, ETIENNE GAUFRES, RICHARD MARTEL, Universite de Montreal, SEBASTIEN FRANCECOEUR, Polytechnique Montreal — Exfoliated black phosphorus layers, or 2D-phosphane, are a lamellar direct-gap semiconductor providing high mobilities and enabling a thickness-controlled band gap tunability ranging from 0.3 up to about 2 eV. Using Raman spectroscopy, we have studied vibrational modes of pristine and non-oxidized 2D-phosphane as a function of the number of layers involved (n), and also as a function of temperature, polarization, and excitation wavelength. The evolution of the width and of the frequency of A$_1^g$ as a function of n presents a clear non-monotonic dependence. This can be explained by the presence of new nearly-degenerate Raman-allowed modes that are symmetry-forbidden in both bulk and monolayer samples. We also present Raman spectra of few-layer samples for excitation wavelengths in the vicinity of the expected band gap.

9:48AM A2.00010 Raman signatures of degradation in mono-, bi- and trilayers of exfoliated black phosphorus$^1$. ALEXANDRE FAVRON, ETIENNE GAUFRES, Universite de Montreal, FREDERIC FOSSARD, Laboratoire d’Etude de Microstructure, ANNE-LAURENCE PHANEUF-L’HEUREUX, Polytechnique Montreal, ANNICK LOISEAU, Laboratoire d’Etude de Microstructure, RICHARD LEONELLI, Universite de Montreal, SEBASTIEN FRANCECOEUR, Polytechnique Montreal, RICHARD MARTEL, Universite de Montreal — Thin layers of black phosphorus have recently raised interest for their two-dimensional (2D) semiconducting properties, such as tunable bandgap with layer thickness and high carrier mobilities. This lamellar crystal of P atoms can be exfoliated down to monolayer 2D-phosphate (also called phosphorene) using procedures similar to that for monolayer graphene. The devices are however challenging to fabricate due to fast degradation of the thin layers upon exposure to light in air. We investigated this degradation process using in-situ Raman and transmission electron spectroscopies and reported on a thickness dependent reactivity of the layers. Moreover, the degradation process was identified to be due to an ubiquitous photo-induced oxidation of the layers by adsorbed oxygen in water. Optimum experimental conditions to prepare n-layer 2D-phosphate in their pristine states were applied to determine the Raman signatures of degradation. Here, we report on the use of the ratio of intensity of the A1g over A2g modes as an assessment of the crystal quality.

$^1$Supported by IBS


10:12AM A2.00012 First-principles study of atomic adsorptions on phosphorene. JUN-HO LEE, YOUNG-WOO SON, Korea Inst for Advanced Study — Phosphorene with a moderate intrinsic band gap around 1eV and appropriate carrier mobility merits a next-generation electronic devices. One of the interesting characters of phosphorene is anisotropic electronic and optical properties due to its puckered atomic structures, providing an interesting realization of self-assembled low-dimensional nanostructure on it. In this study, we investigated electronic and magnetic properties of two-dimensional atomic layer formed on phosphorene by using density-functional theory calculations. We explored adsorption properties of various atoms on phosphorene and calculated energetics to predict two-dimensional atomic arrangements on top of phosphorene. In a strong spin-orbit system, we also found anisotropic spin splitting owing to its structural anisotropic.

10:24AM A2.00013 Electronic band structure of surface-doped black phosphorus$^1$. JIMIN KIM, Pohang University of Science and Technology, SAE HEE RYU, YEONGSUP SOHN, KEUN SU KIM, Pohang University of Science and Technology, Institute for Basic Science — There are rapidly growing interests in the study of few-layer black phosphorus owing to its promising device characteristics that may impact our future electronics technology. The low-energy band structure of black phosphorus has been widely predicted to be controllable by external perturbations, such as strain and doping. In this work, we attempt to control the electronic band structure of black phosphorus by in-situ surface deposition of alkali-metal atoms. We found that surface doping induces steep band bending towards the bulk, leading to the emergence of new 2D electronic states on top of phosphorene. In a strong spin-orbit system, we also found anisotropic spin splitting owing to its structural anisotropic.

1Supported by IBS

10:36AM A2.00014 Van der waals heterostructure of phosphorene and graphene: Tuning the Shottky barrier and doping by electrostatic gating$^1$. JOSE EDUARDO PADILHA DE SOUSA, ADALBERTO FAZZIO, Universidade de Sao Paulo, ANTONIO JOSE ROQUE DA SILVA, Universidade de Sao Paulo/Laboratorio Nacional de Luz Sincrotron — Van der Waals heterostructures of 2D materials is one of the most promising approaches in terms of the new nanodevices. One of these 2D materials that have attracted a lot of attention from a broad community is the phosphorene, an elemental material composed only of phosphorus. If one wishes to build devices, two important points must always be addressed: how to make contacts - and the value of the resulting Schottky Barrier Height (SBH) - and how to control the charge doping level. In the present work we study the structural and electronic properties of single and bilayer phosphorene with graphene. We show that both the properties of graphene and phosphorene are preserved upon its contact, and we also show that via the application of a perpendicular electric field it is possible to tune the position of the band structure of phosphorene with respect to that of graphene. This leads to a great control of the Schottky barrier height and doping of phosphorene, which are important features in the design of new devices based on this kind of structure.

$^1$Work supported by FAPESP and CNPq.

10:48AM A2.00015 Low-frequency interlayer breathing mode in few-layer black phosphorus. XI LING, SHENQI HUANG, MIT, LIANGBO LIANG, VINCENT MEUNIER, RPI, MILDRED DRESSELHAUS, MIT — Black phosphorus (BP), as a layered material, has attracted intense interest recently. Many interesting electronic and optoelectronic properties are being explored based on its unique anisotropic structure. In this work, we studied the Raman spectra in few-layer BP, including the intralayer and interlayer vibrational modes. Besides the three typical Raman modes A$_1^g$ (~ 359 cm$^{-1}$), B$_{2g}$ (~ 437 cm$^{-1}$), and A$_2^g$ (~ 466 cm$^{-1}$), low-frequency modes were observed in few-layer BP, as predicted by the first-principles density functional theory (DFT) calculation. The interlayer breathing mode at around 87 cm$^{-1}$ was assigned as A$_0^g$, since the DFT calculation result showed it has the symmetry of A$_0^g$. In addition, the polarization dependence of the Raman modes in BP is studied systematically. Both the DFT calculation and the experimental results show that the polarization dependence profiles are sensitive to the crystal orientation of BP. In addition, the temperature dependence of the modes is studied in the range of -150 °C to room temperature. It is found that the A$_0^g$ mode has almost no dependence on the temperature change, and the out-of-plane mode (A$_2^g$) has weaker dependence than the in-plane modes (B$_{2g}$ and A$_1^g$).
Data to increase the understanding of the protein's structure. Regulate the kinetics of pore formation in a model bilayer lipid membrane. The FOS-14 Detergent was tested under various conditions to understand its impact.

The experiment analyzes the use of N-tetradecylphosphocholine (FOS-14 Detergent) to stabilize the water soluble protein, protective antigen protein (PA63) to national Institute of Standards and Technology focused on optimization of pore formation of Protective Antigen protein secreted by Bacillus Anthraces. This

Crystal Bailey, American Physical Society

Laser, the power broadening associate with the ionization laser and observe Zeeman splittings in the Doppler width of the Kr atom transition. The ability to absolute frequency of the laser relative to the line center of the Kr transition, the power broadening associated with the cycling of the Kr atoms with the CW supplied by a high resolution CW laser. By observing the portion of the Doppler width that is ionized by this combination of lasers one can determine the distribution of Kr atoms is present in our Ion Imaging apparatus, we will use a three-photon scheme to ionize the Kr atoms, with one of the photon steps being velocity resolution one can use this technique to measure spectroscopic features with 1 MHz resolution. We demonstrate this ability on Kr atoms. A thermal Velocity Mapped Ion Imaging has been used for the measurement of the velocity of molecules with resolution down to 1 meter per second. Because of this high velocity resolution one can use this technique to measure spectroscopic features with 1 MHz resolution. We demonstrate this ability on Kr atoms. A thermal

Further cooling was demonstrated with a one-way wall, realizing the historic thought experiment of Maxwell's Demon. More recently, we showed how to apply this method to compress atomic phase space with almost no loss of atom number. Our approach is fundamentally different than laser cooling as it does not rely

This work

Monday, March 2, 2015 8:00AM - 11:00AM –

Session A4 APS: Undergraduate Research/Society of Physics Students I Mayor Cockrell Room 004 - Crystal Bailey, American Physical Society

Detergent Stabilized Nanopore Formation Kinetics of an Anthrax Protein

KELBY PETERSON, Utah State University — This summer research project funded through the Society of Physics Students Internship Program and The National Institute of Standards and Technology focused on optimization of pore formation of Protective Antigen protein secreted by Bacillus Anthraces. This experiment analyzes the use of N-tetradecylphosphocholine (FOS-14 Detergent) to stabilize the water soluble protein, protective antigen protein (PA63) to regulate the kinetics of pore formation in a model bilayer lipid membrane. The FOS-14 Detergent was tested under various conditions to understand its impact on the protein pore formation. The optimization of this channel insertion is critical in preparing samples of oriented for neutron reflectometry that provide new data to increase the understanding of the protein's structure.
Protein Unfolding reveals the effects of diatom geometry on their optical properties. Finally, the dimensions of the photonic crystal are parametrically swept, allowing for further average geometries of the diatom frustules are used to recreate a 2-dimensional photonic crystal, after which the electric field distribution and optical transmission frustules, a biomimetic photonic crystal derived from diatom frustules can be recreated and modeled with the finite element method. In this approach, the photonic crystals. Through the examination and measurement of the physical characteristics of many scanning electron microscope (SEM) images of diatom frustules, a biomimetic photonic crystal derived from diatom frustules can be recreated and modeled with the finite element method. In this approach, the average geometries of the diatom frustules are used to recreate a 2-dimensional photonic crystal, after which the electric field distribution and optical transmission through the photonic crystal are both measured. The optical transmission is then compared to the transmission spectra of a regular hexagonal photonic crystal, revealing the effects of diatom geometry on their optical properties. Finally, the dimensions of the photonic crystal are parametrically swept, allowing for further control over the transmission of light through the photonic crystal.

Fayetteville, JOSEPH HERZOG, Department of Physics, University of Arkansas Fayetteville — Diatom algae are unicellular, photosynthetic microorganisms. MISHLER, Department of Physics, University of Arkansas, Fayetteville, ANDREW ALVERSON, Department of Biological Sciences, University of Arkansas, Fayetteville, JOSEPH HERZOG, Department of Physics, University of Arkansas Fayetteville — Diatom algae are unicellular, photosynthetic microorganisms with a unique external shell known as a frustule. Frustules, which are composed of amorphous silica, exhibit a unique periodic nano-patterning, distinguishing diatoms from other types of phytoplankton. Diatoms have been studied for their distinctive optical properties due to their resemblance of photonic crystals. In this regard, diatoms are not only considered for their applications as photonic crystals, but also for their use as biomimetic templates for artificially fabricated photonic crystals. Through the examination and measurement of the physical characteristics of many scanning electron microscope (SEM) images of diatom frustules, a biomimetic photonic crystal derived from diatom frustules can be recreated and modeled with the finite element method. In this approach, the average geometries of the diatom frustules are used to recreate a 2-dimensional photonic crystal, after which the electric field distribution and optical transmission through the photonic crystal are both measured. The optical transmission is then compared to the transmission spectra of a regular hexagonal photonic crystal, revealing the effects of diatom geometry on their optical properties. Finally, the dimensions of the photonic crystal are parametrically swept, allowing for further control over the transmission of light through the photonic crystal.

Lipids are organic molecules composed of hydrophobic fatty acid tails and hydrophilic head groups that can form a multitude of structures, including lipid vesicles which provides an excellent model representing cell membranes. In this study, we examine the effects of antimicrobial peptides and drugs on lipid vesicles. Fourier transform infrared spectroscopy measurements are performed with and without the antimicrobial peptide. A change in absorbance corresponding to the wavenumber regimes associated with the stretching of the carbonyl and phosphate groups is observed. Also, a dye leakage assay is performed with vesicles composed of neutral and charged lipids. Calcein dye is enclosed within these vesicles in solution. Different concentrations of the active and inactive antimicrobial peptides, and tamoxifen are incubated with the vesicles. Concentration dependent dye leakage is determined by measuring fluorescence intensity before and after the addition of the peptides and tamoxifen. Different leakage behavior is observed for the active and inactive peptides, and the lipid composition of the vesicle is found to have a large effect.

8:24AM A4.00003 Amphiplex Formation, SHANON PETERSEN, Allegheny College, JENNIFER LAAER, TIMOTHY LODGE, University of Minnesota — Polymer-micelle complexes are currently under heavy investigation due to their potential applications in targeted drug delivery and gene therapy, yet the dynamics of the complex formation is still relatively unstudied. By varying the ratios of poly(styrene sulfonate) chains and cationic poly(dimethylaminoethyl methacrylate)-b-poly(styrene) micelles and the ionic strength of the system, we created a variety of complex configurations of different sizes and charges. The complexes were characterized dynamic light scattering and zeta potential measurements which provided information regarding the hydrodynamic radius, distribution of sizes, and effective charge.

8:36AM A4.00004 Biomimetic Photonic Crystals based on Diatom Algae Frustules, JONATHAN MISHLER, Department of Physics, University of Arkansas, Fayetteville, ANDREW ALVERSON, Department of Biological Sciences, University of Arkansas, Fayetteville, JOSEPH HERZOG, Department of Physics, University of Arkansas Fayetteville — Diatom algae are unicellular, photosynthetic microorganisms with a unique external shell known as a frustule. Frustules, which are composed of amorphous silica, exhibit a unique periodic nano-patterning, distinguishing diatoms from other types of phytoplankton. Diatoms have been studied for their distinctive optical properties due to their resemblance of photonic crystals. In this regard, diatoms are not only considered for their applications as photonic crystals, but also for their use as biomimetic templates for artificially fabricated photonic crystals. Through the examination and measurement of the physical characteristics of many scanning electron microscope (SEM) images of diatom frustules, a biomimetic photonic crystal derived from diatom frustules can be recreated and modeled with the finite element method. In this approach, the average geometries of the diatom frustules are used to recreate a 2-dimensional photonic crystal, after which the electric field distribution and optical transmission through the photonic crystal are both measured. The optical transmission is then compared to the transmission spectra of a regular hexagonal photonic crystal, revealing the effects of diatom geometry on their optical properties. Finally, the dimensions of the photonic crystal are parametrically swept, allowing for further control over the transmission of light through the photonic crystal.

8:48AM A4.00005 Employing Multiple Spectroscopic Techniques Simultaneously to Observe Protein Unfolding, MICHAEL CROWE, BEN KELTY, JUSTIN LINK, Xavier University — A protein’s function is directly related to its native, folded structure. In order to study the structure of proteins, the unfolding process may be characterized. In our study, by using the spectroscopic techniques of circular dichroism (CD), absorption, and fluorescence simultaneously, we examined the unfolding of horse heart cytochrome c, a well-studied, model protein by gradually increasing the concentration of the chemical denaturant, guanidine hydrochloride. The signal changes from these modalities over the course of the unfolding reaction provides some of the thermodynamic properties like Gibbs free energy for insight into the stability of the protein. This allows us to compare the three techniques under the exact same conditions. The objective of this session is to present recent work in developing a protocol to observe the unfolding of cytochrome c using fluorescence, absorbance, and CD simultaneously.

9:00AM A4.00006 The Effect of Magnetic Fields on the Quorum Sensing-Regulated Luminescence of Vibrio fischeri, ADDIE BARRON, STEVE HAGEN, MINJUN SON. None — Quorum sensing (QS) is a mechanism by which bacteria communicate through the secretion and detection of extracellular signaling molecules known as autoinducers. This research focuses on the quorum sensing regulated bioluminescence of Vibrio fischeri, a marine bacterium that lives in symbiosis with certain fish and squid species. Previous studies of V. harveyi, a close relative of V. fischeri, indicate that a strong magnetic field has a positive effect on V.harveyi bioluminescence. However the effect of magnetic fields on quorum sensing-regulated luminescence is in general poorly understood. We grew V. fischeri in solid and liquid growth media, subject to strong static magnetic fields, and imaged the bioluminescence over a period of forty-eight hours. Luminescence patterns were analyzed in both the spatial and time dimensions. We find no indication that a magnetic field influences Vibrio fischeri luminescence either positively or negatively.

This research was funded by the grant number NSF DMR-1156737.

9:12AM A4.00007 Electron mobility in liquid-gated graphene biosensors, CHRISTINA HARMON, Linfield College, MORGAN BROWN, ETHAN MINOT, Oregon State University, MICHAEL CROSSER, Linfield College — We report measurements of the electron mobility in liquid-gated graphene. Graphene field-effect transistor (GFET) biosensors are more sensitive to changes in external fields when the mobility is high; therefore, increasing mobility will improve sensitivity. Mobility can be calculated from the ratio of sheet conductivity to carrier density. Sheet conductivity was measured using a van der Pauw geometry and carrier density was determined from measurements of the liquid-gate capacitance. We show that mobility improves after the graphene surface is cleaned by an annealing process.

9:24AM A4.00008 Detecting a Protein in its Natural Environment with a MOSFET Transistor, BENJAMIN PEREZ, The Society of Physics Students/ NIST, ARVIND BALLEIPALLI, NIST — Our group’s goal is to make a MOSFET transistor that has a nanopore through it. We want to have proteins flow through this device and examine their structure based on the modulation they cause on the current. This process does not harm the protein and allows the protein to be studied in its natural environment. The electric field and electric potential of a point charge were computed within a nano-transistor. The simulations were used to see if the point charge had enough influence on the current to cause a modulation. The point charge did cause a rise in the current making the modulation concept a viable one for medical applications. COMSOL multiphysics software was used to perform all simulations.

1This Society of Physics Students internship program and NIST
2This research was done at NIST through the Society of Physics Students internship program
3He worked as my mentor for my summer at NIST
9:36AM A4.00009 Topological Properties of Some Integrated Circuits for Very Large Scale Integration Chip Designs¹, S. SWANSON, M. LANZEROTTI, Augsburg College, G. VERNIZZI, J. KUJAWSKI, A. WEATHERWAX, Siena College — This talk presents topological properties of integrated circuits for Very Large Scale Integration chip designs. These circuits can be implemented in very large scale integrated circuits, such as those in high performance microprocessors. Prior work considered basic combinational logic functions [1] and produced a mathematical framework based on algebraic topology for integrated circuits composed of logic gates [2]. Prior work also produced an historically-equivalent interpretation of Mr. E. F. Rent’s work for today’s complex circuitry in modern high performance microprocessors, where a heuristic linear relationship was observed between the number of connections and number of logic gates [3]. This talk will examine topological properties and connectivity of more complex functionally-equivalent integrated circuits. References: [1] E. Hitesue, K. Irvin, M. Lanzerotti, G. Vernizzi, J. Kujawski, A. Weatherwax, “Topological Properties of Basic Combinational Logic Functions for Very Large Scale Integrated Circuits,” in 2014 Proc. APS Mtg., Denver, CO, 2014. [2] C. Vernizzi, M. Y. Lanzerotti, J. Kujawski, A. Weatherwax, “Topological Constraints for E. F. Rent’s Work on Microminiature Packaging and Circuitry,” IBM Jnl. Res. Dev., vol. 58, no. 2/3, pp. 13:1-17, Mar/May 2014. ¹The views expressed in this article are those of the author and do not reflect the official policy or position of the United States Air Force, Department of Defense or the U.S. Government.

9:48AM A4.00010 Exploration of Whispering Gallery Modes in an Optically Trapped Aerosol Droplet, ANGELA LUDVIGSEN, LOWELL MCCANN, University of Wisconsin - River Falls — Optical traps use a laser beam to catch and hold small transparent objects. Past observations of optically trapped aqueous aerosol droplets have shown that the droplet moves between two or more stable positions depending upon the power of the trapping laser. It is hypothesized that this movement coincides with a resonance of the light with the droplet called a Whispering Gallery Mode. When the resonance occurs, additional forces act on the droplet. To investigate this behavior, Raman scattered light from the droplet is measured using a spectrometer while simultaneously recording the droplet’s position. The Raman spectrum exhibits a series of peaks that appear due to the very spherical shape of the droplet called Cavity Enhanced Raman Spectroscopy. The location and spacing of the peaks are related to the diameter and the optical properties of the droplet. In order to achieve an accurate determination of the radius from this spectrum, the magnitude of the electric and magnetic fields of the light scattered off the droplet are calculated. This allows for a precise measurement of the droplet’s radius at the moment that the droplet moves between stable positions.

10:00AM A4.00011 Measuring the Temperature of the Ithaca College MOT Cloud using a CMOS Camera, JONATHAN SMUCKER, BRUCE THOMPSON, Ithaca College — We present our work on measuring the temperature of Rubidium atoms cooled using a magneto-optical trap (MOT). The MOT uses laser trapping methods and Doppler cooling to trap and cool Rubidium atoms to form a cloud that is visible to a CMOS Camera. The Rubidium atoms are cooled (by removing the magnetic field). In order to measure the temperature of the MOT we take pictures of the cloud using a CMOS camera as it expands and calculate the temperature based on the free expansion of the cloud. Results from the experiment will be presented along with a summary of the method used.

10:12AM A4.00012 Investigation of Nanowire Thickness and Enhancement Characteristics, CAMERON SAYLOR, DESALEGN DEBU, University of Arkansas Fayetteville, ERIC NOVAK, Shippensburg University, JOSEPH HERZOG, University of Arkansas Fayetteville — This work investigates the effect of nanowire thickness on the optical enhancement of nanowire. We present a study that shows there is potential in altering the thickness of plasmonic structures to improve their optical field enhancement. The study was performed using a finite element method.

10:24AM A4.00013 Nonlinear Interactions between Slender Structures and Axial Flow, LI DU, Nanjing University — For decades, dynamic behaviors of a slender structure with axial flow have been extensively studied. However, the governing equation based on expansions of small quantities is complicatedly-expressed and can be inappropriate as amplitude becomes considerably large. In this research, we are dedicated to finding an approach to study the nonlinear dynamics of a fluid-conveying slender structure with arbitrary amplitude. By introducing the Intrinsic Coordinate, we find a concise way to describe the configuration of the system. Differential relations of such coordinate are studied and the rigorous nonlinear equation of motion is derived. Then rather than small-deflection approximation, linear dynamics are studied using Argand Diagram under a weaker condition named low-varying approximation. Nonlinear properties including Hopf bifurcation, limit-cycle motion and vibration frequencies are studied theoretically and experimentally.

10:36AM A4.00014 ABSTRACT WITHDRAWN —

10:48AM A4.00015 The Importance of Science Policy and its Challenges¹, BENJAMIN PREIS, Tufts University — I worked for physicist and Congressman Bill Foster (D-IL) as the Mather Public Policy Intern through the American Institute of Physics and the Society of Physics Students during the summer of 2014. This internship is meant to connect undergraduate physics students with the policy process in Washington DC. As a Mather Public Policy Intern, I worked for Congressman Foster researching policy initiatives such as science funding, STEM education, and environmental regulations. This talk will discuss my experience and many of the things that I learned as an undergraduate physicist working on Capitol Hill. For example, through my experience with the internship, I attended lectures and hearings that illuminated for me how members of Congress conceive of scientific research. I also met with many physicists on Capitol Hill working to improve government interest in physics research — AAAS Fellows, Members of Congress, and Government Relations Specialists — and I will talk about how I saw physicists impacting governmental policies relating to scientific research and development. This internship is part of the Society of Physics Students internship program and was funded by the John and Jane Mather Foundation for Science and the Arts.

¹This work was part of the Society of Physics Students internship Program

Monday, March 2, 2015 8:00AM - 10:48AM —
Session A5 FIAP: Fractional Quantum Hall Effect I
Juan Gorman Room 005 - John Watson, Purdue University
8:00AM A5.00001 Properties of in-situ back-gated two-dimensional electron gases in GaAs/AlGaAs for the study of electron correlations in the 2d Landau level, JOHN WATSON, Department of Physics and Birck Nanotechnology Center, Purdue University, MICHAEL MANFRA, Department of Physics, Birck Nanotechnology Center, Schools of Electrical and Computer Engineering and Materials Engineering, Purdue University — We report on growth and processing optimization of in-situ back-gated two-dimensional electron gases in GaAs/AlGaAs quantum wells. We find that gate leakage currents as small as 4 pA can cause noticeable heating of the electrons if the lattice is not properly thermally anchored to the cryostat. However, we also show that when the devices are properly optimized gate voltages as large as 4V can be applied before leakage turns on, allowing the density to be tuned over a large range from near depletion to over \( 4 \times 10^{11} \text{ cm}^{-2} \). In these optimized devices heating effects at dilution refrigerator temperatures are negligible and the gap at \( \nu = 5/2 \) can be tuned continuously with density to a maximum >400 mK. Such devices should prove useful for the study of electron transport in nanostructures in the 2d Landau level.

8:12AM A5.00002 Analyzing the Disorder Broadening of the Even Denominator Fractional Quantum Hall States in the Presence of Alloy Disorder, ETHAN KLEINBAUM, NIANPEI DENG, GEOFFREY GARDNER, MICHAEL MANFRA, GABOR CSATHY, Purdue University — The unique character and potential application of the even denominator \( \nu=5/2 \) fractional quantum hall state has elicited significant interest. Yet, the most basic properties of this ground state remain unexplained. One poorly understood effect is that of the various types of disorder. We report energy gaps at the filling factor \( \nu=7/2 \) in a series of samples into which we intentionally added aluminum impurities during the MBE growth. These data, together with the availability of energy gaps at \( \nu=5/2 \) in the same samples, allows us to quantify the disorder broadening and the intrinsic gap of the even denominator fractional quantum Hall states. This work was supported by DOE DE-SC000671.

8:24AM A5.00003 Experimental constraints and a possible quantum Hall state at \( \nu=5/2 \), DIMA FELDMAN, Brown Univ, GUANG YANG, RIKEN — Several topological orders have been proposed to explain the quantum Hall plateau at \( \nu=5/2 \). The observation of an upstream neutral mode on the sample edge [Bid et al., Nature (London) 466, 585 (2010)] supports the non-Abelian anti-Pfaffian state. On the other hand, the tunneling experiments [Radu et al., Science 320, 899 (2008); Lin et al., Phys. Rev. B 85, 165321 (2012); Baer et al., Phys. Rev. B 90, 075403 (2014)] favor the 331 state which exhibits no upstream modes. We find a topological order, compatible with the results of both types of experiments. That order allows both finite and zero spin polarizations. It is Abelian but its signatures in Aharonov-Bohm interferometry can be similar to those of the Pfaffian and anti-Pfaffian states.

1This work was supported by the NSF under Grant No. DMR-1205715.

8:36AM A5.00004 Entanglement Entropy of Quantum Hall Systems with Short Range Disorder, BARRY FRIEDMAN, Department of Physics, Sam Houston State University, GREG LEVINE, Department of Physics and Astronomy, Hofstra University — The critical value of the mobility for which the filling 5/2 quantum Hall effect is destroyed by short range disorder is determined from an earlier calculation of the entanglement entropy. The value agrees well with experiment; this agreement is particularly significant in that there are no adjustable parameters. Entanglement entropy vs. disorder strength for filling 1/2, filling 9/2 and filling 7/3 is calculated. For filling 1/2 there is no evidence for a transition for the disorder strengths considered; for filling 9/2 there appears to be a stripe-liquid transition. For filling 7/3 there again appears to be a transition at similar value of the disorder strength as the 5/2 transition but there are stronger finite size effects.

8:48AM A5.00005 Hall viscosity of hierarchical quantum Hall states, MIKAEL FREMLING, THORS HANS HANSSON, Stockholm University, JUHA SUORSA, Nordita — We construct model wave functions on a torus for all chiral states in the abelian quantum Hall hierarchy. These functions have no variational parameters, and they transform under the modular group in the same way as the multicomponent generalizations of the Laughlin wave functions. Assuming the absence of Berry phases upon adiabatic variations of the modular parameter \( \tau \), we calculate the quantum Hall viscosity and find it to be in agreement with the formula, given by Read, which relates the viscosity to the average orbital spin of the electrons. For the filling factor \( \nu = 2/5 \) Jain state, which is at the second level in the hierarchy, we compare our model wave function with the numerically obtained ground state of the Coulomb interaction Hamiltonian in the lowest Landau level, and find very good agreement in a large region of the complex \( \tau \)-plane. For the same example, we also numerically compute the Hall viscosity and find good agreement with the analytical result for both the model wave function and the numerically obtained Coulomb wave function. We argue that this supports the notion of a generalized plasma analogy that would ensure that wave functions obtained using conformal field theory methods do not acquire Berry phases upon adiabatic evolution.

9:00AM A5.00006 High-mobility hydrogen-terminated Si(111) transistors for measurement of six-fold valley degenerate two-dimensional electron systems in fractional quantum Hall regime, BINHUI HU, MOHAMAD MEQAD YAZDANPANAH, BRUCE E. KANE, Univ of Maryland-College Park — The quality of hydrogen-terminated Si(111)-(H-Si(111)) transistors has improved significantly. Peak electron mobility of 325,000 cm²/Vs was achieved at 90 mK, and the fractional quantum Hall effect (FQHE) at \( 1 < \nu < 2 \) was studied extensively [1]. We have further improved the device by solving gate leakage and contact problems with an updated design, in which a Si piece with thermal oxide acts as a gate through a vacuum cavity, and PN junctions are used to define a hexagonal two-dimensional (2D) region on a H-Si(111) piece. The device operates as an ambipolar transistor, in which a 2D electron system (2DES) and a 2D hole system can be induced at the same \( \nu=5/2 \). The \( \nu=5/2 \) fraction of the various types of disorder. We report energy gaps at the filling factor \( \nu=5/2 \) in a series of samples into which we intentionally added aluminum impurities during the MBE growth. These data, together with the availability of energy gaps at \( \nu=5/2 \) in the same samples, allows us to quantify the disorder broadening and the intrinsic gap of the even denominator fractional quantum Hall states. This work was supported by DOE DE-SC000671.

9:00AM A5.00006 High-mobility hydrogen-terminated Si(111) transistors for measurement of six-fold valley degenerate two-dimensional electron systems in fractional quantum Hall regime, BINHUI HU, MOHAMAD MEQAD YAZDANPANAH, BRUCE E. KANE, Univ of Maryland-College Park — The quality of hydrogen-terminated Si(111)-(H-Si(111)) transistors has improved significantly. Peak electron mobility of 325,000 cm²/Vs was achieved at 90 mK, and the fractional quantum Hall effect (FQHE) at \( 1 < \nu < 2 \) was studied extensively [1]. We have further improved the device by solving gate leakage and contact problems with an updated design, in which a Si piece with thermal oxide acts as a gate through a vacuum cavity, and PN junctions are used to define a hexagonal two-dimensional (2D) region on a H-Si(111) piece. The device operates as an ambipolar transistor, in which a 2D electron system (2DES) and a 2D hole system can be induced at the same \( \nu=5/2 \) surface. Peak electron mobility of more than 200,000 cm²/Vs is routinely achieved at 300 mK. The Si(111) surface has a six-fold valley degeneracy. The hexagonal device is designed to investigate the symmetry of the 2DES. Preliminary data show that the transport anisotropy at \( \nu < 6 \) can be explained by the valley occupancy. The details of the valley occupancy can be caused by several mechanisms, such as miscut, magnetic field, pseudospin quantum Hall ferromagnetism (QHFM), and nematic valley polarization phases [2]. The FQHE is investigated in magnetic fields up to 35T, and the properties of composite fermions will be discussed. [1] T.M. Koti, B.H. Hu, S.H. Brown, B.E. Kane, Phys. Rev. B 89, 041107(R) (2014) [2] D. A. Abanin, S. A. Parameswaran, S. A. Kivelson, and S. L. Sondhi. Phys. Rev. B, 82, 035428 (2010)

9:12AM A5.00007 Quantum Hall Systems on Toroidal Geometries, NIALL MORAN, JOOST SLINGERLAND, Natl Univ of Ireland Maynooth — We present results of recent numerical calculations of second Landau level (LL) states on toroidal geometries. Calculations on the torus generally allow for smaller particle numbers than those on the sphere, due to less powerful symmetries. However, on the torus, different candidate states for particular quantum Hall plateaus appear at equal flux, in contrast to the situation on the sphere or plane. This means that working on the torus allows for more direct comparisons of trial states and reduces the problem of aliasing. Moreover, the torus brings interesting geometry, described by a modular parameter \( \tau \). This potentially allows for a larger variety of phases as well as some interesting limits which can be treated analytically. It also allows for the calculation of the Hall viscosity, a quantity which corresponds to the shift on the sphere. Among fillings considered are \( \nu = 12/5 \) and \( \nu = 3/2 \) where states hosting non-Abelian anyons have been conjectured.
9:24AM A5.00008 Disc configuration exact diagonalization studies of the phase diagram and edge states of the $\nu = 5/2$ fractional quantum Hall state with Landau level mixing and finite well thickness¹, ANTHONY TYLAN-TYLER, YULI LYANDA-GELLER, Department of Physics and Astronomy, Purdue University, West Lafayette, IN 47907 USA — The $\nu = 5/2$ fractional quantum Hall effect is of experimental and theoretical interest as a possible manifestation of non-Abelian statistics. The nature of this state has yet to be fully determined. The leading candidates are the Moore-Read Pfaffian state and its particle-hole conjugate, the anti-Pfaffian. When effects which break particle-hole symmetry are not included, these states are degenerate. We carry out an exact diagonalization calculation in a disk of neutralizing charge configuration, which breaks this degeneracy, and include Landau level mixing interactions arising from a diagrammatic expansion of the Coulomb potential and the effects of finite thickness. The Pfaffian sector is shown to favor strong interactions with the neutralizing background and strong Landau level(LL) mixing, while the anti-Pfaffian state occurs at weak LL mixing and background interactions. We find that there is a phase transition from the anti-Pfaffian to the Pfaffian state through a series of compressible stripe states as LL mixing is turned on. Furthermore, LL mixing interactions lead to an increased quasihole size and can overcome the effects of edge reconstruction. When the effects of the finite thickness of the confining quantum well are included, we observe enhancement these properties.

¹Research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0010544.

9:36AM A5.00009 Non-Abelian statistics of Luttinger holes in quantum wells², GEORGE SIMION, Purdue University, YULI LYANDA-GELLER, Department of Physics, Purdue University, West Lafayette, IN 47907 USA — Non-Abelian quasi-particle excitations represent a key element of topologically protected quantum computing. Such exotic states appear in fractional quantum Hall (FQH) effect as eigenstates of N-body interaction potential. These potentials can be obtained by renormalization of electron-electron interactions in the presence of Landau level (LL) mixing. The properties of valence band holes makes them fundamentally different from electrons. In the presence of magnetic field, low-lying states do not exhibit fan-like diagram and several of the levels cross. Variation of magnetic field in the vicinity of level crossings serves as a knob that tunes LL mixing and enhances the 3-body interaction. 1/2 filling factor FQH is a state that was not observed in electron liquid, but has been observed for holes. The properties of the two dimensional charged quantum hole liquid in the presence of magnetic field are studied using the spherical geometry. The properties of the novel 1/2 state are discussed.

²Research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0010544.

9:48AM A5.00010 Competing quantum Hall phases in the second Landau level in low density limit³, WEI PAN, Sandia National Labs, A. SERAFIN, J.S. XIA, L. YIN, N.S. SULLIVAN, University of Florida and NHMFL, K.W. BALDWIN, K.W. WEST, L.N. PFEIFFER, D.C. TSUI, Princeton University — We present here the results from two high quality, low density GaAs quantum wells. In sample A of electron density $n = 5.0 \times 10^{10}$ cm$^{-2}$, anisotropic electronic transport behavior was observed at $\nu = 7/2$ in the second Landau level. We believe that the anisotropy is due to the large Landau level mixing effect in sample A. In sample B of density $4.1 \times 10^{10}$ cm$^{-2}$, strong $8/3$, $5/2$, and $7/3$ fractional quantum Hall states were observed. Furthermore, our energy gap data obtained in various samples of different densities suggest that the $5/2$ state may be spin unpolariized in the low density limit. The results from both samples show that the strong electron-electron interactions and a large Landau level mixing play an import role in the competing ground states in the second landau level. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

³This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

10:00AM A5.00011 Heterostructure design and growth conditions necessary for electron mobility exceeding $30\times10^6$ cm$^2$/Vs in GaAs quantum wells, SAEED FALLAH, Department of Physics and Birck Nanotechnology Center, Purdue University, GEOFFREY GARDNER, Schools of Materials Engineering and Birck Nanotechnology Center, Purdue University, JOHN WATSON, Department of Physics and Birck Nanotechnology Center, Purdue University, MICHAEL MANFRA, Department of Physics, Birck Nanotechnology Center and Schools of Materials Engineering and Electrical and Computer Engineering, Purdue University — Ultra-high purity GaAs/AlGaAs heterostructures remain the material purity for the achievement of high mobility. In our work high mobility has been achieved primarily through improvements in starting source materials and heterostructure design rather than improvements in vacuum quality, it does not encode all information necessary to quantify disorder relevant to the fractional quantum Hall effect. Here we describe the heterostructure design considerations and molecular-beam-epitaxy growth conditions needed to achieve an electron mobility $>30\times10^6$ cm$^2$/Vs. In particular, we report on the impact of several modulation doping schemes on mobility and the quality of transport in the 2nd Landau level. We also detail constraints on starting source material purity for the achievement of high mobility. In our work high mobility has been achieved primarily through improvements in starting source materials and heterostructure design rather than improvements in vacuum quality.

10:12AM A5.00012 Phase Diagram of Fractional Quantum Hall Effect of Composite Fermions in Multi-Component Systems¹, AJIT COIMBATORE BALRAM, Pennsylvania State University, CSABA TŐKE, Budapest University of Technology and Economics, ARKKADIUSZ WOJŚ, Wrocław University of Technology, JAINENDRA JAIN, Pennsylvania State University — The fractional quantum Hall effect (FQHE) of composite fermions (CFs) produces delicate states arising from a weak residual interaction between CFs. We study the spin phase diagram of these states, motivated by the recent experimental observation by Liu et al. [1] of several spin-polarization transitions at 4/5, 5/7, 6/5, 9/7, 7/9, 8/11 and 10/13 in GaAs systems. We show [2] that the FQHE of CFs is much more prevalent in multicomponent systems, and consider the feasibility of such systems for states with N components for an SU(N) symmetric interaction. Our results apply to GaAs quantum wells, wherein electrons have two components, to AlAs quantum wells and graphene, wherein electrons have four components (two spins and two valleys), and to an H-terminated Si(111) surface, which can have six components. We provide a fairly comprehensive list of possible incompressible FQH states of CFs, their SU(N) spin content, their energies, and their phase diagram as a function of the generalized “Zeeman” energy. The results are in good agreement with available experiments.

¹DOE Grant No. DE-SC0005042, Hungarian Scientific Research Funds No. K105149 (CT), the Polish NCN grant 2011/01/B/ST3/04504 and the EU Marie Curie Grant PCIG09-GA-2011-294186
The Phase Diagram of the $\nu = 5/2$ Fractional Quantum Hall Effect: Effects of Landau Level Mixing and Non-Zero Width$^1$. MICHAEL PETERSON, Cal State Univ- Long Beach, KIRYL PAKROUSKI, ETH Zurich, THIERRY JOLICOUR, CNRS and Universite Paris-Sud, VITO SCAROLA, VA Tech, CHETAN NAYAK, Microsoft, University of California Santa Barbara, MATTHIAS TROYER, ETH Zurich — We study the phase diagram of the $\nu = 5/2$ state by exactly diagonalizing an effective Hamiltonian describing the fractional quantum Hall effect of electrons under realistic conditions in GaAs semiconductors. The effective Hamiltonian takes Landau level mixing into account to lowest-order perturbatively in $\kappa$, the ratio of the Coulomb energy scale to the cyclotron gap and we incorporate non-zero width $\omega$ of the quantum well and sub-band mixing. Using the torus and sphere, we analyze the non-trivial competition between candidate ground states with 4 criteria: overlaps with trial wave functions; the size of energy gaps; the sign of an order parameter for particle-hole symmetry breaking; and entanglement spectrum. We find the ground state is in the universality class of the Moore-Read Pfaffian state, rather than anti-Pfaffian, for $\kappa < \kappa_c(\omega)$, where $0.6 < \kappa_c(\omega) < 1$. Landau level mixing and non-zero width suppress the excitation gap with Landau level mixing having a larger effect. Our findings have important implications for the identification of non-Abelian fractional quantum Hall states.

We thank DARPA, Microsoft, Swiss National Science Foundation (NCCR QSIT), Swiss National Supercomputing Centre (CSCS), European Research Council, AFOSR, and the Centre National de la Recherche Scientifique.
9:00AM A6.00004 Standing wave plasmon modes interact in an antenna-coupled nanowire \(^1\). JARED DAY, NICOLAS LARGE \(^2\), PETER NORDLANDER, NAOMI HALAS, Rice University — In a standing wave optical cavity, the coupling of cavity modes, e.g. through a nonlinear medium, results in a rich variety of nonlinear dynamical phenomena, such as frequency pushing and pulling, mode-locking and pulsing, and modal instabilities. Metallic nanowires of finite length support a hierarchy of longitudinal surface plasmon modes with standing wave properties: the plasmonic analog of a Fabry-Perot cavity. Here we show that positioning the nanowire within the gap of a plasmonic nanoantenna introduces a passive, hybridization-based coupling of the standing-wave plasmonic modes with the antenna structure, mediating an interaction between the nanowire plasmon modes themselves. Frequency pushing and pulling, and the enhancement and suppression of specific plasmon modes, can be controlled and manipulated by nanoantenna position and shape. Dark-field spectroscopy, CL spectroscopy and imaging, and finite-difference time-domain calculations are performed to investigate these surface plasmon “drift.” Near-field coupling of nanoantennas to nanowire optical cavities shows that plasmon hybridization is a powerful strategy for controlling the radiative LDOS of nanowires, and could ultimately enable strategies for active control of emission properties in nanowire-based devices.

\(^1\)Work funded by the Welch Foundation (C-1220, C-1222), the NSSEFF (N00244-09-1-0067), the ONR (N00014-10-1-0989), and the NSF (ECCS-1040478, CNS-0821727).

9:12AM A6.00005 Accurate modeling of photodynamic processes enhanced by plasmonic nanoantennas \(^3\). CHRISTOS ARGYROPOULOS, University of Nebraska-Lincoln, GLEB AKSELROD, Duke University, CRISTIAN CIRACI, Istituto Italiano di Tecnologia, THANG HOANG, MAIKEN MIKKELSEN, DAVID SMITH, Duke University — Plasmonic nanoantennas are powerful platforms to enhance fluorescence and spontaneous emission rates leading to exciting nanophotonic applications. Strong fields confined in highly subwavelength regions in the nanoantenna geometry are ideal conditions to increase the Purcell factor. However, the accurate modeling of the interaction between fluorescence molecules or quantum-dots and plasmonic nanoantennas is a complicated task. In our talk, we will demonstrate efficient numerical techniques to accurately compute the total spontaneous emission rate and radiation efficiency by multiple fluorescence molecules and quantum-dots randomly positioned nearby the plasmonic nanoantennas [G. Akselrod, C. Argyropoulos et al., Nat. Phot. 8, 835-840 (2014)]. This is a complex problem because in plasmonic systems the Purcell factor has contributions from an increased radiative rate and from an increased nonradiative rate due to the inherent metallic losses. We will demonstrate ways to accurately compute the useful fraction of energy emitted as radiation, known as the radiative quantum yield. When we combine the knowledge of the Purcell factor and the quantum yield, the enhancement in the emitters’ radiative rate can be computed, which consists the key property to obtain efficient ultrafast nanophotonic communication systems. The presented numerical results are in excellent agreement with experimental results obtained by similar nanoantenna systems.

\(^3\)Current affiliation: Northwestern University

9:24AM A6.00006 Surface Plasmon Propagation in Nanostructured Metallic Waveguides \(^4\), Y.M. CALM, J.M. MERLO, A.H. ROSE, N.T. Nesbitt, A.M. BOYCE, G. McMahan, M.J. BURNS, K. KEMP, M.J. NAUGHTON \(^1\), Boston College — Visible frequencies of light can be routed on subwavelength scales with nanostructured, metallic waveguides by coupling optical energy to surface plasmon (SP) modes at a metal-insulator interface. Epitaxially-grown Ag nanowires and nanocables provide a low-loss, “model” system to characterize the propagation of SP waves. We have studied these structures by electron, focused ion, scanning probe, and optical microscopies, and have observed propagation lengths exceeding 15 \(\lambda\), which extracts near-field (evanescent) information and propagates it into the far-field, is presented.

\(^4\)Supported by the W.M. Keck Foundation

9:36AM A6.00007 Investigation of nanogap localized field enhancement in gold plasmonic structures \(^5\). DESALEGN TADESE DEBU, STEPHEN BAUMAN, CAMERON SAYLOR, University of Arkansas, ERIC NOVAK, Shippensburg University, DAVID FRENCH, JOSEPH HERZOG, University of Arkansas — Nanogaps between plasmonic structures allow confining the localized electric field with more enhancements. Based on previously implemented two-step lithography process, we introduce a nano-masking technique to fabricate nanostructures and nanogaps for various geometrical patterns. This new method can fabricate gold nanostructures as well as nanogaps that are less than 10nm, below the limiting scale of lithography. Simulation from finite element method (FEM) shows strong gap dependence of optical properties and peak enhancement of these devices. The fabricated plasmonic nanostructure provides wide range of potential future application including highly sensitive optical antenna, surface enhanced Raman spectroscopy and biosensing.

\(^5\)Current affiliation: Northwestern University

9:48AM A6.00008 Purcell factors exceeding 1,000 in directional and efficient plasmonic nanoantennas \(^6\). GLEB AKSELROD, CHRISTOS ARGYROPoulos, THANG HOAng, CRISTIAN CIRACi, CHAO FANG, JIANI HUANG, DAVID SMith, MAIKEN MIKKELSEN, Center for Metamaterials and Integrated Plasmonics, Duke University — To move nanophotonic devices such as nano-lasers, ultrafast LEDs, and single photon sources into the practical realm, a challenging list of requirements must be met, including directional emission, room temperature and broadband operation, and high radiative quantum yield, while having a large spontaneous emission rate. To achieve these features simultaneously, a platform is needed in which the various decay channels of embedded emitters can be fully understood and controlled. In this work we show that all these device requirements can be satisfied by a plasmonic nanoantenna with emitters embedded in the nanoscale gap (\(\sim 10 \text{ nm}\)) between a metal film and a silver nanocube. Fluorescence lifetime measurements on ensembles of emitters reveal Purcell factors exceeding 1000 while maintaining high quantum yield (\(> 0.5\)) and directional emission (84% collection efficiency). Using angle resolved fluorescence measurements, we independently determine the orientations of emission dipoles in the nanoscale gap. By incorporating this information along with the three-dimensional spatial distribution of dipoles into simulations, we predict the emission dynamics in excellent agreement with experiment.

Nanoparticles on Au Nano-cavity Arrays

Our analysis shows the power dependent enhancement in upconversion luminescence can almost entirely be accounted for by a constant shift in the effective excitation intensity, which is maintained over five orders of magnitude variation in excitation intensities in the spectroscopic images on and off the nano-cavity arrays provides an estimate of the average enhancement factor independent of fluctuations in intensity. The variations in upconversion luminescence enhancement with power are modeled by a 3-level-system near the saturation limit, and by simultaneous off-resonance scattering from Au nanoparticles. Our hybrid nanostructures with tunable optical properties can be useful for various optoelectronic applications such as photothermal nanoreactors and ultrafast optical switches.

10:12AM A6.00010 VO2 Semishells/Au Nanohemispheres Hybrid Nanostructure with Tunable Optical Property

10:00AM A6.00009 Study of plasmonic and magnetic modes in non-symmetric gold nano-ring geometries

10:00AM A6.00012 Virus templated plasmonic nanoclusters with icosahedral symmetry via directed assembly

10:36AM A6.00013 Spectroscopic Imaging of NIR to Visible Upconversion from NaYF4: Er3+, Yb3+ Nanoparticles on Au Nano-cavity Arrays

10:24AM A6.00011 Cluster Ion Beam Induced Nano Metallic Rippled Structures for Localized Surface Plasmon Resonance (LSPR) Based Sensors

10:00AM A6.00008 Nanoparticles on Au Nano-cavity Arrays

10:00AM A6.00007 Optical Property

10:24AM A6.00006 Optical Property

10:00AM A6.00005 Optical Property

10:00AM A6.00004 Optical Property

10:00AM A6.00003 Optical Property

10:00AM A6.00002 Optical Property

10:00AM A6.00001 Optical Property

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This work has been supported under the grant from Volkswagen Foundation

We use spectroscopic imaging to assess the spatial variations in upconversion luminescence from NaYF4:Er3+, Yb3+ nanoparticles embedded in PMMA on Au nano-cavity arrays. The nano-cavity arrays support a surface plasmon (SP) resonance at 980nm, coincident with the peak absorption of the Yb3+ sensitizer. Spatially-resolved upconversion spectra show a 30X to 3X luminescence intensity enhancement on the nano-cavity array compared to the nearby smooth Au surface, corresponding to excitation intensities from 1 W/cm2 to 300kW/cm2. Our analysis shows the power dependent enhancement in upconversion luminescence can be almost entirely accounted for by a constant shift in the effective excitation intensity, which is maintained over five orders of magnitude variation in excitation intensity. The variations in upconversion luminescence enhancement with power are modeled by a 3-level-system near the saturation limit, and by simultaneous solution of a system of coupled nonlinear differential equations, both analyses agree well with the experiments. Analysis of the statistical distribution of emission intensities in the spectroscopic images on and off the nano-cavity arrays provides an estimate of the average enhancement factor independent of fluctuations in nanoparticle density.

1Funding provided by NSF award # 0903685 (IGERT).

1This work has been supported under the gift from Volkswagen Foundation.
8:00AM A7.00001 Realization of high-precision and more robust quantum anomalous Hall state in a hard ferromagnetic topological insulator. CUI-ZU CHANG, Massachusetts Institute of Technology. The discovery of the integer quantum Hall (QH) effect in 1980 led to the realization of a topological electronic state with dissipationless currents circulating in one direction along the edge of a two-dimensional electron layer under a strong magnetic field. The quantum anomalous Hall (QAH) effect shares a similar physical phenomenon as the QH effect, whereas its physical origin is a result of intrinsic spin-orbit coupling of the topological insulator (TI) and when it is in ferromagnetic state. Since the QAH effect does not require an external field and the associated Landau levels, it is believed that this effect has unique potential for applications in electronic devices with low-power consumption. In this talk, we shall describe the experimental observation of the QAH state in V-doped (Bi$_2$Sb)$_2$Te$_3$ TI films. We find that in zero-field longitudinal resistance decreases to 0.00013 ± 0.00007 $\Omega^{-2}$ at $T=25$mK, thus realizing the anomalous Hall transport with negligible dissipation in the absence of any initial magnetic field. The advantage of this system comes from the fact that it is a hard ferromagnet with a large coercive field ($H_c=1$Oe) and a relative high Curie temperature. These results were unexpected from the theoretical calculations. This high-precision realization of a more robust QAH state in hard FMTIs is a major step towards dissipationless electronic applications without external applied fields.


Supported by funding from NSF (DMR-1207469), NSF (DMR-0907007), ONR (N00014-13-1-0301), NSF (DMR-0820404, Penn State MRSEC), and the STC Center for Integrated Quantum Materials under NSF grant DMR-1231319.

8:36AM A7.00002 Transport studies on Cr-doped (Bi,Sb)$_2$Te$_3$ thin films with nearly quantized anomalous Hall effect. MINHAO LIU, Physics Department, Princeton University, ANTHONY RICHARDELLA, ABHINAV KANDALDA, Physics Department, Pennsylvania State University, WUDI WANG, ALI YAZDANIB, Physics Department, Princeton University, NITIN SAMARTH, Physics Department, Pennsylvania State University, N. PHUAN ONG, Physics Department, Princeton University. We describe measurements of the quantum anomalous Hall effect in ferromagnetic Cr-doped (Bi,Sb)$_2$Te$_3$ thin films (6-8 QL thickness) grown on (111) SrTiO$_3$ (STO) substrates by molecular beam epitaxy. The Fermi level is tuned close to the neutrality point by tuning the growth flux ratios of Cr, Bi and Sb. Transport measurements were carried out in a dilution fridge at a base temperature of 20 mK. By tuning the chemical potential with a back gate on the STO substrate, we observed an anomalous Hall effect as high as 0.95 $\Omega^{-2}$/s, with a coercive field ~ 0.15 T and a narrow transition between positive/negative Hall plateaus. Transport measurements in a non-local configuration showed a Hall-effect-like non-local resistance with a systematic dependence on the back gate voltage and with pronounced peaks which resembled the non-local resistance of the quantum Hall effect. The non-local signal has a maximum that coincides with the maximum in Hall conductivity, indicating the edge channel as its origin. Our results show that the edge channel manifests itself in various transport properties even though the Hall resistance is not perfectly quantized.

1Supported by DARPA SPAWAR Grant No. N66001-11-1-4110 and MURI grant on Topological Insulators (ARO W911NF-12-1-0461).

8:48AM A7.00003 Spin-Orbital texture and magnetic proximity effect of Bi$_2$Se$_3$/EuS heterostructure. ALEX TAEKYUNG LEE, Columbia Univ, MYUNG JOON HAN, Department of Physics, KAIST, KYUNGWHA PARK, Department of Physics, Virginia Tech. A topological insulator Bi$_2$Se$_3$ has gapless Dirac surface states topologically protected by time reversal symmetry with the helical spin texture. The spin texture has a unique orbital dependence and it allows topological insulator hybrid structures to be used for spintronics or spin transfer torque devices. Recently, an interface between a topological insulator Bi$_2$Se$_3$ and a ferromagnetic insulator EuS, has been experimentally realized, which provides an opportunity to study effects of magnetic interface on Dirac surface states of Bi$_2$Se$_3$. In this talk, we present our study of magnetic proximity effects and spin-orbital texture of the topological surface states of Bi$_2$Se$_3$ at the Bi$_2$Se$_3$/EuS interface, by using first-principles calculations and an low-energy effective model [A. T. Lee et al., Phys. Rev. B. 90, 155103 (2014)]. We discuss an energy gap opening due to the out-of-plane magnetic moment induced by the EuS, and a new Dirac cone occurring for thick Bi$_2$Se$_3$ slabs. Furthermore, we show an interesting coupling between the out-of-plane spin moment and the orbitals caused by broken time reversal symmetry.

2Funding from NSF DMR-1206354

9:00AM A7.00004 Giant anisotropic magneto-resistance in the magnetic topological insulator Cr$_y$(Bi$_{1-x}$Sb$_x$)$_2$I$_2$Te$_3$. ABHINAV KANDALDA, ANTHONY RICHARDELLA, CHAOXING LIU, NITIN SAMARTH, Penn State University. We demonstrate magnetization control of edge state transport and report the observation of a gate-tunable giant anisotropic magneto-resistance (GAMR) effect in the magnetic topological insulator Cr$_y$(Bi$_{1-x}$Sb$_x$)$_2$I$_2$Te$_3$ as an external field (and the magnetization $M$) is rotated from out-of-plane (polar angle $\theta = 0^\circ$) to in-plane ($\theta = 90^\circ$). The angular dependence of the GAMR deviates from the standard $\cos^2 \phi$ form (where $\phi$ is the angle between $M$ and the current density $J$), and is instead explained by a Landauer-Büttiker formalism that accounts for bulk-edge mixing. However, the rotation of the magnetization in-plane produces a weak, conventional AMR. These results serve as evidence for a field tilt-tuned crossover between an “imperfect” quantum anomalous Hall insulator (QAH) and a gapless, ferromagnetic topological insulator. We expect the GAMR to become stronger in the ideal QAH regime where edge state conduction dominates over bulk conduction, thus providing a route toward proof-of-concept ferromagnetic topological insulator transistors and magnetic field sensors. Funded by DARPA.

9:12AM A7.00005 Magnetization in Intrinsic Topological Insulators Induced by Exchange Interaction with Ferromagnetic Insulator. VALERIA LAUTER, Oak Ridge National Laboratory, Oak Ridge, USA, FERHAT KATMIS, Francis Bitter Magnet Laboratory, MIT, Cambridge, USA, BADIH ASSAF. Ecole Normale Supérieure, Paris France, DON HEIMAN, Department of Physics, Northeastern University, Boston, USA, JAGADEESH MOODERA, Department of Physics, MIT, Cambridge, MA-02139, USA. — We examine the magnetic proximity-induced symmetry breaking via the exchange interaction in heterostructures of the topological insulator (TI) Bi$_2$Se$_3$ and the ferromagnetic insulator (FMI) EuS [1]. We observed the emergence of a ferromagnetic phase in TI with the excess of magnetic moment at the interface using depth and element sensitive Polarized Neutron Reflectometry (PNR). We find that the magnetization, penetrating into the TI originates through exchange interaction, without structural perturbation at the interface. Due to the different interlayer exchange coupling as well as the properties of the bulk and surface magnetizations, we investigated several different heterostructures after cooling in zero field (ZFC) and in an external magnetic field (FC). The significantly enhanced magnetic properties of the heterostructures as revealed by the PNR studies, as well as the temperature and external magnetic field dependence will be presented.


3This work was supported by the Scientific User Facilities Division, BES, DOE, NSF ECCS-1402738, DMR-1207469, ONR N00014-13-1-0301.
9:24AM A7.00006 Observation of ferromagnetic domains in magnetic topological insulator1, WENBO WANG, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, 08854 USA, FANG YANG, CHUNLIE GAO, JINFENG JIA, Department of Physics and Astronomy, Shanghai Jiao Tong University, 800 Dongchuan Road, Shanghai 200240, China, WEIDA WU, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, 08854 USA — The breaking of time reversal symmetries in a topological insulator can lead to exotic quantum effects, such as magnetic monopoles, quantum anomalous Hall effect (QAHE), and so on. Recently QAHE has been experimentally observed in a ferromagnetic topological insulator Cr doped Bi$_{1-y}$Sb$_y$Te$_3$[1]. Although a lot of studies have conducted on characterizing the ferromagnetic properties in these fascinating materials, direct observation of ferromagnetic ordering is still lacking. Here, we report variable temperature magnetic force microscopy (VT-MFM) studies on thin film of Cr doped Bi$_{1-y}$Sb$_y$Te$_3$ synthesized by molecular beam epitaxy (MBE). Small bubble-like ferromagnetic domains were observed below Tc $\sim$ 30 K. The evolution of these domains at various temperatures and magnetic fields will be presented.


9:36AM A7.00007 Study of magnetism in Cr doped (Bi$_{1-y}$Sb$_y$)$_2$Te$_3$ — ANTHONY RICHARDELLA, ABHINAV KANDALA, SUSAN KEMPINGER, NITIN SAMARTH, Pennsylvania State Univ., University Park PA, ALEX GRUTTER, JULIE BORCHERS, NCNR, NIST Gaithersburg MD — The quantum anomalous Hall (QAH) effect was first observed in Cr doped films of the topological insulator (TI) (Bi$_{1-y}$Sb$_y$)$_2$Te$_3$. This ferromagnetic T-I opens a gap at the Dirac point and, when the Fermi energy lies inside this gap, a quantized QAH conductance can be observed. The origin of ferromagnetism in this material is still not well understood with the mechanism typically attributed to either a high van-Vleck susceptibility or a carrier mediated RKKY like interaction. To elucidate this we have studied Cr$_x$(Bi$_{1-y}$Sb$_y$)$_2$Te$_3$ thin films grown by MBE on SrTiO$_3$ (STO) substrates using polarized neutron reflectivity (PNR) while in-situ backgating the film to change the position of the Fermi energy. The films are also characterized by XRD, AFM, TEM and low temperature transport measurements. PNR measurements provide a direct measure of the depth dependent magnetization of a sample. We use this to study how the magnetization changes as the Fermi energy is moved towards the Dirac point. Funded by DARPA and ARO-MURI.

9:48AM A7.00008 Electrical Transport Properties of Mn doped Bi$_2$Se$_3$ Thin Films — SERCAN BABAKIRAY, TRENT JOHNSON, PAVEL BORISOV, DAVID LEDERMAN, West Virginia University — Magnetic impurity doping in topological insulators manifest itself with a gap opening in the Dirac cone as a result of breaking the time reversal symmetry. Moreover, the magnetic impurities affect the structural and quantum transport properties of topological insulators by increasing the disorder and by changing the bulk charge carrier type, charge carrier density and Hall mobility. Here, we report magnetotransport properties of Bi$_2$-xMnxSe$_3$ thin films which are 12 quintuple layers thick and grown on Au(001) single crystal substrates via molecular beam epitaxy (MBE). Hikami-Larkin-Nagaoka (HLN) formalism was used to study the weak antilocalization (WAL). Increasing Mn doping concentration was found to increase the bulk charge carrier density and to decrease the Hall mobility. A decrease was also observed in the phase coherence length related to WAL as a function of Mn content $x$. Values of another WAL parameter, the pre-factor alpha, showed that the top and bottom surfaces were coupled through the bulk conducting channels. The temperature dependence of phase coherence length indicated the electrical transport was dominated by 2D electron-electron scattering for the undoped, and by bulk weak localization effects for the Mn doped samples, respectively.

10:00AM A7.00009 Probing interface ferromagnetism of EuS/Bi$_2$Se$_3$ heterostructures with magnetic second harmonic generation1, CHANGMIN LEE, Department of Physics, MIT, FERHAT KATMIS, Francis Bitter Magnet Lab, MIT, PABLO JARILLO-HERRERO, Department of Physics, MIT, JAGADEESH S. MOODERA, Francis Bitter Magnet Lab and Department of Physics, MIT, NUH GEDIK, Department of Physics, MIT — Ferromagnet / topological insulator interfaces are novel heterostructures that can host various interesting physical phenomena, such as massive Dirac fermions, the quantum anomalous Hall effect, and the topological magneto-electric effect. By using magnetic second harmonic generation (MSHG), we separately measure the in-plane and the out-of-plane magnetization at the interface between a ferromagnetic insulator EuS and Bi$_2$Se$_3$. In contrast to bulk-sensitive linear magneto-optics, such as the Faraday and Kerr effects, MSHG allows a selective measurement of ferromagnetism and crystal symmetry of the interface, at which inversion symmetry is broken. Our technique can thus be used to study magnetism and crystal structure of such “buried” interfaces to which other conventional probes do not have direct access.

1Work supported by the STC Center for Integrated Quantum Materials (NSF DMR-1231319), NSF (DMR-1207469), and MIT MRSEC through the MRSEC Program of the NSF (DMR-0819762).

10:12AM A7.00010 Investigation of the structural and magnetic properties of MBE-grown Cr-doped Bi$_2$Se$_3$ thin films — LIAM COLLINS-MCINTYRE, PIET SCHOENHERR, SHILEI ZHANG, ALEXANDER BAKER, University of Oxford, ADRIANA FIGUEROA, GIANNANTONIO CIBIN, GERRIT VAN DER LAAN, Diamond Light Source, NINA-JULIANA STEINKE, CHRISTY KINANE, TIMOTHY CHARLTON, DIEGO ALBA-VENERO, SEAN LANGRIDGE, ISIS Neutron Source, AKASH PUSHP, ANDY KELLOCK, STUART PARKIN, IBM Almaden Research Center, SARA HARRISON, JAMES HARRIS, Stanford University, THORSTEN HESJEDAL, University of Oxford — We report a study of the structural and magnetic properties of Cr-doped Bi$_2$Se$_3$ films grown by MBE. We present a thorough exposition of the electronic character of the magnetic ground state of this material as determined by x-ray magnetic circular dichroism (XMCD) as well as complementary measurements by polarised neutron reflectometry, X-ray diffraction and SQUID magnetometry. We observe the formation of a ferromagnetic ground state (via SQUID), below a measured Tc $\sim$ 8.5 K with a saturation magnetization of 2.1 $\mu_B$/Cr. By XRD we observe a reduction in c-axis lattice parameter with increasing Cr concentration up to 12 at.% of dopant. XMCD and EXAFS studies indicate that, contrary to expectations, the Cr dopes into the system as Cr$_2$Te$_3$. This material demonstrates ferromagnetic proximity coupling.

10:24AM A7.00011 ABSTRACT MOVED TO M31.00008 —

10:36AM A7.00012 Critical Mechanism of Magnetic Doped Cr$_x$Bi$_{2-x}$Te$_3$ Topological Insulator Thin Films1, ZHEN ZHANG, YAN NI, RAVI HADIMANI, DAVID JILES, Department of Electrical and Computer Engineering, Iowa State University, CAJETAN NLEBEDIM, Ames Laboratory, US Department of Energy — Introducing magnetic dopants into topological insulators can lead to the opening of the surface band gap which can induce interesting phenomena such as the quantized anomalous Hall effect (QAHE) and magnetoelectric effect. However, the critical properties of ferromagnetism in magnetic doped TIs are not well studied. In this work, we investigated the effect of magnetic doping on magnetic and transport response in Bi$_2$Te$_3$ thin films. Cr$_x$Bi$_{2-x}$Te$_3$ thin films with x = 0.03, 0.14, and 0.29 were grown with low surface roughness ($\sim$ 0.4 nm). It is found that Cr is an n-type doping element, which reduces the carrier density of p-type Bi$_2$Te$_3$. Moreover, doping Cr induces long range ferromagnetism when x = 0.14 and 0.29, where anomalous Hall effect and weak localization of magnetoconductance were observed. The Arrrott-Noakes plot for Cr$_x$Bi$_{2-x}$Te$_3$ demonstrates that the critical mechanism of the ferromagnetism can be described well with 3D-Heisenberg model. Our work may benefit for the practical applications of ferromagnetic TIs with opened surface band gap in spintronics and magnetoelectric devices.

1Authors would like to thank the financial support from the U.S. National Science Foundation under the Award No. 1201883.
10:48AM A7.00013 Electrostatic control of spin polarization in a quantum Hall ferromagnet: a new platform to realize non-Abelian excitations. ALEXANDER KAZAKOV, Purdue University, V. KOLKOVSKY, Z. ADAMUS, G. KARCZEWSKI, T. WOJTOWICZ, Institute of Physics, Polish Academy of Sciences. LEONID ROKHINSON, Purdue University — Several experiments detected signatures of Majorana fermions in nanowires, and the focus of current research is shifting toward systems where non-Abelian statistics of excitations can be demonstrated. To achieve this goal we are developing a new platform where non-Abelian excitations can be created and manipulated in a two-dimensional plane, with support for Majorana and higher order non-Abelian excitations. The system is based on CdTe quantum wells non-uniformly doped with paramagnetic impurities, which result in a complex field-dependence of Zeeman splitting. A unique property of the system is that at high fields we can form a quantum Hall ferromagnet with gate-controllable spin polarization. Helical 1D edge channels formed along the edges of electrostatic gates may support generalized non-Abelian excitations in the fractional quantun Hall regime, and Majorana and parafermion excitations in the presence of induced superconductivity. We will present results on the gate control of s-d exchange in specially designed heterostructures, demonstrate gate control of spin polarization at filling factor $\nu = 2$, and show spatially separated design of quantum Hall states with different spin polarization using lithographically defined gates.

Monday, March 2, 2015 8:00AM - 11:00AM — Session A8 DCMP: Semiconductor Surfaces and Interfaces 006C - Francesca Cavallo, University of New Mexico

8:00AM A8.00001 Unusual Dramatic Surface Restructuring of Silicon Substrate during Epitaxy1. TANYA GUPTA, DANIEL STEINGART, Princeton University. JAMES HANNON, IBM, PRINCETON UNIVERSITY COLLABORATION, IBM COLLABORATION — Interfacial strain is unavoidable in heteroepitaxial growth and can have a profound impact on the morphology and properties of thin films. In fact, "engineering" thin-film strain is a critical component in many advanced technologies. For example, straining the silicon in advanced CMOS devices can increase the device speed by as much as 90 percent. In order to control interfacial strain, its effects on growth must be understood. The common picture is that the growth substrate is essentially passive: its role is to provide the lattice mismatch that the growing film must respond to. As the film grows thicker, the stress in the film evolves, which can lead to morphological changes in the film, e.g., dislocations, or a change in growth mode from 2D, planar growth to 3D, quantum dot growth. In both of these examples, the action is in the growing film. In this work we describe a growth system that behaves in a completely unexpected manner that does not fit into this conventional picture. Interfacial strain that accompanies the growth of SiC nanoparticles is relieved by a dramatic 3D, quantum dot growth. In fact, "engineering" thin-film strain is a critical component in many advanced technologies. For example, straining the silicon in advanced CMOS devices can increase the device speed by as much as 90 percent.  

8:12AM A8.00002 A joint first principles and Kelvin probe force microscopy study of stepped silicon surfaces with unprecedented resolution1. STEFAN WIPPERMANN, Max-Planck-Institute for Iron Research, CARMEN PEREZ LEON, HOLGER DREES, MICHAEL MARZ, REGINA HOFFMANN-VOGEL, Karlsruhe Institute of Technology — Stepped well-ordered surfaces are important model systems of this kind. It contains (7x7) reconstructed areas equivalent to the well characterized and understood Si(111)-(7x7) surface. Thereby this system essentially contains its own calibration, providing an ideal testbed for surface characterization techniques and understanding in depth the rich morphology of the structural features present in this system. Here we present a joint experimental and theoretical investigation of the structural properties of the vicinal Si(7710) surface. We carried out Kelvin probe force microscopy (KPFM) measurements with unprecedented atomic resolution, and first principles calculations of the local work function as a function of the lateral position of the tip above the surface. These calculations allowed us to interpret the experimental KPFM data in terms of specific structural features and electronic properties of surface states, such as e.g., defects, dangling bond angles and occupations of dangling bonds.

1 R. H.-V. acknowledges ERC starting grant NANOCONTACTS No. ERC 2009-Stg 239838.

8:24AM A8.00003 A novel ground state of the (2√3x2√3)/R30° Sn double layer on Si(111) induced by modulation hole-doping. FANGFEI MING, DANIEL MULUGETA, PAOLO VILMERCATI, University of Tennessee, Knoxville, HANNO H. WEITERING, University of Tennessee, Knoxville and Oak Ridge National Laboratory, PAUL C. SNIJ德ERS, Oak Ridge National Laboratory — Charge doping provides a tuning knob of the delicate interactions between spin, orbital, charge and lattice degrees of freedom in low-dimensional systems, which dictate many intriguing quantum phenomena. Using scanning tunneling microscopy/spectroscopy, we characterize the (2√3x2√3)/R30° Sn double layer grown on a (√3x√3)-B reconstructed Si(111) surface, where 1/3 monolayer B dopants resides in the subsurface layer without forming direct chemical bonds with the Sn layer. The B atoms donate holes to the Sn double layer and shift the Fermi level toward the valence band edge. Surprisingly, it further induces a fraction of the 2√3x2√3 phase to gradually transform to a new 4√3x2√3 phase below 80 K. The two phases coexist down to 2.5 K, indicating a phase-separated ground state for the hole doped Sn double layer, in contrast to a homogeneous 2√3x2√3 phase for the undoped one. The new 4√3x2√3 phase has a larger band gap than the 2√3x2√3 phase and the valence band edge shifts a few tens meV away from the Fermi level to higher binding energy, suggesting that the transition to the 4√3x2√3 structure is accompanied by an electronic structure rearrangement.

8:36AM A8.00004 Structure of the modulation hole doped (2√3x2√3)/R30° Sn double layer on Si(111)1. PAUL C. SNIJ德ERS, Oak Ridge National Lab, YING-TZU HUANG, University of Pennsylvania, State College, FANGFEI MING, DANIEL MULUGETA, WEISONG TU, University of Tennessee, Knoxville, PAUL R.C. KENT, Oak Ridge National Lab, RENEE D. DIEHL, University of Pennsylvania, State College, HANNO H. WEITERING, University of Tennessee, Knoxville — Over the years, a large collection of temperature dependent phase transitions has been identified in atomically thin metal overlayers on semiconductor surfaces. However, studying their doping dependence remains difficult due to the symmetry breaking nature of dopant atoms located on top of these structures, and the associated local lattice deformations localizing the doped carriers. Here we have used a subsurface modulation doping approach using B on Si(111) to hole-dope an overlaying Sn double layer. STM, LEED-I(E), and XPS were used to characterize the structure of a (2√3x2√3)/R30° Sn double layer on a Si(111) (√3x√3)-B surface. STM images 4 atoms in the top Sn layer. Using the tip to remove this top layer, a second layer consisting of 3 triangular structures becomes visible, resulting in a total of 13 Sn atoms per unit cell, consistent with an XPS core level intensity analysis. An extensive LEED-I(E) analysis using 20 independent beams with an energy range of 7126 eV points to a structural model consistent with the STM and XPS data and having a Pendry R-factor of 0.34.

1 Research sponsored by NSF DMR-1005488 (FM, DM, WT, HHW), and by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division (PCS,PRCK).
9:00AM A8.00006 The effect of Al content on the work function engineering at TiAlN/HfO$_2$ interface$^1$, GEUN-MYEONG KIM, YOUNG JUN OH, KEE JOO CHANG, Department of Physics, KAIST — In high-k/metal gate stacks of metal-oxide-semiconductor field-effect transistors, it is important to control the metal work function such that it should be close to the valence and conduction band edges of Si in p- and n-channel devices. It was reported that depositing TiAl on top of TiN/HfO$_2$ stack in gate-last process can effectively induce the n-type shift of work function, while the work function is of p-type at TiN/HfO$_2$ stack. In this work, we perform first-principles density functional calculations to investigate the Schottky barrier height at TiAl/HfO$_2$. In bulk TiN, it is found that a substitutional Al is the most stable form of Al impurity. When substitutional Al atoms are introduced at TiN/HfO$_2$ interface, the effective work function tends to decrease. At TiAIN/HfO$_2$ interface, the n-type shift of the work function increases almost linearly with the Al content. This is attributed to the change of interface bonds by Al incorporation and the dipole field induced at the interface. On the other hand, relative thicknesses of TiAl and Ti on abrupt TiAl/TiN/HfO$_2$ interface do not significantly affect the effective work function.

$^1$The authors are supported by the National Research Foundation of Korea (2005-0093845)

9:24AM A8.00008 Reversible hydrogenation of silicene, JINGLAN QIU, HUIXIA FU, LAN CHEN, KEHUI WU, Institute of Physics, Chinese Academy of Sciences — The hydrogenation of monoatomic silicene sheet on Ag$(111)$ was studied by scanning tunneling microscopy and density functional theory calculations. It was observed that hydrogenation of silicene-4×4 structure at room temperature results in a perfectly ordered γ-4×4 superstructure. A theoretical model, which involves 7 H atoms and rearranged buckling of Si atoms, was proposed and agrees with experiments very well. Unlike silicene-4×4, the hydrogenation of $(\sqrt{7}\times\sqrt{7})$silicene/(2×3) was found to be reversible at room temperature. This separation (lack of intermixing) between Ba and Ge layers is retained through successive annealing experiments up to 770 K with a gradual ordering of the Ba layer at 570 K and above and a decrease in Ba layer density. Annealing above 770 K produces the 2-D surface alloy phase accompanied by strain relief through monolayer height trench formation. At 1070 K the surface morphology changes again but remains a 2-D surface alloy phase.

9:36AM A8.00009 The STM investigations of hydrogenation on monolayer silicene with r7x7 superstructure, LAN CHEN, Institute of Physics, The Chinese Academy of Sciences — The early investigations revealed the monolayer silicene with r7x7 superstructure on Ag$(111)$ can extend over the whole substrate. But this phase was considered to be highly defective due to the strong strain, which limit the applications of this phase. In this presentation, I will report our works about the hydrogenations on the monolayer silicene with r7x7 superstructure on Ag$(111)$ by scanning tunneling microscopy (STM). The STM images show the ordered structures with lattice identical to silicene-1×1 unit cell after hydrogenation on silicene at room temperature, which reveals that the original silicene with r7x7 superstructure is an ideal defectless single-crystal monolayer film. Combined with density functional theory calculations, the structures of hydrogenation can be explained by the “sub-lattice adsorption-picture,” in which H atoms only adsorb on Si atoms in one sub-lattice of silicene. Moreover, by annealing to a moderate temperature, about 450 K, de-hydrogenation process occurs and the clean silicene surface can be fully recovered. Such reversible hydrogenation suggests that silicene may be a potential candidate as hydrogen storage materials.

9:48AM A8.00010 The Role of a Buried Interface in the Growth of Metallic Nanocrystals: Quantum Size Effects in Ag/Si$(111)$7x7, YIYAO CHEN, MICHAEL GRAMLICH, SHAWN HAYDEN, PAUL MICELI, University of Missouri-Columbia — It is shown that the buried interface between a metallic nanocrystal and its supporting substrate plays an essential role in understanding the stability of nanomaterials that grow on a wetting layer in the Stranski-Krastanov growth mode. These in situ x-ray scattering studies reveal a minimum tri-layer height for stable commensurate FCC Ag islands that are in coexistence with a commensurate Ag wetting layer. The minimum height without an oscillating height preference is explained by electron quantum confinement effects, which is manifested differently for Ag$(111)$ than for other metals, such as Pb$(111)$, that can exhibit oscillations of height preference with thickness. The results suggest that quantum size-effects are broadly important for the growth of metallic nanocrystals. Support is gratefully acknowledged from NSF DMR-0706278 and DGE-1069091. The Advanced Photon Source at Argonne National Laboratory is supported by the US-DOE W-31-109-Eng-38.
10:00AM A8.00011 A multi-scale approach to the electronic structure of doped semiconductor surfaces, OFER SINAi, Weizmann Institute of Science, Rehovoth, IL, OLIVER T. HOFMANN, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, DE, PATRICK RINKE, Aalto University School of Science, Aalto, FI, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, DE, GEORG HEIMEL, Humboldt-Universität zu Berlin, Berlin, DE, LEEOR KRONIK, Weizmann Institute of Science, Rehovoth, IL — The inclusion of the global effects of semiconductor doping poses a unique challenge for first-principles simulations, because the typically low concentration of dopants renders an explicit treatment intractable. Furthermore, the width of the space-charge region (SCR) at charged surfaces often exceeds realistic supercell dimensions. We present a multi-scale technique that addresses these difficulties. It is based on the introduction of excess charge, mimicking free charge carriers from the SCR, along with a fixed sheet of counter-charge mimicking the SCR-related field. Self-consistency is obtained by imposing charge conservation and Fermi level equilibration between the bulk, treated semi-classically, and the electronic states of the slab/surface, which are treated quantum-mechanically. The method, called CREST - the Charge-Reservoir Electrostatic Sheet Technique - can be used with standard electronic structure codes. We validate CREST using a simple tight-binding model, which allows for comparison of its results with calculations encompassing the full SCR explicitly. We then employ it with density functional theory, obtaining insight into the doping dependence of the electronic structures of the metallic clean-cleaned Si(111) surface and its semiconducting (2x1) reconstructions.

10:12AM A8.00012 First principles studies of the stability and Shottky barriers of metal/CdTe(111) interfaces, ODKHU-DORJ, M.S. MIAO, N. KIOUSSIS, California State University Northridge, S. TARI, F. AQUARIA, Y. CHANG, Sivananthan Laboratories, C. GREIN, University of Illinois at Chicago — CdZnTe and CdTe based semiconductor X-Ray and Gamma-Ray detectors have been intensively studied recently due to their promising potentials for achieving high-resolution, high signal-to-noise ratios and low leakage current, all are desirable features in applications ranging from medical diagnostics to homeland security. Understanding the atomic and electronic structures of the metal/semiconductor interfaces is essential for the further improvements of performance. Using density functional calculations, we systematically studied the stability, the atomic and electronic structures of the interfaces between Cd-terminated CdTe (111) surface and the selected metals. We also calculated the Shottky barrier height (SBH) by aligning the electrostatic potentials in semiconductor and metal regions. Our calculations revealed the importance of intermixing between semiconductor and metal layers and the formation of Te-metal alloys at the interface. The obtained SBH does not depend much on the choice of metals despite the large variation of the work functions. On the other hand, the interface structure is found to have large effect to the SBH, which is attributed to the metal induced states in the gap. The position of such states is insensitive to the metal work functions, as revealed by the analysis of the electronic structures.

10:24AM A8.00013 Band offsets at the crystalline / hydrogenated amorphous silicon interface from first-principles, EBRAHIM HAZRATI, KAROL JAROLIMEK, GILLES A. DE WIJJS, Roadbed University, Nijmegen, The Netherlands, INSTITUTE FOR MOLECULES AND MATERIALS TEAM — The heterojunction formed between crystalline silicon (c-Si) and hydrogenated amorphous silicon (a-Si:H) is a key component of a new type of high-efficiency silicon solar cell. Since a-Si:H has a larger band gap than c-Si, band offsets are formed at the interface. A band offset at the minority carrier band will mitigate recombination and lead to an increased efficiency. Experimental values of band offsets scatter in a broad range. However, a recent meta-analysis of the results (W. van Sark et al. pp. 405, Springer 2012) gives a larger valence offset (0.40 eV) than the conduction offset (0.15 eV). In light of the conflicting reports our goal is to calculate the band offsets at the c-Si/a-Si:H interface from first-principles. We have prepared several atomistic models of the interface. The crystalline part is terminated with (111) surfaces on both sides. The amorphous structure is generated by simulating an annealing process at 1100 K, with DFT molecular dynamics. Once the atomicistic model is ready it can be used to calculate the electronic structure of the interface. Our preliminary results show that the valence offset is larger than the conduction band offset.

10:36AM A8.00014 Interface Formation for a Ferromagnetic/Antiferromagnetic Bi-layer System Studied by Scanning Tunneling Microscopy and First Principles Theory, ANDRADA-OANA MANDRU, JONATHAN GUERRERO-SANCHEZ, JEONGHIM PAK, NOBORU TAKEUCHI, ARTHUR SMITH, Nanoscale and Quantum Phenomena Institute, Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701, USA — We investigate the initial stages of interface formation for Fe/Mn$_2$N$_2$(001) ferromagnet/antiferromagnet bi-layer system down to the atomic scale using a combination of molecular beam epitaxy, scanning tunneling microscopy and first principles theoretical calculations. Sub-monolayer iron deposits on onto manganese nitride nanoparticle surfaces induce the formation of one monolayer high islands that are present on all terraces. Unexpectedly, the chemical composition of the observed islands does not consist of Fe, as determined using Auger electron spectroscopy, conductance imaging and theoretical models. Further theoretical calculations reveal how Fe atoms incorporate into specific subsurface layers. In addition, theory finds the magnetic alignment of the Fe atoms within a particular layer and with adjacent Mn$_2$N$_2$(001) layers. This study suggest that these complex structural rearrangements at the interfaces between such magnetic bi-layer systems are important to take into account when considering the exchange coupling between the layers.

10:48AM A8.00015 ABSTRACT WITHDRAWN —

Monday, March 2, 2015 8:00AM - 11:00AM — Session A9 DCMP: Majorana Fermions and Superconductivity 006D - Christian Platt, Stanford University

8:00AM A9.00001 Topological Shiba chain in a spin-orbit coupled superconductor, PHILIP BRYDON, HOI-YIN HUI, JAY SAU, Condensed Matter Theory Center, University of Maryland, College Park — The impurity band formed from a chain of classical spins embedded in a superconductor can be topological, depending on the magnetic texture of the spins. Previous proposals require a helical texture [1] which is, however, unstable towards a ferromagnetic or antiferromagnetic configuration [2]. We show that including surface spin-orbit coupling permits a topological gap in a broad range. However, a recent meta-analysis of the results (W. van Sark et al. pp. 405, Springer 2012) gives a larger valence offset (0.40 eV) than the conduction offset (0.15 eV). In light of the conflicting reports our goal is to calculate the band offsets at the c-Si/a-Si:H interface from first-principles. We have prepared several atomistic models of the interface. The crystalline part is terminated with (111) surfaces on both sides. The amorphous structure is generated by simulating an annealing process at 1100 K, with DFT molecular dynamics. Once the atomicistic model is ready it can be used to calculate the electronic structure of the interface. Our preliminary results show that the valence offset is larger than the conduction band offset.

1. We acknowledge support from JQI-NSF-PFC and LPS-CMTC.

References:
8:12AM A9.00002 Zero-bias peak splitting in InSb nanowires , JUN CHEN, PENG YU, University of Pittsburgh, Pittsburgh, PA, 15260, USA, MOIRA HOCEVAR, Institut Niel CNRS, Grenoble, France, SEBASTIEN PLISSARD, CNRS, LAAS, Toulouse, France, DIANA CAR, ERIK BAKKERS, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands, SERGEY FROLOV, University of Pittsburgh, Pittsburgh, PA, 15260, USA — Zero-bias conductance peak (ZBP) has been reported as a signature of Majorana fermions in InSb nanowires. Other features like ZBP phase diagram in chemical potential vs. magnetic field and peak splitting are proposed as additional evidences of Majorana fermions. We make superconductor-InSb nanowire hybrid devices with the aim of exploring these features and beyond. By means of high-k HfOx as the dielectric layer, we obtain large gate-tunability of magnetic properties and use it to map out ZBP phase diagram. Here we report observation of ZBP at finite magnetic field. Such peak is tunable with gates underneath the superconductor. In particular, it splits and merges again as a function of the center gate. We study such splitting in the context of a pair of coupled Majorana bound states.

8:24AM A9.00003 Electrostatic effects in Majorana hybrid structures , PIYAPONG SITHSONN, TUDOR STANESCU, West Virginia University — We study the electrostatic effects that emerge in proximity-coupled semiconductor (SM-SC) structures due to the charge transfer induced by the work function difference between the two materials. The effects are described theoretically using a tight-binding model of the heterostructure solved within a self-consistent Poisson-Schrödinger scheme. We find that these effects are responsible for i) generating an effective Rashba-type spin-orbit coupling and ii) modifying the spatial dependence of the low-energy wave functions near the SM-SC interface. This change in the wave-function amplitude at the interface strongly affects the proximity-induced superconducting gap. Both effects have critical consequences on the stability of the Majorana-hosting topological superconducting phase that is predicted to emerge in this type of structures. For a thin-film geometry, we determine the dependence of the effective spin-orbit coupling and induced superconducting gap on the film thickness and on the strength of the SM-SC coupling.

8:36AM A9.00004 Majorana bound states on a self-organizing helical magnonic wire on the surface of a superconductor with spin-orbit coupling , MORTEN HOLM CHRISTENSEN, JENS PAAESKE, BRIAN M. ANDERSEN, Niels Bohr Institute, University of Copenhagen — Recent STM experiments [1] have observed zero-energy modes consistent with Majorana bound states at the ends of ferromagnetically aligned Fe-chains grown on the surface of lead. We consider a chain of magnetic moments on top of an s-wave superconductor with spin-orbit coupling and study their magnetic ordering self-consistently. In the absence of spin-orbit coupling we find that a topologically non-trivial helical state appears for sufficiently high values of the chemical potential, in agreement with Ref. [2], while including spin-orbit coupling and imposing ferromagnetic order we find a non-trivial phase with Majorana bound states in agreement with Ref. [3]. We report numerical results for the general case, with non-zero spin-orbit coupling and self-organized magnetic order, allowing the moments to minimize the free energy. A range of different magnetic orders are identified and topologically non-trivial regions are found to prevail in a large parameter region. [1] Yazdani et. al Science, 6209 (2014) [2] I. Reis et. al. Phys. Rev. B. 90, 085124 2014 [3] Brydon et. al. arXiv:1407.6345 (2014)

8:48AM A9.00005 Majorana modes and transport across junctions of superconductors and normal metals1 , DIPTIMAN SEN, MANISHA THAKURATHI, OINDRILA DEB, Indian Institute of Science, Bengaluru, India — We study Majorana modes and transport in one-dimensional systems with junctions of p-wave superconductors (SCs) and normal metal (NM) leads. For a system with a SC lying between two NM leads, it is known that there exists a Majorana mode at the junction between the SC and each NM. If an impurity is present or the p-wave pairing amplitude changes sign at some point in the superconductor, two additional Majorana modes appear near that point. We study the effects of all these modes on the normal and Cooper pair conductances. The main effect is to shift the conductance peaks away from zero bias due to hybridization between the Majoranas, the shift oscillates and also decays exponentially as the length of the SC is increased. Using bosonization and the renormalization group (RG) method, we study the effect of interactions between the electrons on the Majorana modes and the conductances. We then consider a system with a junction of three SC regions connected to NM leads. The junction is parameterized by a scattering matrix. Depending on the relative signs of the pairing amplitudes in the three SCs, there may be one or three Majorana modes at the junction. We study the effect of interactions on these modes using an RG analysis which is valid for weak interactions.

1 We thank DST, India and CSIR, India for financial support.

9:00AM A9.00006 Majorana Correlation as a Signature of a Topological Phase Transition1 , AMIT NAG, JAY D. SAU, Condensed matter theory center, University of Maryland- College Park — Spin orbit coupled semiconductor nanowires in proximity to ordinary s-wave superconductor exhibit a topological phase which supports Majorana fermions at the two ends of the nanowire. A signature of Majorana fermions would be a zero bias conductance peak. Indeed such a peak has been observed in recent experiments but at the same time alternate non topological mechanisms have been suggested to explain appearance of the zero bias peak. Here we demonstrate that the zero bias conductance peak from Majorana fermions must appear in a correlated way between the two ends. We analyze how this peculiarity can be used as a signature of the topological phase transition linked to the appearance of Majorana modes and thus can be used to experimentally distinguish between competing theoretical mechanisms.

1 We acknowledge support from Physics Frontier Center and Maryland Startup Fund.

9:12AM A9.00007 Topological Kondo effect in transport through superconducting wire with multiple Majorana end states , OLEKSII KASHUBA, CARSTEN TIMM, Institute of Theoretical Physics, TU Dresden — The transport through the interface between normal metal and topological superconducting wire can be affected by the interaction of the lead electrons and edge states in the wire. For a minimum of three Majorana fermions at the interface, we find nontrivial renormalization physics. Classification of the tunneling processes by spin-1/2 and spin-3/2 irreducible representations of the SU(2) group allows to identify two different renormalization behaviors associated with the representations. Renormalization triggered by the interaction enhances one group of the tunneling amplitudes and suppresses another one, depending on whether the coupling is ferro- or antiferromagnetic. The nontrivial RG processes manifest themselves in distinct temperature dependencies and different spin polarizations of the current through the interface depending on the sign of the interaction.

9:24AM A9.00008 Modulation of the phase in SC order parameter in Kitaev chain and its consequences , SHO NAKOSAI, Univ of Tokyo, YUKIO TANAKA, Nagoya Univ, NAOTO NAGAOSA, RIKEN — Kitaev’s superconducting chain model, one dimensional spinless p-wave superconductor, is a prototype of topological superconductors and supports Majorana modes at the ends of the system. There have been intensive researches on the model since the role of topology in condensed matter physics is highlighted, and recently not a few experimental results show the model can be effectively generated in designed systems. Anytime soon, we will arrange it as we like. A simple extension of the model is two-parallel-aligned chains. It possesses four Majorana states in total. When we take into account the modulation of the phase in the superconducting order parameter, however, the degeneracy of the energy levels is resolved. We investigate the physical consequence of it. The phase should change along the chain to reduce the total energy of the system, and the deterministic equation for it is in the form of sine-Gordon equation. The distribution of the supercurrent due to the modulation leaves the degeneracy in the ground states. Then we can regard the system as a flux qubit. In the presence of external magnetic field, these modulations will couple with the spontaneous field associated with the phase modulation, and result in control of states and an unusual Josephson effect.
Topological Superconductivity in Ferromagnetic Metal Chains: Part I

JIAN LI, Princeton University, HUA CHEN, University of Texas at Austin, Ilya Drozdov, Ali Yazdani, Bogdan Bernevig, Princeton University, Alllan MacDonald, University of Texas at Austin — Recent experiments have demonstrated superconductivity induced in ferromagnetic atomic chains as a new route to the research of Majorana physics. In this talk we discuss the theory behind these experiments. We will present a generic picture for how superconductivity is induced in ferromagnetic metal chains through coupling to a superconductor with strong spin-orbit coupling, and explain why this hybrid system is a plausible new platform in searching for topological superconductivity. We will then present a tight-binding model associated with the existing experiments. We reveal a new chain magnetic symmetry that is able to stabilize multiple Majorana end modes in the absence of disorder, resulting in a one-dimensional crystalline topological superconductor. We show phase diagrams in terms of such topological phases and point out their relevance to the existing experiments. In the last part of this talk we will briefly discuss some other directions of research based on the new platform, including braiding Majorana quasi-particles in ferromagnetic chains, as well as realizing topological superconductivity in two-dimensional ferromagnetic thin films.

Impurity-induced bound states in superconductors with spin-orbit coupling1

YOUNGHYUN KIM, University of California - Santa Barbara, JUN HUA ZHANG, E. ROSSI, College of William and Mary, ROMAN LUTCHYN, Microsoft Research Station Q — We study the effect of strong spin-orbit coupling on bound states induced by impurities in superconductors. The presence of spin-orbit coupling breaks the SU(2)-spin symmetry and causes the superconducting order parameter to have generically both singlet (s-wave) and triplet (p-wave) components. As a result, impurity-bound states corresponding to different angular momentum channels hybridize and display a number of qualitatively different features from that of the well-known Yu-Shiba-Rusinov states in conventional s-wave superconductors. In particular, we find that in the presence of spin-orbit coupling the spectrum of the impurity-bound states depends on the orientation of the magnetic moment of the impurity. Our predictions can be used to distinguish the order parameter and have implications for the Majorana proposals based on chains of magnetic atoms placed on the surface of superconductors with strong spin-orbit coupling [1].

1 We acknowledge support from ONR-N00014-13-1-0321.

Effect of spin-orbit coupling on the topological phase diagram of a Shiba chain1

TEEMU OJANEN, JOEL RONTYNEN, ALEX WESTSTROM, KIM POYHONEN, School of Science, Aalto University, O. V. LOUNASMAA LABORATORY TEAM — Topological superconductivity was recently observed in a system consisting of a 1D magnetic adatoms on top of a superconducting surface. Anticipating further developments, we show that a 2D array of magnetic atoms support a variant of px +ipy superconductivity and exhibit very complex phase diagram with high Chern numbers. We also present a detailed study of Majorana bound states in 1D chains.

1 The authors acknowledge the Academy of Finland for support.

Weak and strong coupling regimes in Majorana hybrid structures1

JOHN STENGTER, TUDOR STANESCU, West Virginia University — We study the proximity-induced low-energy physics that emerges in semiconductor - superconductor hybrid structures. We find that the proximity-induced gap has a non-monotonic dependence on the effective semiconductor - superconductor coupling strength. To identify the qualitative difference between weak and strong coupled regimes characterized by similar values of the induced gap, we determine the dependence of the differential conductance of a metal - semiconductor - superconductor structure capable of hosting zero-energy Majorana bound states on the heterostructure parameters (semiconductor wire thickness, semiconductor - superconductor coupling strength, etc.) and apply an effective energy theory. We apply this effective theory by properly integrating out the high-energy degrees of freedom (rather than simply ignoring them), which results in a strong renormalization of the low-energy sector. Using this effective theory, we describe the qualitative differences between the Majorana signatures emerging in the weak and strong coupling regimes.

Universal Nonequilibrium Signatures of Majorana Zero Modes in Quench Dynamics1

ROMAIN VASSEUR, JAN DAHLHAUS, JOEL MOORE, UC Berkeley — The quantum evolution after a metallic lead is suddenly connected to an electron system contains information about the excitation spectrum of the combined system. We exploit this type of “quantum quench” to probe the presence of Majorana fermions at the ends of a topological superconducting wire. We obtain an algebraically decaying overlap (Loschmidt echo) Ζ(t) = (|ψ(0)|ψ(t))² ∼ t^−α for large times after the quench, with a universal critical exponent α = 1/4 that is found to be remarkably robust against details of the setup, such as interactions in the normal lead, the existence of additional lead channels or the presence of bound levels between the lead and the superconductor. As in recent quantum dot experiments, this exponent could be measured by optical absorption, offering a new signature of Majorana zero modes that is distinct from interferometry and tunneling spectroscopy.

1 This work was supported by the Quantum Materials program of LBNL (R. V.), NSF DMR-1206515 and the Simons Foundation (J.E.M.), the Netherlands Organization for Scientific Research NWO (J. P. D.), and the German Academic Exchange Service DAAD (J. P. D.)

New Topological Superconducting phase in Superconductor/2D Topological Insulator/Superconductor Junction

YAO LU, KAM TUEN LAW, The Hong Kong University of Science and Technology — It is well known that a Josephson junction built on top of helical edge states of the topological insulator traps two Majorana fermions when the phase difference between the two superconductors is π and the system can be considered as a DIII class topological superconductor. In this work, we show that a narrow strip of two dimensional topological insulator coupled to two superconductors, forming a Josephson junction, can support a new topological phase in the presence of an in-plane magnetic field. In this phase, each end of the strip of the topological insulator supports a single Majorana fermion for a wide range of phase difference between the two superconductors. This topological phase can be revealed by Josephson current measurements and tunneling spectroscopy experiments.
Monday, March 2, 2015 8:00AM - 11:00AM — Session A10 DCMP: Topological Matters 007A - Jason Alicea, California Polytechnic Institute

8:00AM A10.00001 Composite Dirac liquids: parent states of symmetric surface topological orders

ANDREW ESSIN, DAVID MROSS, IQIM, Caltech, JASON ALICEA, Caltech — In the absence of interactions, topological insulators surfaces must be gapless or break symmetry. With the addition of strong interactions at the surface, a third possibility is a gapped, symmetric surface that supports anyons, as has been recognized in a number of recent developments. The composite Dirac liquid (CDL) provides a natural stepping stone to identifying such states. The CDL consists of neutral, fractional Dirac fermions coupled to gapped charges, and the addition of pairing to the neutral sector produces a gap for all excitations without breaking any symmetry. The quasi-1D technology we have used in the study of the CDL also allows us to construct and characterize such gapped surface phases, and generalizes naturally to (bosonic) symmetry protected topological phases as well.

1 This work was supported by the Institute for Quantum Information and Matter, an NSF Physics Frontiers Center with support of the Gordon and Betty Moore Foundation through Grant GBMF1250

8:12AM A10.00002 Composite Dirac liquids: exotic gapless states at an electronic topological insulator surface

DAVID MROSS, ANDREW ESSIN, JASON ALICEA, Caltech — We introduce exotic gapless states 'composite Dirac liquids' that can appear at a strongly interacting surface of a three-dimensional electronic topological insulator. Composite Dirac liquids exhibit a gap to all charge excitations but nevertheless feature a single massless Dirac cone built from emergent electrically neutral fermions. These states thus comprise electronic insulators that preserve all symmetries and, interestingly, retain thermal properties similar to those of the non-interacting topological insulator surface. To controllably access the composite Dirac liquid we exploit a quasi-1D deformation of the original electronic Dirac cone that enables us to analytically address the fate of the strongly interacting surface.

8:24AM A10.00003 Axion field theory and \( Z_{16} \) classification of time reversal invariant topological superconductors

YINGFEI GU, XIAOLIANG QI, Stanford Univ — Time-reversal invariant topological superconductors (TRI TSC) are gapped superconductors with topologically robust gapless modes on the boundary. In the work by X. L. Qi et al, [PRB, 87, 134519(2013)], a topological field theory description was proposed for 3+1-dimensional TRI TSC, which contains an axionic coupling between superconducting phase and electromagnetic field. In my talk, I will describe a generalization of this theory to include interaction effects which provides a physical explanation why the integer classification is reduced to \( Z_{16} \). I will also attempt to generalize our results to higher dimensions and give constraints on the possible collapsing of topological classification induced by interaction effects.

8:36AM A10.00004 Possible realization of interacting symmetry-protected topological phases in topological crystalline insulators

HIROKI ISOBE, University of Tokyo, LIANG FU, Massachusetts Institute of Technology — The effects of electron-electron interaction in edge states of mirror-symmetry protected topological crystalline insulators (TCIs) are discussed. The analysis is performed by using bosonized Hamiltonian following the Tomonaga-Luttinger liquid theory. When two pairs of helical edge states exist, electron-electron interaction could gap out one edge mode, which is a possible realization of interacting symmetry-protected topological (SPT) phases. This type of SPT phase is closely related to a Luther-Emery liquid in spinful 1D system. We also propose a method of detecting the SPT phases by STM. The other focus of the study is the classification of SPT phases in mirror-symmetry protected TCIs. By adopting the Chern-Simons theory, we find that electron-electron interaction reduces the classification from \( Z \) to \( Z_{16} \). It means that the edge states can be gapped out when four pairs of edge states exist. In other cases, the edge modes cannot be fully gapped. Each of these states corresponds to a different SPT phase depending on the relevant interaction process.

8:48AM A10.00005 Topological crystalline insulators from crystal field effect in monolayer IV-VI semiconductors

JUNWEI LIU, XIAOFENG QIAN, LIANG FU, MIT — Two-dimensional (2D) topological crystalline insulators (TCIs) were recently predicted in thin films of the SnTe class of IV-VI semiconductors, which can host metallic edge states protected by mirror symmetry. As thickness decreases, quantum confinement effect will increase and surpass the inverted gap at a critical thickness, turning 2D TCIs into normal insulators. Surprisingly, based on first-principles calculation, here we demonstrate that (001) monolayers of rocksalt IV-VI semiconductors XY (X=Ge, Sn, Pb and Y= S, Se, Te) are 2D TCIs with the fundamental band gap as large as 260 meV in monolayer PbTe. This unexpected nontrivial topological phase stems from the strong crystal field effect in the monolayer, which lifts the degeneracy between \( p_x \) and \( p_y \) orbitals and leads to band inversion between cation and anion \( p_z \) orbitals. Our work offers a new strategy to find atomically thin 2D topological materials.

9:00AM A10.00006 ABSTRACT WITHDRAWN —

9:12AM A10.00007 Probing Topological Superconductors

DAVID SCHMELTZER, C.C.N.Y. — The presence of attractive interaction on the surface of a 3D topological insulator which is characterized by spinors carrying a Berry phase of \( \pi \) stabilizes gapped symmetric surface topological superconductors with topologically robust gapless modes on the boundary. We construct the effective dual action for the superconductor with the vortices, and show that the \( 2n \) Majorana fermions are localized and can be replaced with \( n \) spinless fermions. The effect of the Majorana zero modes can be observed through the Andreev cross reflection when metallic leads are attached to the superconductor. The presence of the Majorana fermions can be detected with transverse sound waves. We have computed the effect of elastic strain fields and obtain an anomalous response indicating the presence of the Majorana fermions.

9:24AM A10.00008 Time-reversal invariant topological superconductivity in doped Weyl semimetals

PAVAN HOSUR, Stanford Univ, XI DAI, ZHONG FANG, Institute of Physics, Chinese Academy of Sciences, XIAO-LIANG QI, Stanford Univ — Time-reversal invariant topological superconductors are a new state of matter which have a bulk superconducting gap and robust Majorana fermion surface states. These have not yet been realized in solid state systems. In this paper, we propose that this state can be realized in doped Weyl semimetals or Weyl metals. The Fermi surfaces of a Weyl metal carry Chern numbers, which is a required ingredient for such a topological superconductor. By applying the fluctuation-exchange approach to a generic model of time-reversal invariant Dirac and Weyl semimetals, we investigate what microscopic interactions can supply the other ingredient, viz., sign changing of the superconducting gap function between Fermi surfaces with opposite Chern numbers. We find that if the normal state is inversion symmetric, onsite repulsive and exchange interactions induce various nodal phases as well as a small region of topological superconductivity on the phase diagram. Unlike the 3D Dirac topological superconductor, the phase here does not rely on any special momentum dependence of the pairing amplitude. Breaking inversion symmetry precludes some of the nodal phases and the topological superconductor becomes much more prominent, especially at large ferromagnetic interaction.

1 We acknowledge support from the David and Lucile Packard Foundation, the Department of Energy Office of Basic Sciences, National Science Foundation, National Science Foundation of China and 973 Program of China for financial support
9:36AM A10.00009 Topological Crystalline Metal in Orthorhombic Perovskite Iridates, YIGE CHEN, University of Toronto, YUAN-MING LU, University of California, Berkeley, HAE-YOUNG KEE, University of Toronto — Since topological insulators were theoretically predicted and experimentally observed in semiconductors with strong spin-orbit coupling, more and more attention has been drawn to topological materials which host exotic surface states. These surface excitations are stable against perturbations since they are protected by global or spatial/lattice symmetries. Succeeded in achieving various topological insulators, a tempting challenge now is to search for metallic materials with novel topological properties. Here we predict that orthorhombic perovskite iridates realize a new class of metals dubbed topological crystalline metals, which support zero-energy surface states protected by certain lattice symmetry. These surface states can be probed by photoemission and tunneling experiments. Furthermore, we show that by applying magnetic fields, the topological crystalline metal can be driven into other topological metallic phases, with different topological properties and surface states.  

9:48AM A10.00010 Crystalline Topological Insulators and Superconductors – The Role of Nonsymmetric Symmetries, DANIEL VARJAS, FERNANDO DE JUAN, YUAN-MING LU, Univ of California - Berkeley — We investigate how the presence of nonsymmetric lattice symmetries affects the classification of topological insulators and superconductors in 2 and 3 dimensions. We use the representation theory of space groups, the classification of 1D fermionic symmetry protected topological phases and analyze tight binding models that exhibit gapless surface modes protected by unitary or antiunitary space group symmetries.

10:00AM A10.00011 New classes of three-dimensional topological crystalline insulators with unpinned surface Dirac cones, CHEN FANG, TIMOTHY HSIEH, LIANG FU, Massachusetts Institute of Technology — We theoretically predict two new classes of 3D topological crystalline insulators (TCI) that have protected, robust surface states. In first class, the surface states are protected by a single glide mirror symmetry. On a symmetry-preserving surface, a single Dirac point can appear at any position along either one of the two mirror symmetric lines inside the surface Brillouin zone (SBZ). In the second class, the surface Dirac point is protected by a combination of twofold rotation and time-reversal symmetry, and appears on the crystal surface perpendicular to the rotation axis. Its position in the SBZ is completely free to move by symmetry-preserving perturbations. In each class, we prove the existence of a $Z_2$ bulk invariant and find its explicit analytic expression. These new classes of TCI do not presume the presence or the absence of spin-orbital coupling.

10:12AM A10.00012 Topological phase transition in thin-film topological crystalline insulators, AI YAMAKAGE, HIDEYUKI OZAWA, MASATOSHI SATO, YUKIO TANAKA, Department of Applied Physics, Nagoya University — Topological crystalline insulator is one of the recent breakthrough ideas [1], in which Dirac fermions on the surface protected by crystalline symmetry, not by time-reversal symmetry. Another direction of the topological expansion is nanofabrication. In this work, we reveal the topological phase diagram of a thin-film topological crystalline insulator Pb$_x$Sn$_{1-x}$Te. Odd numbers of layers of Pb$_x$Sn$_{1-x}$Te exhibit the topological phase transition between two-dimensional trivial and topological crystalline insulators protected by the mirror-Chern number, which is consistent with the previous work [2]. In addition, we have found a new topological phase in the even numbers of layers, which is protected by the glide symmetry [3]. This glide topological phase can be realized in the thin film not in the bulk system.

10:24AM A10.00013 Interface gapless states from interfacial symmetries, RYUJI TAKAHASHI, University of Applied Physics, Tokyo, SHUICHI MURAKAMI, Department of Physics, Tokyo Institute of Technology — Previously we have shown that at an interface between two topological insulators with opposite Dirac velocities, gapless interface states protected by mirror symmetry appear [1]. We can calculate the interface dispersion using the Fu-Kane-Mele (FKM) tight-binding model, and it typically consists of Dirac cones. In this presentation, we report another kind of interface metallic states; the Fermi surface forms loops (‘Fermi loop’) [2], rather than isolated Dirac points, sometimes seen in the interface of the FKM models. Such a degeneracy along a loop is unexpected. This Fermi loop appears when the whole junction system preserves particle-hole symmetry, while each system breaks particle-hole symmetry. We call this symmetry “interfacial particle-hole symmetry” (IPHS). We discuss the IPHS in general systems and show that the Fermi loop results from a sign change of a Pfaffian of some matrix, defined only in junctions with IPHS symmetry [2].

10:36AM A10.00014 Quantum anomalous Hall insulators and transitions in spin-orbit coupled double perovskites, ARUN PARAMEKANTI, ASHLEY COOK, CIARAN HICKEY, University of Toronto — Motivated by the interest with strong spin-orbit coupling and ferromagnetism, we study quantum anomalous Hall insulators and their quantum phase transitions in clean systems. We show that certain quantum anomalous Hall critical points support quadratic band touching points, which can lead to interaction induced emergent phases which form a domino around the critical point. This yields the simplest example of the ubiquitously observed formation of novel phases around an underlying metallic quantum critical point. We explore double perovskites with high Tc ferromagnetism and strong spin-orbit coupling, including Sr$_2$FeMoO$_6$, as possible candidate materials in which to explore this physics.

3We acknowledge funding from NSERC and CIFAR.

10:48AM A10.00015 Transport Signatures of Fermi Surface Topology in BiTeI, LINDA YE, University of Tokyo, JOSEPH CHECKELSKY, Massachusetts Institute of Technology, FUMITAKA KAGAWA, YOSHINORI TOKURA, RIKEN Center for Emergent Matter Science — The giant bulk Rashba spin-orbit coupling in BiTeI makes it not only an interesting spintronics system but also a host of an effect Dirac-like electronic structure of fundamental interest. As a function of lowering the Fermi level $E_F$ across the associated Dirac point ($E_F = 0$), the Fermi surface of BiTeI changes its topology: from a spindle-torus ($E_F > 0$) through a horn-torus ($E_F = 0$) to a ring-torus ($E_F < 0$). Here we report a systematic evolution of the magnetoresistance across these energy boundaries in high quality single crystals exhibiting Shubnikov-de Haas oscillations. We further discuss the physical origin of the detailed $E_F/field$/temperature dependencies and remark on the relevance of this study to band crossings generally occurring in 3D systems.
8:00AM A11.00001 Origin of charge density wave instability in the underdoped cuprates\textsuperscript{1}. VIVEK MISHRA, M. R. NORMAN, Materials Science Division, Argonne National Laboratory, Lemont, IL 60439. — The exact nature of the normal state in the underdoped cuprates is still debatable. Recent experimental results favor the existence of an unconventional charge density wave with d-wave form factor above the superconducting transition. Here we study the charge density wave instability within the Eliashberg framework. We find the full momentum structure of the leading charge density wave order and compare its strength to the superconductivity driven by spin-fluctuation mediated pairing interaction.

\textsuperscript{1}This work was supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the US DOE, Office of Science, under Award No. DE-AC0298CH1088.

8:12AM A11.00002 ABSTRACT WITHDRAWN

8:24AM A11.00003 Interplay between pair-density-wave and charge-density-wave orders in underdoped cuprates. DANIEL AGTERBERG, University of Wisconsin-Milwaukee, YUXUAN WANG, Univ of Wisconsin, Madison, ANDREY CHUBUKOV, University of Minnesota — We analyze the interplay between charge-density-wave (CDW) and pair-density-wave (PDW) orders within the spin-fermion model for the cuprates. We show that both orders do emerge in the spin-fermion model as preemptive orders to antiferromagnetism, and are constructed out of pairs of “hot” fermions on the Fermi surface. We that the two orders are nearly degenerate and are related by an approximate SU(2) particle-hole symmetry of the spin-fermion model. The SU(2) symmetry is exact if one neglects the curvature of the Fermi surface in hot regions, in which case the CDW and PDW, each breaking translational U(1) symmetry, become components of an O(4)-symmetric super-vector. We show that the curvature of the Fermi surface breaks this degeneracy and that the mean-field transition temperature is higher for the PDW order. However, we also argue that both CDW and PDW order break additional discrete $Z_2$ symmetries and show that the feedback from the $Z_2$ order on the CDW order is stronger. This feedback increases the critical temperature for CDW order compared to that for PDW order. Which state develops first depends on system parameters. We also consider the case when both orders are present at low $T$ and argue that simultaneous presence of CDW and PDW orders induce a variety of states.

8:36AM A11.00004 Composite Charge Order In Cuprate Superconductors. ANDREY CHUBUKOV, University of Minnesota, YUXUAN WANG, Univ of Wisconsin, Madison — We analyze charge order in hole-doped cuprates. We argue that magnetically-mediated-interaction, which is known to give rise to d-wave superconductivity, also gives rise to charge-density-wave instabilities with momenta $Q_x = (Q, 0)$ and $Q_y = (0, Q)$, as seen in the experiments. We show that the emerging charge order with $Q_x/Q_y$ is of stripe type and that a stripe charge order parameter by itself has two components: one is incommensurate density variation, another is incommensurate current. Both components are non-zero in the CDW-ordered state, with the relative phase $\pm \pi/2$. Such an order breaks time reversal symmetry. We further show that, before a true incommensurate CDW order sets in, the system develops a pre-emptive composite order which breaks lattice rotational symmetry and time-reversal symmetry but preserves a translational $U(1)$ symmetry. We discuss the interplay between our CDW order and superconductivity and the spin-fluctuation scenario for the pseudogap phase.

8:48AM A11.00005 Ginzburg-Landau Theory of multi-component order parameter in the cuprate pseudo-gap regime. LAIMEI NIE, Stanford University, SUBIR SACHDEV, Harvard University, STEVEN KIVELSON, Stanford University — We study a Landau-Ginzburg-Wilson effective field theory of a quasi-2D system with potential disorder in which incommensurate charge-density-wave and superconducting orders are intertwined. The model is shown to exhibit a rich phase diagram at a large-N mean-field level, where both superconducting and nematic, but not charge-density-wave order, can persist in the presence of the quenched disorder. We select three representative sets of input parameters and compute the corresponding CDW structure factors. Where nematicity and SC coexist, the peak height of the CDW structure factor decreases monotonically as a function of increasing $T$, unlike what is seen in X-ray experiments in YBCO. In the parameter regime where no nematic phase occurs, we compute to one-loop order the nematic correlation length, which is shown to be much shorter than CDW correlation length.

9:00AM A11.00006 Quasiparticle transport coefficients from a mean field bond density wave state in high-Tc cuprates. GIRISH SHARMA, Clemson University, Clemson, SC 29634, USA, KANGJUN SEO, School of Natural Sciences, University of California at Merced, Merced, California 95343, USA, SUMANTA TEWARI, Clemson University, Clemson, SC 29634, USA, COLLABORATION WITH K.SEO COLLABORATION — The pseudogap regime in low hole doped high Tc cuprate superconductors exhibits peculiar experimental signatures like the detection of enhanced negative signals for Hall, Seebeck and Nernst coefficients. This has been ascribed to a competing density wave order near 1/8 hold doping and low temperature regimes. Starting with a mean field quasiparticle model describing a bi-axial bond density wave (BDW) state with $Q_1 = (0, 2\pi/3)$ and $Q_2 = (2\pi/3, 0)$, we show that the Fermi surface is reconstructed with the emergence of electron and hole-like pockets in the Brillouin zone. Employing semi-classical Boltzmann dynamics, the emergence of an enhanced negative Hall, Seebeck and Nernst coefficients is shown which is consistent with experimental data. This type of response is not seen for a uni-axial BDW order of type Q1 or Q2.

9:12AM A11.00007 Monte Carlo studies of diamagnetism and charge density wave order in the cuprate pseudogap regime. LAUREN HAYWARD SIERENS, ANDREW ACHKAR, DAVID HAWTHORN, University of Waterloo, ROGER MEIKO, University of Waterloo / Perimeter Institute for Theoretical Physics, SUBIR SACHDEV, Harvard University / Perimeter Institute for Theoretical Physics — The pseudogap regime of the hole-doped cuprate superconductors is often characterized experimentally in terms of a substantial diamagnetic response and, from another point of view, in terms of strong charge density wave (CDW) order. We introduce a dimensionless ratio, $R$, that incorporates both diamagnetic susceptibility and the correlation length of CDW order, and therefore reconciles these two fundamental characteristics of the pseudogap [PRB 90, 094515 (2014)]. We perform Monte Carlo simulations on a classical model that considers angular fluctuations of a six-dimensional order parameter [Science 343, 1336 (2014)], and compare our Monte Carlo results for $R$ with existing data from torque magnetometry and x-ray scattering experiments on YBa$_2$Cu$_3$O$_{6+x}$. We achieve qualitative agreement, and also propose future experiments to further investigate the behaviour of this dimensionless ratio.

9:24AM A11.00008 The charge susceptibility in the cuprate pseudogap phase: Similarieties and differences between Fermi pockets and Fermi arcs scenarios. PETER SCHERPELZ, ADAM RANCON, James Franck Institute, University of Chicago, YAN HE, College of Physical Science and Technology, Sichuan University, K. LEVIN, James Franck Institute, University of Chicago — Recent experimental results have provided a variety of evidence for incommensurate charge ordering in underdoped cuprates. To understand these experimental findings, here we address the calculation of charge response functions. We perform these calculations for both the Fermi arcs approach, and the Fermi pockets scenario of Yang, Rice, and Zhang. Critically, we include vertex corrections that have previously been omitted, and which are shown to exactly satisfy the sum rules. We show that these corrections lead to a double-peak structure in the susceptibility, as well as significant suppression of the susceptibility for low $q$. These effects have a straightforward physical interpretation: They represent the inclusion of charged bosonic, spin singlet degrees of freedom. See also Scherpelz et al., PRB 90 060506(R) (2014).
9:36AM A11.00009 Fully consistent theory of response functions in the cuprate pseudogap phase: Implementing the Ward Takahashi identity

CHIEN-TE WU, RUFUS BOYACK, PETER SCHERPELZ, KATHRYN LEVIN, James Franck Institute, University of Chicago — There is a multiplicity of pairing-based theories of the cuprate pseudogap associated with Fermi surface reconstruction or charge ordering, which have a simple mean-field-like self energy. These include the scenario of Yang, Rice and Zhang and the recent Amperian pairing scenario of Lee. We demonstrate here how to arrive at precise response functions for this class of theories which include vertex corrections, where necessary. Thus one can address two body physics experiments at the same level of accuracy that one addresses the one body physics of photoemission spectroscopy. We do so by exploiting the Ward Takahashi identity. As an illustration, we present the spin dynamical response functions of neutron scattering for three different scenarios, finding that a recently proposed pair Amperian pairing scheme is readily distinguishable from other related scenarios.

9:48AM A11.00010 Emergent loop current order from pair density wave superconductivity

MANOJ KASHYAP, Univ of Wisconsin, Milwaukee, DREW MELCHERT, Univ of Chicago, Chicago, DANIEL AGTERBERG, Univ of Wisconsin, Milwaukee — In addition to charge density wave (CDW) order, it is clear that the pseudogap phase in the cuprates breaks time reversal symmetry. Here we show that pair density wave (PDW) states give rise to a translational invariant non-superconducting order parameter that breaks time reversal and parity symmetries, but preserves their product. This secondary order parameter has a different origin, but shares the same symmetry properties as a magnetoelectric loop current order that has been proposed earlier in the context of the cuprates to explain the appearance of intra-cell magnetic order. We further show that, due to fluctuations, this secondary loop current order, which represents the breaking of discrete symmetries, can preempt PDW order, which breaks both continuous and discrete symmetries. In such a phase, the emergent loop current order coexists with spatial short range CDW and short range superconducting order. Finally, we propose a PDW phase that accounts for intra-cell magnetic order and the Kerr effect, has CDW order consistent with x-ray scattering and nuclear magnetic resonance observations, and quasi-particle properties consistent with resolved photoemission scattering.

10:00AM A11.00011 Vortices and charge order in high-Tc superconductors

MATTHIAS EINENKEL, Ruhr-Universität Bochum, National University of Science and Technology “MISIS,” Moscow, HENDRIK MEIER, Yale University, CATHERINE PÉPIN, CEASaclay, KONSTANTIN B. EFETOV, Ruhr-Universität Bochum, National University of Science and Technology “MISIS,” Moscow — We theoretically investigate the vortex state of the cuprate high-temperature superconductors in the presence of magnetic fields. Assuming the recently derived nonlinear σ-model for fluctuations in the pseudogap phase, we find that the vortex cores consist of two crossed regions of elliptic shape, in which a static charge order emerges. Charge density wave order manifests itself as satellites to the ordinary Bragg peaks directed along the axes of the reciprocal copper lattice. Quadrupole density wave (bond order) satellites, if seen, are predicted to be along the diagonals. The intensity of the satellites should grow linearly with the magnetic field, in agreement with the result of recent experiments.

10:12AM A11.00012 Orbital symmetry of charge density wave order in La1.875Ba0.125CuO4 and YBa2Cu3O6.67

DAVID HAWTHORN, ANDREW ACHKAR, University of Waterloo, FEIZHUO HE, RONNY SUTARTO, Canadian Light Source, CHRISTOPHER MCMAHON, University of Waterloo, MARTIN ZWIEBLER, Leibniz Institute for Solid State and Materials Research IFW Dresden, MARKUS HÜCKER, GENDA GU, Brookhaven National Laboratory, RUXING LIANG, DOUG BONN, WALTER HARDY, University of British Columbia, JOCHEN GETK, Leibniz Institute for Solid State and Materials Research IFW Dresden — Recent theories of charge density wave (CDW) order in high-temperature superconductors have predicted a primarily d CDW orbital symmetry. Here, we report on the orbital symmetry of CDW order in the canonical cuprate superconductors La1.875Ba0.125CuO4 (LBCO) and YBa2Cu3O6.67 (YBCO), using resonant soft x-ray scattering and a model mapped to the CDW orbital symmetry. From measurements sensitive to the O sublattice, we conclude that LBCO has predominantly s′ CDW orbital symmetry, in contrast to the d orbital symmetry recently reported in other cuprates. Additionally, we find that the C2 orbital symmetry of the Cu sublattice scattering is approximately preserved in LBCO and broken in YBCO. This work highlights orbital symmetry as an additional key property of CDW order that distinguishes the different cuprate families. We discuss how the CDW symmetry may be related to the “1/8-anomaly” and to static spin ordering.


WEI-LIN TU, Doctoral Candidate, Department of Physics, National Taiwan University, TING-KUO LEE, Director, Institute of Physics, Academia Sinica — One of the most puzzling facts about the cuprate high temperature superconductors is the observation of a variety of low-energy states in coexistence with the superconductivity and/or antiferromagnetism in the underdoped regime. These states could have a unidirectional charge density wave like structure or a bidirectional checkerboard structure. Some of them like the stripe state could also have an intertwined charge density and spin density waves together. Can all these different states caused by different mechanisms and competing with the superconducting state? Can these states also be consistent with the recently observed d-form factor density wave in cuprates? In this talk we will present reasons to show that these states are all originated from the same strong correlation inherent in the cuprates.

10:36AM A11.00014 Spin-Fluctuation-Driven Nematic Charge-Density-Wave in Cuprate Superconductors: Charge-Orbital-Spin Multimode Fluctuations Caused by Vertex Corrections

YOSUKE YAMAKAWA, MASASHI TSUCHIIZU, HIROSHI KONTANI, Department of Physics, Nagoya University — We explain the recently discovered nematic charge-density-wave (CDW) state in cuprate superconductors on the basis of the three-orbital d-Γ Hubbard model, by including the vertex correction (VC) [1]. Due to the strong charge-spin interference given by the VC, the CDW instability at $q = (\Delta_{FS} \cdot 0, 0, \Delta_{FS})$ is strongly promoted near the magnetic critical point. Here, $\Delta_{FS}$ is the wavenumber connected by the neighboring hot spots. The obtained spin-fluctuation-driven CDW is described as the “intra-unit-cell orbital order” accompanied by the charge transfer between the neighboring atomic orbitals. The obtained nematic-type charge pattern is similar to the STM results. The CDW in cuprates has a close relation to the nematic orbital order in Fe-based superconductors. [1] Y. Yamakawa and H. Kontani, arXiv:1406.7520.
10:48AM A11.00015 Charge Order Instability in Doped Resonating Valence Bond State and Magnetic Orbits from Reconstructed Fermi Surface in Underdoped Cuprates1, LONG ZHANG, Tsinghua Univ, JIA-WEI MEI, Perimeter Institute for Theoretical Physics — Recent experiments reveal incommensurate charge density wave (CDW) and quantum oscillations (QO) in the pseudogap phase of underdoped cuprates. In this work, we take a phenomenological synthesis of the resonating valence bond (RVB) state and the CDW order. Starting from the Yang-Rice-Zhang (YRZ) ansatz for the Green’s function of the RVB state, we show that the CDW instability at wavevectors connecting the tips of the Fermi arcs can induce Fermi surface reconstruction. We find three primary magnetic orbits in the QO spectrum, the CDW-induced electron-like \( \alpha \) and hole-like \( \beta \) orbits and the \( \gamma \) orbit enclosing the initial nodal YRZ hole pockets due to magnetic breakdown. Their combinations naturally explain the multi-component QO pattern observed in experiments. The \( \gamma \) orbit encloses an area satisfying the generalized Luttinger theorem. The cyclotron mass of the \( \gamma \) orbit increases monotonically with doping in agreement with the optical Hall angle measurements, while that of the \( \alpha \) orbit is enhanced as the CDW order vanishes on approaching two critical dopings. However, we find that the enhancement of \( m_{\gamma}^* \) is overestimated in QO experiments due to the ignorance of the impact of the CDW order suppression with increasing temperature.

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Monday, March 2, 2015 8:00AM - 11:00AM — Session A12 DMP: Focus Session: Iridates and Ruthenates 007C - Gang Cao, University of Kentucky

8:00AM A12.00001 X-ray scattering and spectroscopy studies of strongly correlated iridates, YOUNG-JUNE KIM, University of Toronto — Due to strong spin-orbit coupling and electronic correlation, iridates host a number of interesting quantum phases of matter. A broad overview of recent x-ray scattering and spectroscopy studies of iridates on honeycomb, pyrochlore, and square lattice will be given. In particular, we will focus on square lattice iridates, which exhibit physical and magnetic properties remarkably similar to those of cuprates, such as quasi-two-dimensional magnetism and very large magnetic exchange. Various studies found unusual metallic phases in \( \text{Sr}_2\text{IrO}_4 \) doped with charge carriers [1-3]. We examine the case of partially replacing \( \text{Ir}^{4+} \) ions with \( \text{Rh}^{3+} \) ions, which corresponds to a hole-doping. Our magnetic x-ray scattering and x-ray absorption spectroscopy investigation reveal that the suppression of magnetic order and the rise of metallicity is described by a percolation picture [3]. We also obtained magnetic excitation spectra using resonant inelastic x-ray scattering (RIXS), which will be compared with those of cuprates and possible routes to high temperature superconductivity will be discussed [4].

1-3. We examine the case of partially replacing \( \text{Ir}^{4+} \) ions with \( \text{Rh}^{3+} \) ions, which corresponds to a hole-doping. Our magnetic x-ray scattering and x-ray absorption spectroscopy investigation reveal that the suppression of magnetic order and the rise of metallicity is described by a percolation picture [3]. We also obtained magnetic excitation spectra using resonant inelastic x-ray scattering (RIXS), which will be compared with those of cuprates and possible routes to high temperature superconductivity will be discussed [4].


8:36AM A12.00002 High-energy electronic excitations in \( \text{Sr}_2\text{IrO}_4 \) observed by Raman scattering1, JHIH-ANG YANG, YI-PING HUANG, MICHAEL HERMELE, Univ of Colorado - Boulder, TONGFEI QI, GANG CAO, University of Kentucky, DMITRY REZNIK, Univ of Colorado - Boulder — The interplay between spin-orbit interaction, on-site coulomb correlation, crystal field splitting, and inter-site hopping leads to a novel insulating behavior in \( \text{Sr}_2\text{IrO}_4 \) as the realization of the \( J_{\text{eff}} = 1/2 \) state. We report results of a large-shift Raman scattering investigation of electronic excitations in \( \text{Sr}_2\text{IrO}_4 \). We found two high-energy excitations at 690 meV and 680 meV with \( A_{1y} \) and \( B_{1y} \) symmetry respectively. The two peaks have different temperature and Rh-doping dependences. Symmetry analysis of the dd transitions that contribute to Raman signals will also be presented. The observed peaks are consistent with the scenario of excitons associated with inter-site dd transitions without pseudospin-flip.

1NSF, DOE, and BES

8:48AM A12.00003 Evolution of Magnetism in Single-Crystal \( \text{Ca}_2\text{Ru}_1-x\text{Ir}_x\text{O}_4 \) \( (0 \leq x \leq 0.65) \), S.J. YUAN, J. TERZIC, J.C. WANG, L. LI, T.F. QI, W.H. SONG, S. ASWARTHAM, G. CAO, Center for Advanced Materials, Department of Physics and Astronomy, University of Kentucky, Lexington, Kentucky 40506, USA — We report structural, magnetic, transport and thermal properties of single-crystal \( \text{Ca}_2\text{Ru}_1-x\text{Ir}_x\text{O}_4 \) \( (0 \leq x \leq 0.65) \). \( \text{Ca}_2\text{Ru}_1-x\text{Ir}_x\text{O}_4 \) is a structurally-driven Mott insulator with a metal-insulator transition at \( T_{\text{MI}} = 357 \) K, followed by a well-separated antiferromagnetic order at \( T_N = 110 \) K. Substituting Ru with Ir enhances the spin-orbit coupling (SOC) and causes further orthorhombic distortions. As a result, a pronounced weak ferromagnetic behavior occurs, which enhances dramatically with increasing Ir concentration. The magnetic ordering temperature \( T_N \) increases from 110 K at \( x = 0 \) to 215 K at \( x = 0.65 \), along with enhanced magnetic anisotropy due to SOC. In addition, with increasing \( x \), the metal-insulator transition \( T_{\text{MI}} \) increases initially and vanishes eventually.

1This work was supported by the National Science Foundation (NSF) under Grants No. DMR-0856234, and No. DMR-1265162.

9:00AM A12.00004 Ground State Tuning by Spin-Orbit Coupling and Lattice Degrees of Freedom in Single-Crystal \( \text{Ba}_x\text{Ru}_{1-x}\text{O}_3 \) \( (0 \leq x \leq 1) \), K. BUTROUNA, S.J. YUAN, T.F. QI, J. TERZIC, S. ASWARTHAM, L.E. DELONG, G. CAO, Center for Advanced Materials, Department of Physics and Astronomy, University of Kentucky, Lexington, Kentucky 40506, USA — \( \text{Ba}_x\text{Ru}_{1-x}\text{O}_3 \) is a magnetic insulator driven by spin-orbit coupling (SOC) whereas \( \text{Ba}_2\text{RuO}_3 \) is a paramagnetic metal. The contrasting ground states provide a unique opportunity to study the role of the SOC and the lattice degrees freedom. Our investigation reveals that substitution of Ru\(^{4+}\) \( (4d^5) \) ions for Ir\(^{5+}\) \( (5d^2) \) ions in \( \text{Ba}_2\text{RuO}_3 \) reduces the magnitude of the SOC and the structural distortion. There are two major effects of Ru additions: (1) Light Ru doping \( (0 \leq x \leq 0.15) \) prompts a simultaneous, precipitous drop in both the magnetic ordering temperature \( T_C \) and the electrical resistivity, which exhibits a crossover behavior from a metallic to an insulating state near \( T_C \). (2) Heavier Ru doping \( (0.41 \leq x \leq 0.9) \) induces a robust metallic state with a strong spin frustration.

1This work was supported by the National Science Foundation (NSF) under Grants No. DMR-1265162; L.E.D. is supported by U.S. Department of Energy Grant No. DE-FG02-97ER45653.
9:12 AM A12.00005 Surface Bilateral Symmetry on Orthorhombic Double-layer Sr$_3$(Ru$_{1-x}$Mn$_x$)$_2$O$_7$\(^1\) — CHEN CHEN, JIANDI ZHANG, RONGYING JIN, WARD PLUMMER, Louisiana State University — The double-layered ruthenate Sr$_3$Ru$_2$O$_7$ exhibits very interesting properties especially on the surface because of the broken symmetry (G. Li et al., Scientific Reports 3 2882 (2013)). Compared to the bulk, the surface not only enhances the octahedral rotation but also introduces tilt (not in the bulk). Partial substitution of Mn for Ru reduces the tilt distortion while keeps the rotation angle constant up to ~20% doping. Tilt distortion as expected removes one of the glidelines (associated with rotation) and breaks the mirror symmetry along this broken glideline in the LEED pattern, resulting in a “bilayer symmetry” as a prefect human has. It is surprising that the surface has lost much of the symmetry present in the bulk. When the tilt is removed by increased Mn doping (z) in Sr$_3$(Ru$_{1-z}$Mn$_z$)$_2$O$_7$ the LEED pattern returns to the expected one with two glide planes. In comparison, the LEED pattern of single layer Ca$_1.9$Sr$_0.1$Ru$_2$O$_4$ which has tilt still preserves the mirror symmetry. We assign this difference to the different structures in the first and second octahedral layers.

\(^1\)Supported by NSF DMR-1002622

9:24 AM A12.00006 STM study of lattice distortion effect on Sr$_3$(Ru$_{1-x}$Mn$_x$)$_2$O$_7$ surfaces\(^1\) — JISUN KIM, ZHENGYU DIAO, JIANDI ZHANG, RONGYING JIN, E.W. PLUMMER, Department of Physics and Astronomy, Louisiana State University, Baton Rouge — The Ruddlesden-Popper ruthenates Sr$_{n+1}$Ru$_n$O$_{3n+1}$ (n = 1 to ∞) exhibit a wide range of distinct electronic and magnetic properties due to strong coupling between charge, spin, lattice, and orbital degrees of freedom. For example, substituting Ru with Mn in Sr$_3$Ru$_2$O$_7$ (Sr327) leads to a metal-insulator transition (MIT) at $T_{MIT}$, as well as a magnetic phase transition from paramagnetic at high temperatures to long-range AFM ordering at $T_M$. In the parent compound (x=0), RuO$_2$ octahedra are rotated by ~8° in the bulk and the distortion is enhanced at the surface (12°) with the addition of tilt (~5°). With Mn doping, the rotation of octahedra at the surface does not change but tilt is eliminated. Our recent study of Mn doped Sr327 shows that the surface symmetry and Mn-induced local disturbance observed by scanning tunneling microscope (STM) changes with increasing Mn doping (6 to 16 %), suggesting that the surface electronic properties change with the concentration of Mn doping, driven by the structural change. By studying lower Mn doped Sr327 using STM/STS we delineate the relationship of size of the disturbance induced by Mn to surface metallicity. The result is also compared to 1 % Ti doped Sr327 case.

\(^1\)Supported by NSF

9:36 AM A12.00007 Novel magnetic states in insulating d$^4$ oxides with strong spin-orbit coupling\(^2\) — CHRISTOPHER SVOBODA, NANDINI TRIVEDI, The Ohio State University — The comparable energy scales in 4d and 5d transition metal oxides, arising from Coulomb correlations, spin-orbit coupling and bandwidth, can lead to new phases and phenomena. With this motivation we examine an isovalent substitution of Ti by Zr in the double perovskite Cu$_2$Ir$_2$O$_6$ in order to explore the nature of the ground state, by crystal field splitting. Upon including spin-orbit coupling, the completely filled $d^4$ manifold is nonmagnetic but with a nonzero magnetic susceptibility. Upon introducing hopping between two $d^4$ atoms, we find novel entangled ferromagnetism generated by the superexchange interaction in a significant part of the phase diagram [1]. We further present results for the temperature dependent susceptibility calculated using exact diagonalization to illustrate this novel magnetic behavior and the role Hund’s coupling plays in producing these phases. We make predictions for resonant X-ray scattering and magnetic measurements in pyrochlore osmates.


\(^2\)We acknowledge the support of the CEM, and NSF MRSEC, under grant DMR-1420451.

9:48 AM A12.00008 Electronic, magnetic and optical properties of Sr$_{n+1}$Ir$_n$O$_{3n+1}$ (n = 1, 2, and ∞)\(^1\) — PEITAO LIU, Faculty of Physics, University of Vienna, Vienna, Austria, SERGII KUMELEVSKYI, Department of Applied Physics, Vienna University of Technology, Vienna, Austria, BONGJAE KIM, Faculty of Physics, University of Vienna, Vienna, Austria, XING-QIU CHEN, DIANZHONG LI, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China, CESARE FRANCHINI, Faculty of Physics, University of Vienna, Vienna, Austria — We have studied the crossover between metallic/insulating and non-magnetic/magnetic phases in Ruddlesden-Popper series of iridates Sr$_{n+1}$Ir$_n$O$_{3n+1}$ (n = 1, 2, and ∞) by means of density functional theory including an on-site Hubbard U correction and many-body first principles methods. By systematically investigating the evolution of the orbital and spin properties as a function of U, spin-orbit coupling (SOC) strength, and n we have constructed detailed phase diagrams of the metal-insulator transition (MIT) which provide clear evidence for the crucial role played by SOC and U in establishing a relativistic Mott-Hubbard insulating state in the n = 1 and 2 compounds. Optical spectra computed within a model Bethe-Salpeter scheme show the typical double peak structure observed in experiments and capture well the progressive shrinkage of the band-gap and the widening of the bandwidth going from n = 1 to n = ∞. Finally, we clarify the origin of the canted magnetic ground state of Sr$_2$IrO$_3$ as due to the the synergistic effect of structural distortions (rotation and tetragonal distortion of IrO$_6$ octahedral) and to the competition between exchange and Dzyaloshinskii-Moriya interactions.

\(^1\)This work is supported by the China Scholarship Council and Austria Science fund.

10:00 AM A12.00009 Coherent quasiparticles with a small Fermi Surface in lightly doped Sr$_3$Ir$_2$O$_7$. ALBERTO DE LA TORRE, SIOBHAN MCEWOWN WALKER, ANNA TAMAI, University of Geneva, EMILY HUNTER, University of Edinburgh, ALASKA SUBEDI, Ecole Polytechnique, TIMUR KIM, MORITZ HOESCH, Diamond Light Source, ROBIN PERRY, University College London, ANTOINE GAGNÉS, College de France, FELIX BAUMBERGER, University of Geneva — We characterize the electron doping evolution of Sr$_{2n+1}$Ir$_n$O$_{3n+1}$ by means of angle-resolved photoemission. Concomitant with the metal insulator transition around $x \approx 0.05$ we find the emergence of coherent quasiparticle states forming a closed small Fermi surface of volume $3\pi/2$, where $x$ is the independently measured La concentration. The quasiparticle weight $Z$ remains large along the entire Fermi surface, consistent with the moderate renormalization of the low-energy dispersion and no pseudogap is observed. This indicates a conventional, weakly correlated Fermi liquid state with a momentum independent residue $Z \approx 0.5$ in lightly doped Sr$_3$Ir$_2$O$_7$, in stark contrast with underdoped cuprates.

10:12 AM A12.00010 Experimental bandstructure of the 5d transition metal oxide IrO$_2$. JASON KAWASAKI, YUEFENG NIE, Cornell University, MASAKI UCHIDA, University of Tokyo, DARRELL SCHLOM, KYLE SHEN, Cornell University — In the 5d iridium oxides the close energy scales of spin-orbit coupling and electron-electron correlations lead to emergent quantum phenomena. Much research has focused on the ternary iridium oxides, e.g. the Ruddlesden-Poppers A$_{n+1}$B$_n$O$_{3n+1}$, which exhibit behavior from metal to antiferromagnetic insulator ground states, share common features with the cuprates, and may host a number of topological phases. The binary rutile IrO$_2$ is another important 5d oxide, which has technological importance for spintronics due to its large spin Hall effect and also applications in catalysis. IrO$_2$ is expected to share similar physics as its perovskite-based cousins; however, due to bond-length distortions of the IrO$_6$ octahedra in the rutile structure, the extent of similarities remains an open question. Here we use angle-resolved photoemission spectroscopy to perform momentum-resolved measurements of the electronic structure of IrO$_2$. IrO$_2$ thin films were grown by molecular beam epitaxy on TiO$_2$ (110) substrates using an Ir e-beam source and distilled ozone. Films were subsequently transferred through ultrahigh vacuum to a connected ARPES system. Combined with first-principles calculations we explore the interplay of spin-orbit coupling and correlations in IrO$_2$. 

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This work is supported by the China Scholarship Council and Austria Science fund.
10:24AM A12.00011 Magnetic fluctuations induced insulator-to-metal transition in Ca(Ir,Ru)_{1-x}O_3. DEEPAK SINGH, JAGATH GUNASEKERA, ASHUTOSH DAHAL, University of Missouri, Columbia, LELAND HARRIGER, National Institute of Standards and Technology, Gaithersburg, THOMAS HEITMANN, University of Missouri Research Reactor, Columbia — The Fermi liquid theory dictates the metal-insulator transition in a continuous fashion via the divergence of the quasiparticle mass m*. However, the metallic phase near the Mott insulator in the metal-insulator phase diagram based on the Hubbard model is dominated by the fluctuations of spin, charge and orbital correlations; often termed as the anomalous metallic phase. In this presentation, experimental results manifesting the magnetic fluctuations induced insulator-to-metal transition in Ca(Ir,Ru)_{1-x}O_3 will be discussed in the framework of the Hubbard model. For x = 1, the compound CaIrO_3 is a Mott insulator with antiferromagnetic order below T ~ 110 K. A gradual substitution of Ir by Ru results in the onset of anomalous metallic behavior as a function of the tuning parameter x. At x = 0, the compound CaRuO_3 is a non-Fermi liquid metal with no apparent magnetic order. While the orthorhombic structural integrity is maintained throughout the group, strong magnetic fluctuations is detected below x = 0.8. The role of magnetic fluctuations in the metallic transition is further confirmed by first principle theoretical calculation.

10:36AM A12.00012 Magneto-optical transmission of Bi_2Se_3 at the fundamental absorption edge. GERARD MARTINEZ, MILAN ORLITA, BENJAMIN PIOT, MAREK POTEMSKI, LNCMI, CNRS, France, YEW SAN HOR, Missouri University of Science and Technology, MO, USA, G. STRZELECKA, A. HRUBAN, Institute of Electronic Materials, Warsaw, Poland — Magneto-optical transmission spectroscopy of a series of n-type Bi_2Se_3 samples have been performed, around the fundamental absorption edge, up to 32 T. The absorption edge splits in two components, offset by about 0.2 eV. The first component is associated with the spin splitting of the 3d states of Se_2p. The second component, corresponding to the spin splitting of the 5d states of Bi_5s. The splitting increases linearly with the magnetic field up to a critical value B_c depending on the carrier density, beyond which it remains constant. This corresponds to a complete spin polarization of the compound. The consequences of this specific property put some constrains on the parameters of the Hamiltonian describing the system.

10:48AM A12.00013 Quasi-local critical nature of cooperative paramagnetic fluctuations in CaRuO_3 metal. JAGATH GUNASEKERA, Univ of Missouri - Columbia, LELAND HARRIGER, NIST, THOMAS HEITMANN, MURR, DEEPAK SINGH, Univ of Missouri - Columbia — Ruthenate perovskites of the form ARuO_3, where A is an alkaline earth metal, hold strong promises in developing new paradigm of the quantum magnetism. CaRuO_3 is of special interest among this group. The unusual combination of the absence of magnetic order and the anomalous non-Fermi liquid properties makes it an archetypal perovskite for the exploration of the quantum magnetism. Recently, we performed detailed electric, magnetic and neutron scattering measurements on high quality polycrystalline sample of CaRuO_3. The experimental results suggest that the underlying magnetism is depicted by the quantum mechanical fluctuations of Ru^{4+} spins, confined to field-independent random domains that form a cooperative paramagnetic state at low temperature. The dynamic structure factor, which increases significantly below T ~ 22 K, manifests a linear (E^2T) scaling, implying the Curie-Weiss type fluctuations with temperature as the most relevant parameter. Moreover, the linear dynamic scaling in conjunction with the divergence of the spin fluctuations mean relaxation time as T ~ 0 K suggest the existence of a quasi-local critical behavior in the system.

Monday, March 2, 2015 8:00AM - 11:00AM — Session A13 DMP: Focus Session: Titania Interfaces and Heterostructures 007D - Roman Engel-Herbert, Pennsylvania State University

8:00AM A13.00001 Thermal and photoconductivity at the La_{1-x}Sr_{x}CrO_{3}/SrTiO_{3}(001) interface. SCOTT CHAMBERS, Pacific Northwest National Laboratory — We have investigated the electronic and photophysical properties of interfaces between La_{1-x}Sr_{x}CrO_{3} and SrTiO_{3}(001) as prepared by molecular beam epitaxy. LaCrO_3 is a III-II antiferromagnetic insulator whereas SrCrO_3 is a II-IV metallic oxide. Substituting Sr^{2+} for La^{3+} in LaCrO_3 effectively dopes holes into the top of valence band, reducing the band gap and the resistivity, and generating a p-type oxide semiconductor. In contrast, SrTiO_3 is a wide-gap II-IV semiconductor that is readily made n-type by La doping. Therefore, the La_{1-x}Sr_{x}CrO_{3}/SrTiO_{3}(001) system has much potential for interesting interface physics with regard to studying intrinsic conductivity via electronic reconstruction and electron-hole pair separation under light irradiation. However, there are inherent physical and chemical complexities at these interfaces and within the bulk of the La_{1-x}Sr_{x}CrO_{3} films which can have profound effects on the associated functional properties. In this talk, we present some of our most recent results from this ongoing investigation.

In collaboration with Kelvin Zhang, Du Yingge, Sushko Peter, Bowden Mark, Shuttanandan V, Pacific Northwest National Laboratory; and Shawn Sallis, Louis Piper, Binghamton University.

8:36AM A13.00002 ABSTRACT WITHDRAWN —

8:48AM A13.00004 Extreme high-density electron gas using band engineered complex oxide interfaces. PENG ANDREW XU, Univ of Minn - Minneapolis, TIMOTHY C. DROUBAY, Pacific Northwest National Laboratory, JONG SEOK JEONG, Univ of Minn - Minneapolis, SCOTT A. CHAMBERS, Pacific Northwest National Laboratory, ANDRE K. MKHOYAN, BHARAT JALAN, Univ of Minn - Minneapolis — The study of interfaces between polar and non-polar complex oxides has seen unprecedented growth due to their unique ability to display interface-stabilized ground states including high-density two-dimensional electron gas (equivalent to 0.5 electron/u.c./interface). In this talk, we will present thickness dependent structural and electronic transport study of the MBE-grown NdTiO_3/SrTiO_3 heterostructures. High-resolution x-ray diffraction, atomic force microscopy, reflection high-energy electron diffraction, scanning transmission electron microscopy and different spectroscopy techniques reveal nearly stoichiometric composition and abrupt interfaces. We will review the long-standing question on the origin of carriers at oxide semiconductor interface and present an approach to combine the high carrier density of 2DEG oxides with a higher mobility medium in order to realize the combined benefits of higher mobility and carrier density.

1This work is supported partially by NSF through UMN MRSEC and the office of vice president for research, UMN.

9:00AM A13.00004 Band offset engineering of 2DEG oxide systems on Si. ERIC JIN, LIOR KORNBLUM, DIVINE KUMAH, KE ZOU, Yale Univ, CHRISTINE BROADBRIDGE, Southern Connecticut State Univ, JOSEPH NGAI, Univ of Texas at Arlington, CHARLES AHN, FRED WALKER, Yale Univ — The discovery of 2-dimensional electron gases (2DEGs) at perovskite oxide interfaces has sparked much interest in recent years due to their large carrier densities when compared with semiconductor heterostructures. For device applications, these oxide systems are plagued by low room temperature electrical densities. We present an approach to combine the high carrier density of 2DEGs with a higher mobility medium in order to realize the combined benefits of higher mobility and carrier density. We grow epitaxial films of the interfacial oxide system LaTiO_3/SrTiO_3 (LTO/STO) on silicon by molecular beam epitaxy. Magnetotransport measurements show the sheet carrier densities of the heterostructures scale with the number of LTO/STO interfaces, consistent with the presence of a 2DEG at each interface. Sheet carrier densities of 8.9 x 10^{14} cm^{-2} per interface are measured. Band offsets between the STO and Si are obtained, showing that the conduction band edge of the STO is close in energy to that of silicon, but in a direction that hinders carrier transfer to the silicon substrate. Through modification of the STO/Si interface, we suggest an approach to raise the band offset in order to move the 2DEG from the oxide into the silicon.
9:12AM A13.00005 High-carrier-density phase in LaTiO$_3$/SrTiO$_3$ superlattices$^1$. SE YOUNG PARK, KARIN RABE, Rutgers University, ANDREW MILLIS, Columbia University — We investigate superlattices composed of alternating layers of Mott insulating LaTiO$_3$ and band insulating SrTiO$_3$ from first principles, using the density functional theory plus U (DFT+U) method. For values of U above a critical threshold, we find that melting of the Mott-insulating phase can extend from the interface into the LaTiO$_3$ layer, resulting in a sheet carrier density exceeding the density of 0.5 electrons per in-plane unit cell found in previous studies. The critical U for the melting transition is larger than the critical Coulomb correlation required for the insulating LaTiO$_3$, suggesting the existence of a high sheet carrier density phase in LaTiO$_3$/SrTiO$_3$ superlattices. The effects of in-plane strain and varying layer thickness on the melting transition are discussed. For insulating superlattices, we study the strain and thickness dependence of the polarization and its relation to near-interface local atomic distortions.

1Support: DOE ER 041669, ONR N00014-11-0666

9:24AM A13.00006 Phase diagram and high density two-dimensional electron gas at the LaAlO$_3$/La$_{0.5}$Sr$_{0.5}$TiO$_3$/SrTiO$_3$ heterostructures. HAILIAO MA, NUSNNI-Nanocore and Physics Department, NUS, ZHEN HUANG, SHENGWEI ZENG, ANIL ANNADI, NUSNNI-Nanocore, NUS. THIRUMALAI VENKY VENKATESAN, ARIANDO ARIANDO, NUSNNI-Nanocore and Physics Department, NUS, ARIANDO RESEARCH GROUP TEAM$^1$ — We report a two dimensional electron gas with a high carrier density at the LaAlO$_3$/La$_{0.5}$Sr$_{0.5}$TiO$_3$/SrTiO$_3$ heterostructures, reaching a value of about five times higher than that observed at the LaAlO$_3$/SrTiO$_3$ interface. The La$_{0.5}$Sr$_{0.5}$TiO$_3$ polar layer is introduced to preserve the degeneracy of the Ti $t_{2g}$ orbitals and minimize the disorder at the LaAlO$_3$/La$_{0.5}$Sr$_{0.5}$TiO$_3$/SrTiO$_3$ interface. Various thickness combinations of La$_{0.5}$Sr$_{0.5}$TiO$_3$ and LaAlO$_3$ layers are used for tuning the total internal potential of the polar layer responsible for the charge transfer. Experimental data showed that the carrier density increases by raising the total internal potential, and this is in a good agreement with a simple electrostatic model. A complete metal-insulator phase diagram is obtained, which shows that at least 3.15 eV polar potential is needed to form the metallic interface at the SrTiO$_3$, providing an estimate for the critical thickness needed for the metallic phase. Nonlinear Hall effect was observed below 60 K which can be understood by multiple filling of the degenerated orbitals responsible for multiple band electronic conductions.

9:36AM A13.00007 Induced Itinerant Antiferromagnetism in SrTiO$_3$. BRANDON ISAAC, EVGENY MIKHEEV, CHRIS FREEZE, SUSANNE STEMMER, University of California, Santa Barbara — Interfaces between RTiO$_3$ (R = Gd or Sm) and SrTiO$_3$ grown by molecular beam epitaxy induce a high-density two-dimensional electron gas (2DEG). Such 2DEGs show evidence of strong electron correlation effects, including non-Fermi liquid behavior, and a non-trivial magnetoresistance. Here we present magneto-transport measurements of SmTiO$_3$/SrTiO$_3$/SmTiO$_3$ quantum well structures to investigate induced, itinerant, antiferromagnetic ordering in the SrTiO$_3$ through proximity to the SmTiO$_3$. At low temperatures, the Hall effect, the longitudinal resistance, and the magnetoresistance all show evidence of itinerant antiferromagnetism. For example, the longitudinal resistance shows deviations from the logarithmic correction of weak localization, and the Hall effect indicates opening of a gap and loss of carriers. The results will be discussed in terms of a possible spin-density wave formation and gap opening on the Fermi surface.

9:48AM A13.00008 Pseudogaps in SrTiO$_3$. Quantum Wells. PATRICK MARSHALL, SANTOSH RAGHAVAN, EVGENY MIKHEEV, SUSANNE STEMMER, Univ of California - Santa Barbara — A departure from Fermi liquid behavior appears in molecular beam epitaxy grown SrTiO$_3$ quantum wells embedded in the antiferromagnetic insulator SmTiO$_3$, suggesting proximity to a quantum critical point. We will report on the observation of pseudogap behavior in SmTiO$_3$/SrTiO$_3$/SmTiO$_3$ quantum wells via tunneling spectroscopy measurements. Tunnel junction devices with SrZrO$_3$ barriers grown in-situ were fabricated from quantum wells of varying thickness. The tunneling conductance spectra of these devices revealed the formation of a pseudogap in the density of states upon cooling, indicating the onset of non-Fermi liquid behavior. The pseudogap state was most pronounced in thin quantum wells, persisting up to nearly 200 K in the well containing only 2 SrO layers. The pseudogap was absent in the thickest wells, which showed only a small suppression of the density of states with a logarithmic dependence on bias resulting from disorder. The results are compared to tunneling spectra of GdTiO$_3$/SrTiO$_3$/GdTiO$_3$ quantum wells, providing insight into the role of structural distortion and octahedral tilts on the electronic structure and quantum critical behavior in oxide heterostructures.

10:00AM A13.00009 Tunable Orbital-Selective Magnetic Interaction in Tricolor Oxide Interfaces. YANWEI CAO, MICHAEL KAREEV, XIAORAN LIU, DEBRAJ CHOUHDURY, SRIMANTA MIDDEY, DEREK MEYERS, JAK CHAKHALIAN, University of Arkansas — Several recent theoretical scenarios of orbital-selective magnetic interactions were proposed to understand the emergence of the unexpected interfacial magnetism in the archetypal SrTiO$_3$-based two-dimensional electron gas systems, the origin of which is still intriguing and not an entirely understood phenomenon in oxide interface physics. Experimentally, however, there thus far lacks a material system to directly demonstrate the magnetic interaction with orbital-selection (dxy vs. dxz/dyz) and eventually manipulate this magnetic interaction. To address this, here we induced 2DEG and localized magnetism in the same SrTiO$_3$ layer by devising the heterostructure LaTiO$_3$/SrTiO$_3$/YTiO$_3$. Combined electrical transport and atomic-resolved scanning transmission electron microscope with electron energy loss spectroscopy revealed that the magnetic localized electrons are formed by the spin transfer from the YTiO$_3$ layer into 2DEG formed at the LaTiO$_3$/SrTiO$_3$ interface, with the orbital occupancy and strength of the magnetic interaction controlled by the SrTiO$_3$ layer thickness. Our work provides an ideal platform to explore the orbital physics driven by the interfacial magnetism with prospects for exciting spintronic applications.

10:12AM A13.00010 High electron density 2DEGs at 111 SrTiO$_3$/SmTiO$_3$ interfaces. SANTOSH RAGHAVAN, SUSANNE STEMMER, University of California Santa Barbara, STEMMER RESEARCH GROUP TEAM — (001) SrTiO$_3$ quantum wells formed in structures such as RTiO$_3$/SrTiO$_3$/RTiO$_3$ (R = Gd or Sm) exhibit two dimensional electron gases (2DEGs) that exhibit ferromagnetism and non-Fermi-liquid behavior. 2DEGs are also expected for (111) quantum wells, which furthermore form a honeycomb lattice that is susceptible to geometric frustration and nontrivial band structures. In this work, we present the growth of high quality SrTiO$_3$ and SmTiO$_3$ layers on (111) LSAT substrates using a hybrid molecular beam epitaxy technique. Structural and electrical characterization show atomically sharp (111) interfaces between SrTiO$_3$ and SmTiO$_3$, and the presence of a high charge carrier density of $\sim 3 \times 10^{13}$ cm$^{-2}$. We will discuss results of magneto-transport studies in highly confined quantum wells that are only a few atomic planes thick and compare them with results from (001) interfaces.

10:24AM A13.00011 ABSTRACT WITHDRAWN —
10:36AM A13.00012 Thickness dependent metal-insulator transition in GdTiO$_3$/SrTiO$_3$ superlattices$^1$, ANDERSON JANOTTI, LARS BJAALIE, BURAK HIMMETOGLU, CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — SrTiO$_3$ (STO) is at the core of recent discoveries of two-dimensional electron gas (2DEG) formation at complex oxide interfaces, with the 2DEG residing on the STO side. Experimental results for ultrathin STO layers inserted in GdTiO$_3$ reveal a transition from metallic to insulating behavior, and suggest a strong interplay between electron-electron interaction and lattice distortions. Using first-principles calculations we investigate the evolution of the electronic structure of STO/STO superlattices as a function of the thickness of the STO layer. We show that the metal-to-insulator transition is a bulk property of STO that emerges at extreme doping levels [1]. For thick STO layers, we find a two-dimensional electron gas with a density of 1/2 electron per unit-cell area per interface within the STO. However, once the STO layer thickness is reduced below three layers, we find that the electrons localize on every second interface Ti atom, giving a charge-ordered Mott-insulating phase. This onset of localization is analyzed in terms of the electron density in the STO layer and octahedral distortions at the interface. The Mott-insulator phase is shown to occur both in STO/LaAlO$_3$ and STO/GdTiO$_3$ heterostructures with ultrathin STO layers.


$^1$This work was supported by NSF, ARO and ONR.

10:48AM A13.00013 Mixed-valence magnetism in TiO$_2$/Ti$_2$O$_3$ superlattices, W.C. HSIEH, National Sun-Yat Sen University, Taiwan, P.V. WADEKAR, University of Liverpool, UK, H.C. HUANG, C.F. CHANG, National Sun-Yat Sen University, Taiwan, M.S. WONG, National Dong Hua University, Taiwan, H.W. SEO, University of Arkansas, USA, F.C. CHUANG, Q.Y. CHEN, National Sun-Yat Sen University, Taiwan — Epitaxial TiO$_2$ and Ti$_2$O$_3$ superlattices, ~ 1-nm thick per layer by sputtering at 570°C using pure argon on sapphire substrates. From HR-TEM, the periodically alternating layers are well-defined. XPS analyses based on the binding energy of Ti 2p$_{3/2}$ peaks suggest the co-existence of Ti$^{3+}$ and Ti$^{4+}$, thus verifying the mixed-valence nature. The M(H) curves measured at room temperature using SQUID showed hysteretic loops typical of ferromagnetism. Electrical transport measurements were done at zero field demonstrate transition of charge ordering at low temperatures, reminiscent of what was found in Ti-rich Ti$_{1+x}$O$_2$ single-layer thin films, made by Ti ion implantation into TiO$_2$ crystals, in which randomly distributed TiO$_2$, Ti$_2$O$_3$ and TiO were found to coexist. Preliminary First-principle (ab initio) calculations to understand the roles of oxygen vacancies in various TiO$_2$ super-cells could indeed lead to spontaneous magnetizations. We thus argue that mixed-valence titanium ions are responsible for the magnetism.

Monday, March 2, 2015 8:00AM - 11:00AM – 
Session A14 DMP: Focus Session: Quantum Phase Transitions And Quantum Criticality 008A
- Vivien Zapf, Los Alamos National Laboratory

8:00AM A14.00001 Transport signatures of Majorana ferromagnetism realized by dissipative resonant tunneling, HUAIXIU ZHENG, Departments of Physics and Applied Physics, Yale University, New Haven, Connecticut 06511, USA, SERGE FLORENS, Institut Neel, CNRS and UJF, 25 avenue des Martyrs, BP 166, 38042 Grenoble, France, HAROLD BARANGER, Department of Physics, Duke University, P. O. Box 93055, Durham, North Carolina 27708, USA — We consider theoretically the transport properties of a spinless resonant electronic level coupled to strongly dissipative leads, in the regime of circuit impedance near the resistance quantum [1]. Using the Luttinger liquid analogy, one obtains an effective Hamiltonian expressed in terms of interacting Majorana fermions, in which all environmental degrees of freedom (leads and electromagnetic modes) are encapsulated in a single fermionic bath. A perturbative treatment of the Majorana interaction term yields the appearance of a marginal, linear dependence of the conductance on temperature when the system is tuned to its quantum critical point, in agreement with recent experimental observations [2].


8:12AM A14.00002 Metallic transport near a quantum critical point in organic superconductors from a renormalized Boltzmann theory, MARYAM SHAHBAZI, CLAUDE BOURBONNAIS, Regroupement Québécois des Matériaux de pointe, Département de Physique, Université de Sherbrooke, Sherbrooke, QC, Canada J1K 2R1 — The electrical and thermal transport properties of the normal state of quasi-1D superconductors like Bechgaard salts are investigated by combining the linearised Boltzmann equation and the renormalisation group (RG) method. The collision integral operator is calculated using the Umklapp scattering amplitudes obtained by the RG method yielding the electrical resistivity($\rho$) and Seebeck coefficient ($S$). The power law dependence, $\rho(T) \sim T^\alpha$, for resistivity is obtained by changing the antining parameter $t'_r$, simulating the pressure distance from the quantum critical point (QCP) between spin-density-wave (SDW) and d-wave SC (SCd) in the phase diagram. The resistivity evolves from a linear component ($\alpha \approx 1$) to the QCP towards a Fermi liquid component ($\alpha \approx 2$) with increasing $t'_r$, which confirms an extended region of quantum criticality as a result of interference between SCd and SDW causing an anomalous growth of Umklapp scattering. Its anisotropy is also tied to the $k_z$-dependence of hot/cold scattering regions along the Fermi surface. Similar calculations for the Seebeck coefficient show deviations from the usual linear temperature dependence and also a change of sign near a SDW instability.


8:36AM A14.00004 Higgs criticality in a two-dimensional metal, SUBIR SACHDEV, DEBANJAN CHOWDHURY, Harvard Univ — We analyze a candidate theory for the strange metal near optimal hole-doping in the cuprate superconductors. The theory contains a quantum phase transition between metals with ‘large’ and ‘small’ Fermi surfaces, but the transition does not directly involve any broken global symmetries. The two metals have emergent SU(2) and U(1) gauge fields respectively, and the transition is driven by the condensation of a real Higgs field which carries an adjoint SU(2) charge. We propose a global phase diagram around this Higgs transition, and describe its relationship to a variety of recent experiments on the cuprate superconductors.
Quantum Criticality In Layered YFe<sub>2</sub>Al<sub>10</sub>  
Shao-Kai Jian, Yi-Fan Jiang, and Hong Yao, arXiv:1407.4497

Quantum critical point of Dirac fermions studied using efficient continuous-time projector quantum Monte Carlo method  
Lei Wang, Mauro Iazzì, ETH - Zurich, Philippe Corboz, University of Amsterdam, Matthias Troyer, ETH - Zurich — Quantum phase transition (QPT) of Dirac fermions is a fascinating topic both in condensed matter and in high energy physics. Besides its immediate connection to fundamental problems like mass generation and exotic phases of matter, it provides a common playground where the state of the art numerical simulations can be crosschecked with various effective field theory predictions, thus deepen our understanding of both fields. The universality class of the QPT is fundamentally different from the usual bosonic field theory because of the coupling to the gapless fermionic mode at the critical point. We study lattice models with spinless and multi-flavor Dirac fermions using the newly developed efficient continuous-time projector quantum Monte Carlo method. Besides eliminating the Trotter error, the method also enables us to directly calculate derivative observables in a continuous range of interaction strengths, thus greatly enhancing the resolution of the quantum critical region. Compatible results are also obtained from infinite projected entangled-pair states calculations. We compare these numerical results with predictions of the Gross-Neveu theory and discuss their physical implications.

Quantum phase transitions in the Kondo-necklace model  
Nader Ghassemi, Shayan Hemmatiyan, Department of Physics, Texas A&M University, College Station, TX 77843-4242, Mahsa Rahimi Movassagh, Department of Physics, McMaster University, ON L8S 4L8, Canada, Mahdi Kargarian, Department of Physics, University of Texas at Austin, Austin, Texas 78712-1081, USA, Ali T. Rezakhani, Abdollah Langari, Department of Physics, Sharif University of Technology, Tehran 11155-9161, Iran — Kondo-necklace model, which includes an additional spin degree of freedom, exhibits unique quantum phase transitions due to the strong quantum correlations. We study these phase transitions using the time projector quantum Monte Carlo method. Besides eliminating the Trotter error, the method also enables us to directly calculate derivative observables in a continuous range of interaction strengths, thus greatly enhancing the resolution of the quantum critical region. Compatible results are also obtained from infinite projected entangled-pair states calculations. We compare these numerical results with predictions of the Gross-Neveu theory and discuss their physical implications.

Emergent space-time supersymmetry in 3D Weyl semimetals and 2D Dirac semimetals  
Shao-Kai Jian, Yi-Fan Jiang, Hong Yao, Institute for Advanced Study, Tsinghua University — Supersymmetry (SUSY) interchanges bosons and fermions but no direct evidences of it have been revealed in nature yet. In this paper, we observe that fluctuating pair density waves (PDW) phase of the spinless honeycomb model with nearest neighbor attractions by doing fermionic projected entangled pairing state (PEPS) algorithm for infinite lattices. It was recently shown by renormalization group (RG) analysis that space-time supersymmetry (SUSY) emerges in Dirac fermions at their PDW transition. The connection of our present PEPS studies with the emergent space-time SUSY at the PDW transition shown by RG will be discussed.

Work at Brookhaven National Laboratory was carried out under the auspices of US Department of Energy, Office of Basic Energy Sciences, Contract DE-AC02-98CH1886.

1Sharif University of Technology

2Work at Brookhaven National Laboratory was carried out under the auspices of US Department of Energy, Office of Basic Energy Sciences, Contract DE-AC02-98CH1886.

3Shao-Kai Jian, Yi-Fan Jiang, and Hong Yao, arXiv:1407.4497
10:00AM A14.00011 How Ubiquitous is Total Electron Transmission through Nanostructures (Quantum Dragons)?¹, MARK NOVOTNY, Mississippi State University — In transport through nanostructures connected to two semi-infinite leads, the transmission probability \( T(E) \) as a function of the energy \( E \) of the incoming electron plays a central role in the Landauer calculation of the electrical conductance \( G \). A quantum dragon nanostructure [1] is one which when connected to appropriate leads has total electron transmission for all energies, \( T(E)=1 \).

In two-terminal measurements of single-channel quantum dragons, the quantum of conductance, \( G_0=2e^2/h \), should be observed. A quantum dragon may have strong scattering. In [1] the disorder was along the axis of electron propagation, the \( z \) axis. We show that quantum dragon nanostructures can be found for strong disorder perpendicular to the \( z \) axis. In select types of nanostuctures, we find the ratio of the dimension of the parameter space where quantum dragons exist to that of the complete parameter space. The results use the single-band tight-binding model, and are for the case with only one open channel and homogeneous leads. One type of nanostructure with \( T(E)=1 \) has completely disordered slices perpendicular to the \( z \) axis, but identical slices along the \( z \) direction. [1] M.A. Novotny, Phys. Rev. B 90, 165103 [14 pages] (2014)

¹Supported in part by NSF grant DMR-1206233.

10:12AM A14.00012 Single and Multi-channel Quantum Dragons from Rectangular Nanotubes, ZHOU LI, MARK NOVOTNY, Mississippi State University — Recently quantum dragons have been discovered theoretically [1]. Quantum dragons are nanostructures with correlated disorder that permit energy-independent total quantum transmission of electrons. Hence the electrical conductance \( G \) in a two-terminal measurement should be the conductance quantum \( G_0=2e^2/h \). The single-band tight binding model is used.

An example of a single-channel quantum dragon is a rectangular nanotube with disorder along the direction \( z \) of the electron propagation [1]. Quantum dragons are obtained by solving the time-independent Schrödinger equation to obtain the electrical transmission \( T \) as a function of the incoming electron energy \( E \). A quantum dragon has \( T(E)=1 \) for all energies. This work generalizes the solution of the time-independent Schrödinger equation to the case of more than one open channel, and applies the method to nanotubes formed from rectangular lattices. One can envision such single-walled rectangular nanotubes for iron starting from free-standing single-atom-thick Fe membranes which have recently been obtained experimentally [2].


¹Supported in part by NSF grant DMR-1206233

10:24AM A14.00013 Single and Multi-Channel Carbon-based Quantum Dragons¹, GODFRED INKoom, Mississippi State University, OMADILLO ABDURAZAKOV, NCSU, MARK NOVOTNY, Mississippi State University — In the coherent regime for electrical conductance measurements, two semi-infinite leads are connected to a finite nanostructure, and the nano-device conductance is calculated using the Landauer formula. Any channel \( k \) that has transmission for electrons with energy \( E \), \( T_k(E)=1 \) contributes the conductance quantum \( G_0=2e^2/h \). Any nano-device with at least one \( T_k(E)=1 \) is called a quantum dragon [1]. The transmission probability \( T_k(E) \) can be obtained from the solution of the time-independent Schrödinger equation. Uniform leads connected to armchair single-walled carbon nanotubes (SWCNTs) have \( T(E)=1 \), while when connected to zigzag SWCNTs the \( T(E) \) is less than unity. Appropriately dimerized leads connected to zigzag SWCNTs are quantum dragons, while when connected to armchair SWCNTs \( T(E) \) is less than unity [1]. We have generalized the matrix method and mapping methods of [1] in order to investigate SWCNTs that can be multi-channel quantum dragons. For example, one can use armchair SWCNT leads to connect to an armchair SWCNT to try to produce a multi-channel quantum dragon.


¹Supported in part by NSF grant DMR-1206233

10:36AM A14.00014 Quantum degradation of the second order phase transitions, SERGEI STISHOV, ALLA PETROVA, Institute for High Pressure Physics of RAS, Troitsk, Russia, SERGEY GAVRILKIN, P. N. Lebedev Physical Institute of RAS, Leninsky pr., 53, 119991 Moscow, Russia, LUBOV KLINKOVA, Institute of Solid State Physics of RAS, Chernogolovka, Moscow District, Russia — The specific heat, magnetization and thermal expansion of single crystals of antiferromagnetic insulator EuTe were measured at temperatures down to 2 K and in magnetic fields up to 90 kOe. The Neel temperature, being \(~9.8\) K at \( H=0 \), decreases with magnetic field and tends to zero at \(~76\) kOe, therefore forming the quantum critical point. The heat capacity and thermal expansion coefficient reveal \( \lambda \)-type anomalies at the second order magnetic phase transition at low magnetic fields, evolving to simple jumps at high magnetic fields and low temperatures, well described in a fluctuation free mean - field theory. The experimental data and the corresponding analysis favor the quantum concept of effective increasing space dimensionality at low temperatures that suppresses a fluctuation divergence at a second order phase transition.

10:48AM A14.00015 Dynamic spin susceptibility of interacting electron systems¹, VLADIMIR ZYUZIN, DMITRII MASLOV, University of Florida — We study the dynamic spin susceptibility of interacting electrons in spatial dimensions from one to three. In all cases, backscattering processes result in non-zero imaginary part of the spin susceptibility above the particle-hole continuum of non-interacting electrons. In one dimension, we employ the renormalization group to go beyond the second order and obtain a general expression for the spin susceptibility. In higher dimensions, we show that the imaginary part of the spin susceptibility arises from the same mechanism as non-analytic corrections to the Fermi-liquid theory. We relate the obtained results to the lifetime of collective spin modes.

¹This work was supported by the National Science Foundation via grant NSF DMR-1308972.
8:00AM A15.00001 First-principles interpretation of attosecond time-resolved XUV absorption spectroscopy of laser excited Silicon, SRI CHAITANYA DAS PEMMARAJU, Lawrence Berkeley Natl Lab, SHUNSUKE SATO, KAZUHIRU YABANA, University of Tsukuba, KRUPA RAMASESHA, University of California, Berkeley, MARTIN SCHULTZE, Ludwig-Maximilians-Universitat, STEPHEN R. LEONE, University of California, Berkeley, DAVID PRENDERGAST, Lawrence Berkeley Natl Lab — The availability of ultrafast x-ray pulses both from powerful free electron laser light-sources as well as table top high-harmonic generation, has significantly enhanced the utility of core-level spectroscopies as probes for investigating dynamical processes in functional materials. Theoretical approaches to complement these time-domain experiments are therefore actively being developed. In this study we employ a combination of real-time time-dependent density functional theory (TDDFT), occupancy-constrained density functional theory and many-body perturbation theory approaches to help interpret spectral signatures observed in attosecond time-resolved core-level spectroscopic measurements on laser-excited silicon. Using non-equilibrium electron-hole densities obtained from real-time TDDFT simulations of the valence electronic structure we estimate the transient modulation of L-edge absorption in femtosecond infrared pump - attosecond XUV probe experiments. We further estimate the contribution of electron-phonon and electron-electron scattering mechanisms to the lifetime broadening observed in measured L-edge spectra using occupation-constrained density functional theory and GW calculations respectively.

8:12AM A15.00002 First-principles calculation of electronic structure and optical absorption of BN ZnO, XIAO ZHANG, ANDRE SCHLIEFE, Univ of Illinois - Urbana — The α-BN structure of ZnO, a nonequilibrium phase with a transition pressure of 25 GPa, has been found in nano structures of ZnO. The structural difference between the BN structure and the equilibrium wurtzite structure can play an important role for applications of nanostructured ZnO. In order to understand the difference, first principles calculations have been performed on both phases. The electronic structure is computed using the GW method based on Density Functional Theory and HSE hybrid functional calculations. The GW method includes the quasiparticle effects due to the screened electron-electron interaction which gives an accurate description of the electronic band structure and density of states. After that, by solving the Bethe-Salpeter Equation for the optical polarization function, which take excitonic effects into account, we have achieved an accurate description of optical absorption spectra for both structures. We find a good agreement with experimental and previous computational results for WZ structure, and predict the absorption for the BN structure. The BN structure shows a larger band gap and we found a very large optical anisotropy: The gap for extraordinary light polarization is almost 0.7eV larger than that for ordinary light polarization.

8:24AM A15.00003 Wannier function analysis of charge states in transition metal oxides1, YUNDI QUAN, WARREN PICKETT, Univ of California - Davis — The charge (or oxidation) state of a cation has been a crucial concept in analyzing the electronic and magnetic properties of oxides as well as interpreting “charge ordering” metal-insulator transitions. In recent years a few methods have been proposed for the objective identification of charge states, beyond the conventional (and occasionally subjective) use of projected densities of states, weighted band structures (fatbands), and Born effective charges. In the past two decades Wannier functions (WFs) and particularly maximally localized WFs (MLWFs), have become an indispensable tool for several different purposes in electronic structure studies. These developments have motivated us to explore the charge state picture from the perspective of MLWFs. We will illustrate with a few transition metal oxide examples such as AgO and YNiO3 that the shape, extent, and location of the charge centers of the MLWFs provide insights into how cation-oxygen hybridization determines chemical bonding, charge distribution, and “charge ordering.”

1DOE DE-FG02-04ER46111

8:36AM A15.00004 DFT+U invsitgation of doped-PbPdO2 spin gapless semiconductors, HAN HSU, SHENG-CHIEH HUANG, National Central University — Spin gapless semiconductors (SGSs), with a zero gap in one spin channel and a finite gap in the other, have attracted considerable attention due to their potential in spintronics. Ever since PbPdO2 was predicted a gapless semiconductor by local density approximation (LDA) calculations and confirmed by experiments afterward, it is anticipated to be a backbone material for SGS. Using density functional theory + self-consistent Hubbard U (DFT+U) calculations, we investigate doped PbPdO2 with different kinds of transition-metal dopants, including V, Cr, Mn, Fe, Co, and Ni, at different dopant concentration. We show that doped PbPdO2 can be a SGS with a proper choice of dopant and dopant concentration. Furthermore, different dopant and dopant concentration can lead to different types of SGS.

8:48AM A15.00005 Final-state effect on X-ray photoelectron spectrum of n-doped SrTiO3, CHUNGHWEI LIN, AGHAM POSADAS, ALEXANDER DEMKOV, UT Austin, Physics Department, DEMKOV TEAM — X-ray photoelectron spectroscopy (XPS) is a widely used technique to determine the oxidation states of chemical elements. In stoichiometric SrTiO3, the Ti4+ peak appears at a binding energy of about 459.0 eV for photoelectrons ejected from the Ti 2p core level. In lightly n-doped SrTiO3, a weak shoulder at a binding energy of about 1.5 eV lower than the Ti4+ peak appears in the XPS spectrum which has been conventionally interpreted as a Ti3+ signal. By taking the final-state effect into account, i.e. by considering the response of the valence electrons in the presence of a core hole, we argue that such a Ti3+ peak does not necessarily imply the existence of spatially localized Ti3+ ions, and explicitly show that a spatially uniform Ti(4−z)+ distribution also leads to the multi-peak structure. Spectra from metallic n-doped SrTiO3 (e.g. La replacing Sr, Nb replacing Ti, or even oxygen vacancy doping) should be interpreted as the latter case. Several experiments based on this interpretation are discussed.

9:00AM A15.00006 Test set for materials science and engineering, TOKTAM MORSHEDLOO, Fritz-Haber-Institut der MPG, Berlin, DE; Ferdowsi University of Mashhad, IR, NORINA A. RICHTER, FAWZI MOHAMED, Fritz-Haber-Institut der MPG, Berlin, DE, XINGUO REN, Fritz-Haber-Institut der MPG, Berlin, DE; University of Science and Technology of China, China, SERGEO V. LEVCHENKO, LUCA M. GHIRINGHELLI, ICOR YING ZHANG, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, DE — Understanding of the applicability and limitations of electronic-structure methods needs detailed comparison with highly accurate data of representative test sets. A variety of highly valuable test sets have been established in quantum chemistry for small molecules. However, for crystalline solids they are still lacking. We present a representative test set for materials science and engineering (MSE) which includes first and second row elements and their binaries, comprising various crystal structures. This test set allows for unbiased benchmarking for various chemical interactions. In the MSE test set, we consider cohesive energy, lattice constant, bulk modulus, electronic, band structures and phonons etc. A big effort is made to produce systematically converged results with respect to basis set[1] and k mesh for a hierarchy of electronic-structure methods, ranging from the local-density approximation to advanced orbital-dependent functionals implemented in the all-electron, full-potential FHI-aims code. Furthermore, we use incremental schemes to obtain benchmark values calculated with coupled-cluster approaches.

Berkeley National Laboratory, ARUN BANSIL, Northeastern University, ALESSANDRA LANZARA, University of California, Berkeley and Lawrence National Tsing Hua University and Academia Sinica, ASLIHAN SUSLU, Arizona State University, JUNQIAO WU, University of California, Berkeley and Lawrence TONGAY, Arizona State University, TAY-RONG CHANG, National Tsing Hua University, HSIN LIN, National University of Singapore, HORNG-TAY JENG, calculated electron and hole effective masses. Funded in part by the NSF and the Louisiana Board of Regents, through LASiGMA [Award Nos. EPS-1003897, Γ at the other ionic inputs; hence, the description of w-AlN is provided by a calculation with these ionic species as input. Our calculated, direct band gap for w-AlN, of the calculation leading to the lowest, occupied energies. With Al \( ^{3+} \) states of Al and N, the method led to several sets of calculations with different ionic species as input. LDA requires, for the description of w-AlN, the results of Gaussian orbitals (LCGO), and the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF). With multiple oxidation states of Al and N, the method led to several sets of calculations with different ionic species as input. LDA requires, for the description of w-AlN, the results of Gaussian orbitals (LCGO), and the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF), in our implementation of the LCGO. We discuss electronic energy bands, total (DOS) and partial (pDOS) densities of states, effective masses that are pertinent to transport properties, and the bulk modulus. For a room temperature lattice constant of 6.539 Å, our calculated, direct band gap of the material, at \( \Gamma \), is 2.83 eV. We predict a direct band gap of 3.05 eV for the calculated equilibrium lattice constant of 6.395 Å. The significant decrease of the lattice constant, for a drop in temperature from 300 to 0 K, is understandable with the relatively small, predicted bulk modulus of 43.9 GPa. Acknowledgments: This work was funded in part by the NSF and the Louisiana Board of Regents, through LASiGMA [Award Nos. EPS-1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, the US Department of Energy – NNSA (Award Nos. DE-NA0001861 and DE-NA0002630). LaSPACE, and LONI-SUBR.

9:24AM 15.00008 Electronic structure, spin–orbit coupling, and interlayer interaction in bulk MoS\(_2\) and WS\(_2\). DREW LATZKE, WENTAO ZHANG, University of California, Berkeley and Lawrence Berkeley National Laboratory, SEFAATTIN TONGAY, Arizona State University, TAY-RONG CHANG, National Tsing Hua University and Academy Sinica, ASLIHAN SUSLU, Arizona State University, JUNQIAO WU, University of California, Berkeley and Lawrence Berkeley National Laboratory, ARUN BANSIL, Northeastern University, ALESSANDRA LANZARA, University of California, Berkeley and Lawrence Berkeley National Laboratory — Transition metal dichalcogenides (TMDs) (MX\(_2\) where M = Mo or W and X = S, Se, or Te) are theorized to possess unique spin-split valence bands along with rare spin–valley coupling, making them attractive for applications within the growing fields of spintronics and valleytronics. Despite the importance of the spin valence band that governs the unique spin- and valley-physics of TMDs, there remain many questions regarding its origin and properties in bulk TMDs. In this talk, I will present high-resolution angle resolved photoemission spectroscopy (ARPES) measurements of the electronic band structure of bulk TMDs MoS\(_2\) and WS\(_2\). Detailed comparison with first principle calculations will be shown. The role of the valence band splitting and how it can be controlled will be discussed.

9:36AM 15.00009 Barium disilicides (BaSi\(_2\)) a low-cost, earth-abundant material for thin-film solar cells. MUKESH KUMAR, NAOTO UMEZAWA, MOTOHARU IMAI, Natl Inst for Materials Sci — In order to meet the clean energy requirement, materials consisting of abundant, eco-friendly, and low-cost elements are of great interest. Therefore in this study, we discussed the importance of BaSi\(_2\) and other similar semiconductor compounds which contain inexpensive and earth abundant elements, for solar cell applications. Employing first-principles modeling within the density functional theory, we analyze the structural, electronic and optical properties and find that these compounds have fundamental indirect band gaps and the gap energies are in the region of 0.9–1.3 eV, which is suitable for solar cell applications. Furthermore, a lower energy dispersion of the conduction band (CB), which results in a flat shape of the CB minimum, implies a large optical absorption. In fact, our calculations reveal that the photoabsorption of these compounds is stronger than other common PV materials like Si and Cu(Ga,In)Se\(_2\).

9:48AM 15.00010 Quantifying defect levels in hexagonal boron nitride from simulated x-ray absorption spectroscopy \(^1\). SEBASTIAAN HUBER, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, United States, ROBBERT VAN DE KRUJIS, FRED BIJKERK, Industrial Focus Group XUV Optics, MESA+ Research Institute for Nanotechnology, University of Twente, The Netherlands, ERC GULLIKSON, Center for X-Ray Optics, Lawrence Berkeley National Laboratory, Berkeley, United States, DAVID PRENDERGAST, Molecular Foundry, Lawrence Berkeley National Laboratory, United States — X-Ray Absorption Spectroscopy is a technique that is highly sensitive to the local structural and chemical environment of the probed species. This quality can be exploited to investigate the characteristics of localized structural imperfections such as point defects and grain boundaries. In this study, we simulated X-ray absorption spectra for several hexagonal (h-BN) and amorphous boron nitride (a-BN) samples were recorded. Simulation of X-ray absorption spectra from first principles allows for characteristic features in the measured spectra to be attributed to local defects of the planar hexagonal structure of the material. Analysis of the relative intensities of these features can subsequently provide a quantitative analysis of the levels of various defects in the analyzed structure.

\(^1\)This work is supported by NanoNextNL, a micro and nanotechnology programme of the Dutch Government and 130 partners.

10:00AM 15.00011 Accurate, Electronic and Transport Properties of Wurtzite Aluminum Nitride (w-AIN). IFEANYI NWIGBOJI, YURIY MALOZOVSKY, LASHOUNDA FRANKLIN, Southern University and A&M College, CHINEDU EKUMA, Louisiana State University, DIOLA BAGAYOKO, Southern University and A&M College — We present results from ab-initio, self-consistent calculations of electronic and transport properties of wurtzite aluminum nitride (w-AIN). We utilized a local density approximation (LDA) potential, the linear combination of Gaussian orbitals (LCGO) potential and the linear combination of Gaussian orbitals (LCGO) formalism. We followed the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF). With multiple oxidation states of Al and N, the method led to several sets of calculations with different ionic species as input. LDA requires, for the description of w-AIN, the results of the calculation leading to the lowest, occupied energies. With Al\(^{3+}\) and N\(^{3+}\) as input, the binding energy was 1.5 eV larger, in magnitude, than those for other ionic inputs; hence, the description of w-AIN is provided by a calculation with these ionic species as input. Our calculated, direct band gap for w-AIN, at the \( \Gamma \) point, is 6.28 eV, in excellent agreement with the 6.28 eV experimental value at 5 K. We discuss the bands, total and partial densities of states, and calculated electron and hole effective masses. Funded in part by the NSF and the Louisiana Board of Regents, through LASiGMA [Award Nos. EPS-1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, the US Department of Energy – NNSA (Award No. DE-NA0001861), LaSPACE, and LONI-SUBR.

10:12AM 15.00012 Electronic properties of perovskite absorbers for solar cell applications\(^1\). MARINA FILIP, FELICIANO GIUSTINO, University of Oxford, Department of Materials — Metal halide perovskite absorbers have captured the attention of the photovoltaics community in the past 3 years, reaching efficiencies over 19%. Despite this unprecedented progress, the remarkable physical properties of these materials are not yet fully understood. In this work we show an exhaustive computational study of CH\(_3\)NH\(_3\)PbI\(_3\) within density functional theory and the GW approximation. We show the effect of semicore states and spin-orbit coupling on the quasiparticle band gap of CH\(_3\)NH\(_3\)PbI\(_3\) and describe a straightforward "self-consistent scissor" method to correct the underestimated dielectric screening in the G0W0 approach [1]. Finally, we model the interplay between the structural and electronic properties of lead-iodide perovskites and propose novel lead-iodide perovskite absorbers with different cations at the center of the cuboctahedra cavity facilitating the tuning of the fundamental band gap [2].


\(^{1}\)This work was supported by the ERC (EU FP7 / ERC 239578), UK EPSRC (EP/J009857/1) and the Leverhulme Trust (RL-2012-001).
10:24AM A15.00013 Chemical trends in halide perovskite electronic properties¹. WALTER LAM-BRECHT, LING-YI HUANG, Case Western Reserve University — The halide perovskites ABX₃ with B = Pb or Sn, X = I, and A = Cs or methylammonium (MA), have recently attracted attention as solar cell materials. We discuss the basic bonding, stability and electronic band structure of these materials for different chemical substitutions using first-principles calculations. An important feature of the Pb and Sn based halides is that these element’s 6-electrons strongly hybridize with the halogen p-orbitals leading to a valence band maximum with strong Sn or Pb-p character and small effective mass. The conduction band minimum is Sn or Pb-p-like. We present trends in the electronic band structure with the halogen X = I, Br, Cl and the B cation Pb, Sn, Ge, Si. The gap is remarkably insensitive because of the opposing trends of the increased spin-orbit coupling for heavier elements (reducing the gap) and the decreased valence band width for heavier elements due to the larger B-X distance, which increases the gap. The stability of the perovskite structure vs. competing structures is influenced by the tolerance factor t = RₓA₃/VγBₓC₃. The smaller this factor, the least stable is the perovskite structure. CsSnI₃ is found to be a topological insulator. Its stability with respect to CsI and SnI₂ is discussed.

¹Supported by DOE-BES, No. ER 46874-SC0008933.

10:36AM A15.00014 Electronic structure studies of MX₂ (M=Mo, W; X=S, Se) by ARPES and the band evolution of hydrogen gas exposed MoS₂. BEOM SEO KIM, SOOHYUN CHO, BEOMYOUNG KIM, Yonsei Univ; JONATHAN DENLINGER, Advanced Light Source, BYUNG HOON KIM, SEUNG RYONG PARK, Incheon National Univ, CHANGYOUNG KIM, Yonsei Univ — The physics associated with transition metal dichalcogenides (TMDs) is one of the most intriguing issues in condensed matter physics. These materials have several interesting aspects inter physical properties, especially the direct to indirect band gap transition and spin-orbit coupling induced spin band splitting at the K-point. However, thorough systematic studies on the electronic structures of TMDs regarding those issues have not been done. We present the electronic structure studies of MoS₂ using angle resolved photoemission spectroscopy (ARPES). We investigated the indirect band gap and spin-band splitting sizes of MoS₂. In addition, we present ARPES results from MoS₂+H₂(10h), performed to investigate the evolution of the band structure as a function of hydrogen exposure (from MoS₂ to MoS₂+H₂(10h)). Photon energy dependence and potassium dosing were performed for each system. The results from MX₂ are quite consistent with the published band calculation results. In the MoS₂+H₂ (10h) case, there are two interesting observations from the results. The first is that the indirect band gap size decreases upon exposure to hydrogen. The other observation is that the Γ band appears to have quantized confinement effect.

10:48AM A15.00015 Discrete energy bands in bulk semiconductors. MAOHUA DU, HONGLIANG SHI, Oak Ridge National Lab — Bulk semiconductors typically have continuous valence and conduction bands. Discrete energy levels and bands have been sought after for various applications. For instance, discrete energy levels existing in semiconductor nanocrystals, or quantum dots (QDs) have been proposed as a mechanism to suppress hot carrier thermalization and to enhance carrier multiplication in QD solar cells. Impurity bands in the band gap have been proposed for intermediate-band solar cells and for efficient visible light absorption and photocatalysis. In this talk, we show by first principles calculations that, in a multinary compound, a combination of large electronegativity difference between different cations (anions) and large nearest-neighbor distances in cation (anion) sublattices can lead to the splitting of the conduction (valence) band, resulting in several discrete and narrow energy bands separated by large energy gaps. We also discuss applications that may benefit from such electronic structure.

Monday, March 2, 2015 8:00AM - 11:00AM –
Session A16 DMP DCOMP: Focus Session: Materials by Theoretical Design

8:00AM A16.00001 Theory-guided discovery of new superconducting materials¹. ALEKSEY KOLMOGOROV, Binghamton University, SUNY — Extensive theoretical effort to predict new superconductors has resulted in remarkably few discoveries. Successful examples so far have been restricted primarily to pressure- or doping-driven superconducting transformations in existing materials. In this talk I will describe our work that has led to the prediction [1] and discovery [2] of a brand-new superconducting FeB₄ compound with a previously unknown crystal structure. First measurements supported the predicted phonon-mediated pairing mechanism, rare for an iron-based superconductor. The identification of FeB₄ candidate material was a result of combined high-throughput screening, targeted evolutionary search [3], and rational design. The systematic study of more than 12,000 metal boride phases has identified dozens of synthetizable materials with unusual structural motifs, some of which have been confirmed experimentally [4]. I will overview employed strategies for selecting promising superconducting compounds and describe our ongoing work on accelerating the search for stable materials.

¹This work is supported by the National Research Foundation of Korea (NRF) under Grant No. NRF-2005-003845 and by Samsung Science and Technology Foundation under Grant No. SSTFBA1401-08.

8:36AM A16.00002 Guided design of copper oxyxulfide superconductors. CHUCK-HOU YEE, TURAN BIROL, GABRIEL KOTLIAR, Rutgers University — Using the framework of chemical intuition introduced by Antipov, et. al., in his synthesis of the Hg-based high-temperature superconductors, supplemented with modern first-principles electronic structure tools, materials databases, and evolutionary algorithms capable of exploring large configurational spaces, we design a novel family of copper oxyxulfides. We explore the predictions of theories based on charge-transfer energies, orbital distillation and uniaxial strain on the superconducting transition temperatures of these oxyxulfides.

8:48AM A16.00003 Conformational space annealing scheme in the inverse design of functional materials¹. SUNGHYUN KIM, KAIST; IN-HO LEE, Korea Research Institute of Standards and Science. JOOYOUNG LEE, Center for In Silico Protein Science, School of Computational Science, YOUNG JUN OH, KEE JOO CHANG, KAIST — Recently, the so-called inverse method has drawn much attention, in which specific electronic properties are initially assigned and target materials are subsequently searched. In this work, we develop a new scheme for the inverse design of functional materials, in which the conformational space annealing (CSA) algorithm for global optimization is combined with first-principles density functional calculations. To implement the CSA, we need a series of ingredients, (i) an objective function to minimize, (ii) a ‘distance’ measure between two conformations, (iii) a local enthalpy minimizer of a given conformation, (iv) ways to combine two parent conformations to generate a daughter one, (v) a special conformation update scheme, and (vi) an annealing method in the ‘distance’ parameter axis. We show the results of applications for searching for Si crystals with direct band gaps and the lowest-enthalpy phase of boron at a finite pressure and discuss the efficiency of the present scheme.

¹This work is supported by the National Research Foundation of Korea (NRF) under Grant No. NRF-2005-003845 and by Samsung Science and Technology Foundation under Grant No. SSTFBA1401-08.
9:00AM A16.00004 Computational materials design of negative effective $U$ system in the hole-doped Delafosseite of CuAlO$_2$, AgAlO$_2$ and AuAlO$_2$. AKITAKA NAKANISHI, TETSUYA FUKUSHIMA, HIROKI UEDE, HIROSHI KATAYAMA-YOSHIDA, Osaka University — In order to realize the super-high-$T_c$ superconductors ($T_c$(0)>1.00K) based on the general design rules [1] for the negative $U_{eff}$ system, we have performed computational materials design for the hole-doped one-dimensional (1D) Delafosseite CuAlO$_2$, AgAlO$_2$ and AuAlO$_2$ from the first principles. We find the interesting chemical trend of $T_c$ in 2D and 3D systems; where the $T_c$ increases exponentially in the weak coupling regime ($|U_{eff}|=0.44 eV$) for the band width $W$ (1.7 eV) for hole-doped CuAlO$_2$. [1] H. Katayama-Yoshida et al., Appl. Phys. Express 1 081703, 2008.

9:12AM A16.00005 How to design negative effective $U$ Fermion system in hole doped chalcopryte CuFeSe$_2$? HIROSHI KATAYAMA-YOSHIDA, TETSUYA FUKUSHIMA, HIROKI UEDE, YUKI TAKAWASHI, AKITAKA NAKANISHI, Graduate School of Engineering Science, Osaka University, KAZUNORI SATO, Graduate School of Engineering, Osaka University — Here, we have proposed a general rule of the attractive Fermion system in the purely electronic origin, which is called negative effective $U$ ($U_{eff}<0$) system. Purely electronic-originated $U_{eff}<0$ is caused by (i) the exchange-correlation-induced energy gain in the Hund’s rules, and (ii) the charge-excitation-induced energy gain. Based on the general design rules, we perform ab initio electronic structure calculations for hole-doped Chalcopryte CuFeSe$_2$. It is found that the hole-doped CuFeSe$_2$ has the $U_{eff}<0$ is originated by the charge-excitation- induced mechanism in the hole-doped Cu$^{3+}$ ($d^9$) and $S^2- (e^2p^2)$, and also originated by the exchange-correlation- induced mechanism in the hole-doped Fe$^{4+}$ ($d^5$). The hole-doped paramagnetic and metallic CuFeSe$_2$ with $U_{eff}<0$ may cause a possible super-high-$T_c$ superconductor ($T_c$ $\approx$ 1000 K, if $\Delta/|U_{eff}| \approx 10$ by assuming a strong coupling regime.) because of the strong attractive electron-electron interactions (superconducting gap $\Delta \approx |U_{eff}| \approx 5000$ K). We propose a new computational materials design methodology to design super-high-$T_c$ superconductors starting from the atomic number only. [1] T. Fukushima et al., J. Phys. Condens. Matter, 26 355502, 2014.

9:24AM A16.00006 Direct band gap silicon crystals predicted by an inverse design method. YOUNG JUN OH, Korea Advanced Institute of Science and Technology, IN-HO LEE, Korea Research Institute of Standards and Science. JOOYOUNG LEE, Korea Institute for Advanced Study, SUNGYUN KIM, KEE JONG CHANG, Korea Advanced Institute of Science and Technology — Cubic diamond silicon has an indirect band gap and does not absorb or emit light as efficiently as other semiconductors with direct band bands. Thus, searching for Si crystals with direct band gaps is important to realize efficient thin-film solar cells. In this work, we report various crystalline silicon allotropes with direct and quasi-direct band gaps, which are predicted by the inverse design method which combines a conformation space annealing algorithm for global optimization and first-principles density functional calculations. The predicted allotropes exhibit energies less than 0.3 eV per atom and good lattice matches, compared with the diamond structure. The structural stability is examined by performing finite-temperature ab initio molecular dynamics simulations and calculating the phonon spectra. The absorption spectra are obtained by solving the Bethe-Salpeter equation together with the quasiparticle phonon spectra. The absorption spectra are obtained by solving the Bethe-Salpeter equation together with the quasiparticle phonon spectra.

9:36AM A16.00007 Design of I$_2$-II-IV-VI$_4$ Semiconductors through Element-substitution: the Thermodynamic Stability Limit and Chemical Trend. SHIYOU CHEN, East China Normal University, CONGCONG WANG, Fudan University, HONGKUN XIANG, XIN-GAO GONG, Fudan University, ARON WALSH, University of Bath, SU-HUAI WEI, National Renewable Energy Laboratory — Through element substitution in kesterite Cu$_2$ZnSnS$_4$ or Cu$_2$ZnSnSe$_4$, a class of I$_2$-II-IV-VI$_4$ semiconductors can be designed as novel functional materials. Using the first-principles calculations, we show that this element-substitution design is thermodynamically limited, i.e., although I$_2$-II-IV-VI$_4$ with I=Cu, Ag, II=Zn, Cd, Hg, IV=Si, Ge, Sn and VI=5, 6, Se, Te are stable quaternary compounds, those with I=Mg, Ca, Sr, Ba, IV=Ti, Zr, Hf, and VI=O are unstable against the phase-separation into the competing binary and ternary compounds. Three main phase-separation pathways are revealed. We show that if the secondary II-VI or I-IV-VI$_4$ phases prefer to have non-tetrahedral structures, then the I$_2$-II-IV-VI$_4$ semiconductors tend to phase separate. This finding can be used as a guideline for future design of new quaternary semiconductors.

9:48AM A16.00008 Materials predicted to be topological insulators in hypothetical structures assumed by theorists might be trivial insulators in their stable phases. GIANCARLO TRIMARCHI, Northwestern U., Evanston, IL, XIUWEN ZHANG, ALEX ZUNGER, U. of Colorado, Boulder, CO — The quest for new topological insulators (TIs) has motivated numerous ab initio calculations of the topological metric $Z_2$ of candidate compounds in hypothetical crystal structures, or in assumed pressure or doping conditions. However, TI-ness might destabilize certain crystal structures that would be replaced by other structures, which might not be TIs. Here, we discuss such false-positive predictions in the ab initio search for new TIs. (i) Various ABX compounds, predicted to be TIs in the assumed ZrBeSi-type structure that turns out to be unstable, become trivial insulators in their stable structures. (ii) Band-inversion-inducing structure perturbations destabilize the system which is instead trivial at equilibrium: examples of this scenario are the cubic $\text{Al}_{13}\text{Bi}_3\text{O}_{34}$ perovskites that transform from topological to trivial when they relax to their equilibrium structures. (iii) Doping destabilizes the band-inverted system that relaxes to a trivial atomic configuration (orthorhombic band-inverted $\text{BaBiO}_3$) is a shallow acceptor producing holes yet the hole-killer donor of B-interstitial is unfavorable. (4) When B=N or Co, the compound favors $n$-type due to the dominance of B-interstitial defects (e.g., TiCoSb). We will show the calculated leading defect types and the dependence of carrier concentrations on chemical conditions for newly predicted half-Heusler insulators. This study is supported by DOE, Office of Science, Basic Energy Science, MSE division grant to CU Boulder.

1Work at CU, Boulder supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Grant DE-FG02-13ER46959.

10:00AM A16.00009 Doping designed half-Heusler insulators. YONGGANG YU, XIUWEN ZHANG, LIPING YU, University of Colorado, Boulder, CO, FENG YAN, A. NAGARAJA, T. O. MASON, Northwestern University, Evanston, IL, ALEX ZUNGER, University of Colorado, Boulder, CO — The 18-valence electron 1:1:1 compounds of the type III-X-V, IV-X-IV, IV-IX-V and V-IX-IV include thermoelectric materials, topological insulators, and recently a high mobility $p$-type transparent conductor TaRbGe (arXiv:1406.0872), yet their intrinsic doping trends are poorly known or understood. Using the “modern theory of doping” that addresses via DFT and HSE the thermodynamic formation energies and the DFT-corrected transition levels in the gap, we find the following interesting trends: (1) High atomic number compounds such as TaRbGe made of metallic elements can surprisingly have a large band gap (direct) of $\sim$ 2.5 eV. (2) Half-Heusler such as $\text{A}^{(IV)}\text{B}^{(II)}\text{C}^{(IV)}$ is naturally n-type if its DFT calculated chemical stability field resides within the A-rich or B-rich domain of the stability triangle, while it is n-type within the C-rich domain. Such calculations provide a good metric. (3) When the B atom $[1, 4, 1, 4, 1, 4]$ is as large as Ir or Pt, the compound prefers p-type because the C-on-A antisite [such as Ge$_3$Zn$_{13}$] is a shallow acceptor producing holes yet the hole-killer donor of B-interstitial is unfavorable. (4) When B=N or Co, the compound favors n-type due to the dominance of B-interstitial defects (e.g., TiCoSb). We will show the calculated leading defect types and the dependence of carrier concentrations on chemical conditions for newly predicted half-Heusler insulators. This study is supported by DOE, Office of Science, Basic Energy Science, MSE division grant to CU Boulder.
Trends of semiconductivity in 3d oxides^1. STEPHAN LANY, NREL — Open shell transition metal oxides are usually described as Mott insulators, which are often viewed as being disparate from semiconductors. Based on the premise that the presence of a Mott gap and semiconductivity are not mutually exclusive, this work reviews electronic structure calculations on the binary 3d oxides, so to distill trends and design principles for semiconducting transition metal oxides. This class of materials possesses the potential for discovery, design, and development of novel functional semiconducting compounds, e.g., for energy applications. This presentation gives an overview for the band-structure trends of 3d oxides with special attention on the hybridization between the 3d crystal field symmetries with the sp bands, and on how this interactions affect the effective masses and the likelihood of self-trapping of electrons or holes.

^1Supported by DOE-SC-BES as part on an Energy Frontier Research Center.

Discovery of earth abundant light absorbers for solar water splitting: Mn,V₂O₇ and beyond^1. QIMIN YAN, Molecular Foundry, Lawrence Berkeley National Laboratory, PAWL F. NEWHOUSE, California Institute of Technology, GUO LI, JIE YU, WEI CHEN, KRISTIN PERSSON, Lawrence Berkeley National Laboratory, JOHN GREGOIRE, California Institute of Technology, JEFFREY NEATON, Lawrence Berkeley National Laboratory — Utilizing a first-principles data driven discovery approach with high-throughput computations and machine learning techniques, we screen for transition metal oxide (TMO) compounds with low band gaps and optimal band edges for solar water splitting applications. Combining the computational screening with the high-throughput experimental synthesis efforts, we identify the complex oxide β-Mn₂V₂O₇ as exhibiting a band gap and band edges that are near optimal for photocatalytic water splitting. Experiments, corroborated by theory, indicate that β-Mn₂V₂O₇ has a near-direct band gap near 1.8 eV. Our calculations further reveal a valence band maximum composed of mixed O-p/Mn-d states, and a conduction band maximum of V d-character, leading to dipole-allowed direct transitions at the band edges. Photoelectrochemical measurements indicate appreciable photocurrent from Mn₂V₂O₇ samples, corroborating our predictions. We further discuss design principles for guiding the discovery of more promising metal oxides with optimal band energetics for solar fuels applications.

^1This work was supported by the DOE through the Materials Project and the Joint Center for Artificial Photosynthesis. Computational resources provided by NERSC.

Theoretical prediction of stable tin oxides: stoichiometry, electronic structure and possible applications. JUNJIE WANG, NAOITO UMEZAWA, National Institute for Materials Science, THEORETICAL DESIGN OF ENVIRONMENTAL REMEDIATION MATERIALS TEAM — We have carried out a computational materials search for stable crystal phases of tin oxides in different composition ratios under ambient pressure condition. By employing density-functional theory calculations combined with evolutionary algorithm, we have identified several thermodynamically stable phases of tin oxides and investigated their dynamical stabilities by computing phonon vibration frequencies. We revealed the mechanism of determining the electronic structures of tin oxide crystals/van der Waals heterostructures through a systematic computational study of chemical bonding, band structure and Bader charges. Based on our theoretical analysis, we demonstrated that the predicted structures can lead to a desirable band structure for photocatalytic hydrogen evolution from water solution. Therefore, the tin oxides proposed in the present work have great potential as an abundant, cheap and environmentally-benign solar-energy conversion catalyst.

Pentahexoctite: A New Two-dimensional Allotrope of Carbon. ADITYA MANJANATH, Centre for Nano Science and Engineering/Materials Research Centre, Indian Institute of Science, BABU RAM SHARMA, ABHISHEK K. SINGH, Materials Research Centre, Indian Institute of Science — Structures with carbon atoms can be arranged in various shapes (polygons) that exhibit unique properties. This has spawned search in exploring such newer allotropes across dimensions. Although research has been extensive in bulk graphitic structures, there are several 2D allotropes that are yet to be unearthed. Here, we report a new allotrope consisting of 5-6-8 rings of carbon atoms, named as “pentahexoctite.” This sp² hybridized 2D allotrope has mechanical strength comparable to graphene. Electronically, the sheet is metallic with direction-dependent flat and dispersive bands at the Fermi level. It serves as a precursor for a stable 1D nanotubes with chirality-dependent electronic and mechanical properties. With these unique properties, the pentahexoctite sheet is another exciting addition to the family of robust novel 2D allotropes of carbon.

Monday, March 2, 2015 8:00AM - 11:00AM — Session A17 DMP: Focus Session: Carbon Nanotubes & Related Materials: Growth, Separation, and Assembly 102AB — Andrew Rinzler, University of Florida

Modulating diameter of single-walled carbon nanotubes in alcohol catalytic chemical vapor deposition. RONG XIANG, KEHANG CUI, JIE YU, HUA AN, XIAO CHEN, SHOHEI CHIASHI, SHIGEO MARUYAMA, Department of Mechanical Engineering, the University of Tokyo — Modulating the diameter of a single walled carbon nanotube (SWNT) is essential for its applications in optical and electronic devices. We demonstrate that the average diameter of vertically aligned SWNTs can be successfully reduced from 2.5 to 1.2 nm by changing catalyst component ratio in a Co/Mo bimetallic system, no matter the catalyst is dip-coated or spray-coated onto a substrate. Meanwhile, the diameter can be further reduced after replacing the conventional ethanol carbon source by acetonitrile. Recently, Cu is found to be effective in reducing diameter of mechanical and dispersive bands at the Fermi level. It serves as a precursor for a stable 1D nanotubes with chirality-dependent electronic and mechanical properties.

Ethanol decomposition on transition metal nanoparticles during carbon nanotube growth: ab initio molecular dynamics study. YASUSHI SHIBUTA, The University of Tokyo, KOHEI SHIMAMURA, Kumamoto University, TOMOYA OGURI, The University of Tokyo, RIZAL ARIFIN, FUUYUKI SHIMOJO, Kumamoto University, SHU YAMAGUCHI, The University of Tokyo — The growth mechanism of carbon nanotubes (CNT) has been widely discussed both from experimental and computational studies. Regarding the computational studies, most of the studies focuses on the aggregation of isolate carbon atoms on the catalytic metal nanoparticle, whereas the initial dissociation of carbon source molecules should affect the yield and quality of the products [1]. On the other hand, we have studied the dissociation process of carbon source molecules on the metal surface by the ab initio molecular dynamics simulation [2,3]. In the study, we investigate the ethanol dissociation on Pt and Ni clusters by ab initio MD simulations to discuss the initial stage of CNT growth by alcohol CVD technique. [1] Y. Shibuta, Diamond and Related Materials, 20 (2011) 334-338. [2] T. Oguri, K. Shimamuray, Y. Shibuta, F. Shimojo, S. Yamaguchi, J. Phys. Chem. C 117 (2013) 9983. [3] T. Oguri, K. Shimamuray, Y. Shibuta, F. Shimojo, S. Yamaguchi, Chem. Phys. Lett., 595-596 (2014) 185.
variety of feedstock materials. Conditions, collapsed BN nanotubes (i.e., nanoribbons), and closed shell BN capsules (i.e., nanococoons) are also obtained. The process is adaptable to a large system has been developed and used to produce high-quality boron nitride nanotubes (BNNTs) at continuous production rates of 35 g/h. Under suitable conditions, the graphene is tuned through precise feedstock application. Through careful materials synthesis, the interfaces of these hybrid carbon nanotube – graphene systems are investigated through ultra-high resolution electron microscopy. As a result the graphene embryos incorporate in their hexagonal network various polygons to accommodate the curved 3D geometry that initiates cap formation following by elongation of the circumferential rims. Based on these results, also on the census of nanotube caps and the fact that given cap fit only one nanotube wall, we consider carbon cap responsible for the helicity of carbon nanotube. This understanding could provide new avenues towards engineering particles to explicitly accommodate certain helicities via exploitation of the angular distribution of catalyst adjacent facets. Our recent progresses in production of carbon nanotubes, nanotube reinforced composites and their potential applications also will be presented.

9:36 AM A17.00007 Crystallographic growth and alignment of carbon nanotubes on few-layer graphene, ARAM ARASH, PATRICK D. HUNLEY, MOHSEN NASSERI, MATTHIAS J. BOLAND, ABHISHEK SUNDARARAJAN, BETHANY M. HUDAK, BETH S. GUITON, DOUGLAS R. STRACHAN, Univ of Kentucky — Hybrid carbon nanotube and graphene structures are emerging as an exciting material system built from a common sp2 carbon backbone. Such hybrid systems have promise for use in improving the performance of energy storage and high-speed electronic applications. Towards the attainment of such hybrid materials, the catalytic growth and crystallographic alignment of these integrated structures are investigated along with the atomic-scale features of their interfaces. The catalytic activity of nanoparticles to form carbon nanotubes on the surface of few-layer graphene is tuned through precise feedstock application. Through careful materials synthesis, the interfaces of these hybrid carbon nanotube – graphene systems are investigated through ultra-high resolution electron microscopy.

9:48 AM A17.00008 Sealed Synthesis of Boron Nitride Nanotubes, Nanoribbons, and Nanococones Using Direct Injection into an Extended-Pressure, Inductively-Coupled Thermal Plasma, AIDIN FATHALIZADEH, THANG PHAM, WILLIAM MICKELSON, ALEX ZETTL, Department of Physics, University of California at Berkeley; Materials Sciences Division, Lawrence Berkeley National Laboratory — A variable pressure (up to 10 atm) powder or gas injection inductively coupled plasma system has been developed and used to produce high-quality boron nitride nanotubes (BNNTs) at continuous production rates of 35 g/h. Under suitable conditions, collapsed BN nanotubes (i.e., nanoribbons), and closed shell BN capsules (i.e., nanococones) are also obtained. The process is adaptable to a large variety of feedstock materials.
10:00AM A17.00009 Electronic and optoelectronic devices based on chirality-enriched wafer-scale single-wall carbon nanotube thin films, WEILU GAO, XIAOWEI HE, LIJUAN XIE, QI ZHANG, ECE Department, Rice University, ERIK HAROZ, STEPHEN K. DOORN, Los Alamos National Laboratory, JUNICHIRO KONO, ECE Department, Rice University — The unique and rich material properties of single-wall carbon nanotubes (SWCNTs) make them attractive for nano-electronic and optoelectronic applications. Slight changes in tube diameter and wrapping angle, defined by the chirality indices \((n,m)\), can dramatically modify the bandstructure, which can be utilized for designing devices with tailored properties. However, it remains to be a challenge to fabricate macroscopic, single-chirality devices. Here, we introduce a simple way of producing chirality-enriched wafer-scale SWCNT films by combining recently developed solution-based polymer-modified sorting method\(^1\) and vacuum filtration. The produced thin films can be easily transferred onto any substrate to have a CMOS compatible wafer. We fabricated a transistor of \((6,5)\)-enriched SWCNTs with an on/off ratio \(>10^{11}\). Large-scale photothermoelectric-effect-based and photovoltaic-effect-based photodetectors made of \((6,6)\)- and \((6,5)\)-enriched films, respectively, will also be discussed.

\(^1\)C. Y. Khripin et al., JACS 18, 6822 (2013)

10:12AM A17.00010 Single Chirality Resolution Separation of Single-Wall Carbon Nanotubes up to 1.7+ nm in Diameter using Aqueous Two-Phase Extraction, JEFFREY FAGAN, National Institute of Standards and Technology — The recent development of aqueous two-phase extraction (ATPE) as a method for separating single-wall carbon nanotubes (SWCNTs) provides a scalable method for isolating many individual species of SWCNT via solution processing. In this presentation I will demonstrate that the ability of ATPE is not limited to the separation of small diameter SWCNTs \(<1\text{nm}\), but enables the extraction of single metallic and semiconducting SWCNT species from plasma torch, laser ablation, electric arc and even large diameter CVD grown SWCNTs. The separation range of the technique thus extends to the isolation of individual species of nanotubes up to at least 1.7 nm in diameter, a dramatic improvement beyond previous SWCNT separation methods. Optical characterization of the refined populations, and analysis of the order of \((n,m)\) extraction with respect to the mechanism underlying the ATPE method will be presented.

10:24AM A17.00011 Molecular Dynamics Study of Surfactant Self-Assembly on Single-Walled Carbon Nanotubes (SWCNTs), FREDERICK PHELAN JR., NIST - Natl Inst of Stds & Tech — Single-walled carbon nanotubes (SWCNTs) are materials with structural, electronic and optical properties that make them attractive for a myriad of advanced technology applications. Increased adaptation of these materials requires advancement in separation techniques which enable them to be sorted with increased reliability into monodisperser fractions with respect to length and chirality. Most separation techniques currently in use rely on dispersion of tubes in aqueous solution using surfactants. This results in a colloidal mixture in which tubes are packed and individually dispersed in a surfactant shell. Understanding the structure and properties of the SWCNT-surfactant complex at the molecular level, and how this is affected by chirality, will help to improve separations processes. In this work, we study the structure and properties of SWCNT-surfactant colloidal complexes using all-atom molecular dynamics. Self-assembled structures are computed for a number of combinations SWCNT/surfactant, and also, co-surfactant mixtures for the bile salt surfactant sodium deoxycholate (DOC) and the anionic surfactant sodium dodecyl sulfate (SDS). From the radial distribution function we estimate the size of the SWCNT hydration layer, and use that information to compute the buoyant densities of unfilled tubes for a number of concentrations. Estimates of the change in hydrodynamic radius with increased surfactant packing and the binding energies of the individual surfactants are also obtained.

10:36AM A17.00012 Integration of Nanotubes, Etch Tracks, and Nanoribbons in Crystallographic Alignment, MATHIAS J. BOLAND, D. PATRICK HUNLEY, ABHISHEK SUNDRARAJAN, MOHSEN NASSERI, DOUGLAS R. STRACHAN, Univ of Kentucky — Three nanomaterial components, carbon nanotubes (CNTs), few-layer graphene (FLG), and etch tracks exposing insulating SiO\(_2\) regions, are integrated to form crystallographically-aligned nanoscale systems. These integrated systems consist of CNTs grown across nanogap etch tracks and nanoribbons formed within the FLG films as a result of chemical vapor deposition (CVD) processing. Each nanoscale component is aligned along the underlying graphene lattice, resulting in their orientations being locked into precise values, with CNTs maintaining alignment even after crossing etch tracks. The growth of aligned CNTs across nanogap etch tracks and nanoribbons suggests that integrated formations can be achieved by growing CNTs directly over nanogap etch tracks and nanoribbons. This is supported by calculations of the vibrational energy of CNTs indicating that they should be capable of maintaining atomic registry with an underlying graphene lattice as they grow across a typical etch track, in agreement with our experimental results. Thus, this work is relevant to the integration of semiconducting, conducting, and insulating nano-materials all together into precise nano-electronic systems.

10:48AM A17.00013 High stability of faceted nanotubes and fullerenes of multi-phase layered phosphorus: A computational study, JIE GUAN, ZHEN ZHU, DAVID TOMANEK, Michigan State University — We present a paradigm in constructing very stable, faceted nanotube and fullerene structures by laterally joining nanoribbons or patches of different planar phosphorene phases. Our \textit{ab initio} density functional calculations indicate that these phases may form very stable, non-planar joints. Unlike fullerenes and nanotubes obtained by deforming a single-phase planar monolayer at substantial energy penalty, we find faceted fullerenes and nanotubes to be nearly as stable as the planar single-phase monolayers. The resulting rich variety of polymorphs allows to tune the electronic properties of phosphorene nanotubes (PNTs) and fullerenes not only by the chiral index, but also by the combination of different phosphorene phases. In selected PNTs, a metal-insulator transition may be induced by strain or changing the number of walls.

\(^1\)Supported by the National Science Foundation Cooperative Agreement #EEC-0832785, titled “NSEC: Center for High-rate Nanomanufacturing.”

Monday, March 2, 2015 8:00AM - 11:00AM — Session A18 GQI DAMOP: Invited Session: Recent Advances in Quantum Algorithms

Mission Room 103A - Nathan Wiebe, Microsoft Research
oxide-metal interfaces. They are also used to address key questions associated with corrosion, thin film growth, and heterogeneous catalysis.

...becomes routine. The recently developed charge optimized many body potential (COMB) potentials have significantly enhanced our

...computational simulations of multi-phase systems is increasingly important as our ability to simulate atomic and electronic structure evolution unravels the elementary steps that constitute a chemical reaction. This approach cannot capture many interesting processes that involved excitation of electrons and its effects on the coupled electron-ion dynamics. The time scale needed to accurately resolve the evolution of electron dynamics is atto-seconds. This poses a challenge to the simulation of important chemical processes that typically take place on time scales of pico-seconds and beyond, such as reactions at surfaces and charge transport in macromolecules. We will present a methodology based on time-dependent density functional theory for electrons, and classical (Ehrenfest) dynamics for the ions, that successfully captures such processes. We will give a review of key features of the method and several applications. These illustrate how the quantum information-theoretic lower bound on the number of particles needed for the approximation to hold, asymptotically. This is joint work with Tom Wong.

1This work has been partially supported by AFOSR grant FA9550-12-1-0046.

8:36AM A18.00002 Quantum algorithms for quantum field theories1 — STEPHEN JORDAN, NIST — Ever since Feynman’s original proposal for quantum computers, one of the primary applications envisioned has been efficient simulation of other quantum systems. In fact, it has been conjectured that quantum computers would be universal simulators, which can simulate all physical systems using computational resources that scale polynomially with the system’s number of degrees of freedom. Quantum field theories have posed a challenge in that the set of degrees of freedom is formally infinite. We show how quantum computers, if built, could nevertheless efficiently simulate certain quantum field theories at bounded energy scales. Our algorithm includes a new state preparation technique which we believe may find additional applications in quantum algorithms.

1joint work with Keith Lee and John Preskill

9:12AM A18.00003 Boson Sampling for Molecular Vibronic Spectra — GIAN GIACOMO GUERRESCHI, Harvard University — Quantum computers are expected to be more efficient in performing certain computations than any classical machine. Unfortunately, the technological challenges associated with building a fullscale quantum computer have not yet allowed the experimental verification of such an expectation. Recently, boson sampling has emerged as a problem that is suspected to be intractable on any classical computer, but efficiently implementable with a linear quantum optical setup. Therefore, boson sampling may offer an experimentally realizable challenge to the Extended Church-Turing thesis and this remarkable possibility motivated much of the interest around boson sampling, at least in relation to complexity-theoretic questions. In this work, we show that the successful development of a boson sampling apparatus would not only answer such inquiries, but also yield a practical tool for difficult molecular computations. Specifically, we show that a boson sampling device with a modified input state can be used to generate molecular vibronic spectra, including complicated effects such as Duschinsky rotations.

9:48AM A18.00004 ABSTRACT WITHDRAWN —

10:24AM A18.00005 Hidden subgroups and hidden polynomials — MIKLOS SANDTA, CNRS, Université Paris Diderot and CQT, National University of Singapore — Efficient solutions for the abelian hidden subgroup problem (HSP) constitute probably the greatest success of quantum computing. As a sequel to these results, various generalizations of the abelian HSP have been investigated, such as the non abelian HSP, hidden symmetry problems, and hidden structures of higher degree. In this talk we review an interesting connection between the HSP in certain semidirect product p-groups of constant nilpotency class and the multi-dimensional univariate hidden polynomial graph problem when the degree of the polynomials is constant. Using that connection, we present an efficient quantum solution for both, based on a new randomized algorithm for solving systems of diagonal polynomial equations in finite fields.

Joint work with Gábor Ivanyos.

Monday, March 2, 2015 8:00AM - 11:00AM —

Session A19.00001 Recent advances in Ab initio Molecular Dynamics — ROBERTO CAR, Princeton University — No abstract available.

8:36AM A19.00002 Combining Molecular Dynamics and Density Functional Theory — EFTHIMIOS KAXIRAS1, Harvard University — The time evolution of a system consisting of electrons and ions is often treated in the Born-Oppenheimer approximation, with electrons in their instantaneous ground state. This approach cannot capture many interesting processes that involved excitation of electrons and its effects on the coupled electron-ion dynamics. The time scale needed to accurately resolve the evolution of electron dynamics is atto-seconds. This poses a challenge to the simulation of important chemical processes that typically take place on time scales of pico-seconds and beyond, such as reactions at surfaces and charge transport in macromolecules. We will present a methodology based on time-dependent density functional theory for electrons, and classical (Ehrenfest) dynamics for the ions, that successfully captures such processes. We will give a review of key features of the method and several applications. These illustrate how the atomic and electronic structure evolution unravels the elementary steps that constitute a chemical reaction.

1in collaboration with: G. Kolesov, D. Vinichenko, G. Tritsaris, C.M. Friend, Departments of Physics and of Chemistry and Chemical Biology

9:12AM A19.00003 Material Discovery and Design with Dynamic Charge Reactive Potentials — SUSAN SINNOTT, University of Florida — Atomic scale computational simulations of multi-phase systems is increasingly important as our ability to simulate nanometer-sized systems becomes routine. The recently developed charge optimized many body potential (COMB) potentials have significantly enhanced our ability to carry out atomic-scale simulations of heterogeneous material systems. The formalism of this potential combines variable charge electrostatic interactions with a classical analytical bond-order potential. It therefore has the capacity to adaptively model metallic, covalent, ionic, and van der Waals bonding within the same simulation cell and dynamically determine the charges on individual atoms according to the local environment. The utility of the COMB potentials is illustrated for materials design and discovery by exploring the structure, stability, mechanical properties, and thermal properties of intermetallic systems and oxide-metal interfaces. They are also used to address key questions associated with corrosion, thin film growth, and heterogeneous catalysis.
Small is Different: Nanoscale Computational Microscopy, UZI LANDMAN, School of Physics, Georgia Institute of technology — Finite materials systems of reduced sizes exhibit discrete quantized energy level spectra and specific structures and morphologies, which are manifested in unique, noncalable, size-dependent physical and chemical properties. Indeed, when the scale of materials structures is reduced to the nanoscale, emergent phenomena often occurs, that is not commonly expected, or deduced, from knowledge learned at larger sizes. Characterization and understanding of the size-dependent evolution of the properties of materials aggregates are among the major challenges of modern materials science. Computer-based classical and quantum computations and simulations are tools of discovery of nanoscale emergent behavior [1]. We highlight such behavior in diverse systems, including: (i) Atomistic simulations of nanoscale liquid jets and bridges and the stochastic hydrodynamic description of their properties [2]; (ii) Metal nanoclusters and their self-assembled superlattices exhibiting stabilities and properties originating from superatom electronic shell-closing, atom packing, and interactions between protecting ligands [3]; (iii) Electric-field-induced shape-transitions and electrorcrystalization of liquid droplets [4]; and (iv) Symmetry-breaking and formation of highly-correlated Wigner molecules between electrons in 2D quantum dots and bosons in traps [5].

Monday, March 2, 2015 8:00AM - 11:00AM
Session A20 DPOLY: Invited Session: Interfacing Experiment and Theory in Polymer Physics
Ballroom B - Bryan Boudouris, Purdue University

8:00AM A20.00001 Order and Disorder in Short Block Polymers1, FRANK S. BATES, University of Minnesota — Block polymers have captivated the interest of scientists and engineers for more than half a century. The phase behavior of this class of self-assembling soft material is well understood in the limit of infinite molecular weight, based on the self-consistent mean-field theory pioneered by Leibler. At practical molecular sizes, typically around N ≈ 1000 repeat units, fluctuation effects become highly significant in the vicinity of the order disorder transition. One-loop corrections to mean-field theory, first described by Brazovski and applied to block polymers by Fredrickson and Helfand, are not expected to be applicable in this limit. Moreover, the drive towards ever smaller domain dimensions, and the opportunity to circumvent transport limitations associated with entanglements, have motivated experiments with yet lower molecular weight block polymers, N less than 100. This presentation will describe the consequences of fluctuations and the equilibrium structural properties of short model AB diblock polymers in the symmetric (f = 1/2) and asymmetric (f → 0) regimes above and below the order-disorder transition. The consequences of fluctuations and access to equilibrium states will be described in the 1-dimensional striped (lamellar) phase and the ordering in reduced dimensions. A computer simulation with realistic molecular detail becomes feasible presenting exciting opportunities to compliment the associated theoretical challenges.

1 Research in collaboration with Sangwoo Lee, Chris Leighton and Timothy Gillard and Supported by NSF-DMR-1104368

8:36AM A20.00002 Nanocomposites with Crystalline Polymers, SANAT KUMAR, Columbia University — The creation of ordered (layered) biomimetic materials typically follows a series of steps: first mix nanoparticles with water, organize the NPs by ice templating, evaporate the ice and then back fill with metal or polymer. We propose a simple method exploiting the in situ self-assembly of a crystalline polymer in the presence of nanoparticles to facilitate this process, and provide a completely new pathway for the synthesis of biomimetic materials. A suite of complementary experimental tools are used in this analysis. In parallel, we are developing theoretical tools to a priori predict the morphologies adopted by semicrystalline polymers. The convergence of these novel experimental and theoretical developments in the venerable field of semicrystalline polymers could lead to new applications for this largest class of commercially relevant polymeric materials. With Jacques Jestin, Brian Benicewicz, Dan Zhao, Longxi Zhao

9:12AM A20.00003 Segmental Interactions between Polymers and Small Molecules in Batteries and Biofuel Purification, NITASH BALSARA, UC Berkeley — Polymers such as poly(ethylene oxide) (PEO) and poly(dimethyl siloxane) (PDMS) have the potential to play an important role in the emerging clean energy landscape. Mixtures of PEO and lithium salts are the most widely studied non-flammable electrolyte for rechargeable lithium batteries. PDMS membranes are ideally suited for purifying bioethanol and biobutanol from fermentation broths. The ability of PEO and PDMS to function in these applications depends on segmental interactions between the polymeric host and small molecule guests. One experimental approach for studying these interactions is X-ray absorption spectroscopy (XAS). Models for interpreting XAS spectra of amorphous mixtures and charged species such as salts must quantify the effect of segmental interactions on the electronic structure of the atoms of interest (e.g. sulfur). This combination of experiment and theory is used to determine the species formed in during charging and discharging lithium-sulfur batteries; the theoretical specific energy of lithium-sulfur batteries is a factor of four larger than that of current lithium-ion batteries. Selective transport of alcohols in PDMS-containing membranes is controlled by the size, shape, and connectivity of sub-nanometer cavities or free volume that form and disappear spontaneously as the chain segments undergo Brownian motion. We demonstrate that self-assembly of PDMS-containing block copolymers can be used to realistic molecular detail becomes feasible presenting exciting opportunities to compliment the associated theoretical challenges.
9:48AM A20.00004 Using multi-scale molecular simulations to guide experimental design of biomaterials for drug and DNA delivery. ARTHI JAYARAMAN, University of Delaware — In this talk I will present molecular simulations studies that guide experimental synthesis of polymers for efficient DNA delivery. Viruses, while effective at delivery and transfection of DNA, can elicit harmful immunogenic responses, thus motivating design of non-viral transfection agents. Polycations are a promising class of non-viral vectors that bind to the negatively charged DNA backbone to form a complex (polyplex) that is then internalized into the target cell. Combinatorial approaches have generated various polycations with differing DNA transfection efficiencies, but there is a need for general design guidelines that can relate the molecular features of the polycation to its DNA transfection efficiency. Using atomistic and coarse-grained molecular dynamics simulations we connect the thermodynamics of polycation-DNA binding and polyplex structure to experimentally observed transfection efficiency as a function of polycation chemistry and architecture.

10:24AM A20.00005 Ion Containing Polymers for Battery Technology. JANNA K. MARANAS, Departments of Chemical Engineering and Materials Science and Engineering, The Pennsylvania State University — Polymer electrolytes have potential for use in next generation lithium and sodium batteries. Replacing the liquid electrolyte currently used has several advantages: it allows use of high energy density solid lithium as the anode, removes toxic solvents, improves safety, and eliminates the need for heavy casings. Despite their advantages, the conductivity of solid polymer electrolytes is not sufficient for use in batteries. As a result, considerable effort towards improving conductivity and understanding mechanisms of lithium transport has taken place over the last 30 years. This talk considers the interplay of conductivity, crystallinity, local coordination and polymer dynamics in solid polymer electrolytes. Using a combination of experimental and computational technique, we propose the possibility of high charge mobility using ion aggregates and percolated nanofiller networks.

Monday, March 2, 2015 8:00AM - 11:00AM —
Session A21 GIMS: Focus Session: Advances in Scanned Probe Microscopy I: Novel Approaches and Ultrasensitive Detection
201 - Nikolai Zhitenev, National Institute of Standards and Technology

8:00AM A21.00001 Cryogen-free low temperature STM/AFM based on a closed cycle cryostat . BYOUNG CHOI, STEFEN ULRICH, RYAN MURDICK, RHK Technology, Inc, RHK TECHNOLOGY, INC. TEAM — Closed cycle cryogenic scanning tunneling microscope (CCC-STM) and atomic force microscope (AFM) will be presented. By using He heat exchange gas, thermally linked and mechanically decoupled CCC-STM/AFM enables atomically resolved microscopy and spectroscopy on various surfaces. We will present the noise measurement of the tunneling current and the thermal drift analysis. Temperature as low as 14K on the sample and the tip-sample distance fluctuation as low as 2 picometer have been achieved.

8:12AM A21.00002 Construction of a 3He Magnetic Force Microscope with a Vector Magnet . JINHO YANG, YUNWON KIM, ILKYU YANG, JUYOUNG JEOUNG, DONGWOO SHIN, DIRK WULFERDING, YOONHEE JEOUNG, HANWOONG YEOM, JEEHOON KIM, CALDES, IBS, POSTECH, Pohang, Korea — We have built a 3He magnetic force microscope (MFM) with a base temperature of 300 mK, operating in a vector magnet with the field of Z=9 T, X=2 T, Y=2 T for each axis. We employed a fiber interferometer system for detection of a cantilever motion that includes two autotcobe types of walkers for alignment between the fiber end and a cantilever tip. We apply our novel microscope to investigate unconventional magnetic materials and superconductors such as centrosymmetric skyrmmion crystals and Heavy Fermion Superconductors. We will show some preliminary MFM images in these systems.

8:24AM A21.00003 Mapping surface charge density with a scanning nanopipette . LASSE HYLDGAARD KLAUSEN, THOMAS FUHLS, FLEMMING BESENBACKER, MINGDONG DONG, Interdisciplinary Nanoscience Center, Aarhus University, Denmark — Characterisation of the surface charge density (SCD) is important in interface and colloid science, and especially local variations in SCD of biological samples are of keen interest. The surface charge of lipid bilayers governs the uptake of charged particles and guides cell-cell interactions. As the electrostatic potential is screened by high physiological salt concentrations, direct probing of the potential can only be performed at a sub nanometer distance; therefore it was impossible to directly measure the SCD under physiological conditions. Yet the charged surface attracts counter ions leading to an enhanced ionic concentration near the surface, creating a measurable surface conductivity. In this study we measure SCD using a scanning ion-conductance microscope (SICM) setup, where the electrolyte current through a nanopipette is monitored as the pipette is positioned in the vicinity of the sample. We investigate the current dependency of SCD and pipette potential using numerical solutions to Poisson and Nernst-Planck equations and characterise a complex system governed by a multitude of factors such as pipette size, geometry and charge. We then propose an imaging method and prove its feasibility by mapping the surface charge density of phase separated lipid bilayers.

8:36AM A21.00004 The SQCRMscope: Probing exotic materials with quantum gases1 . SHENGLAN QIAO, RICHARD TURNER, JACK DISCIACCA, BENJAMIN LEV, Stanford University — Microscopy techniques co-opted from nonlinear optics and high energy physics have complemented solid-state probes in elucidating exotic order manifest in condensed matter materials. Up until now, however, no attempts have been made to use modern techniques of ultracold atomic physics to directly explore properties of strongly correlated or topologically protected materials. Our talk will present the SQCRMscope, a novel Scanning Quantum Cryogenic Atom Microscope technique for imaging magnetic and electric fields near cryogenically cooled materials. With our SQCRMscope, we aim to image inhomogeneous transport and domain percolation in technologically relevant materials whose order has evaded elucidation.

1We are grateful to the Moore Foundation and the Department of Energy for their generous support.

8:48AM A21.00005 Simulated imaging of intermolecular bonds using high throughput real-space density functional calculations . ALEX LEE, The University of Texas at Austin, MINJUNG KIM, Yale University, JAMES CHELIKOWSKY, The University of Texas at Austin — Recent experimental noncontact atomic force microscopy (AFM) studies on 8-hydroxyquinoline (8-hq) assemblies have imaged distinct lines between molecules that are thought to represent intermolecular bonding. To aid the interpretation of these images, we calculate simulated AFM images of an 8-hq dimer with a CO functionalized tip using a real-space pseudopotential formalism. We examine the effects of Pauli repulsion and tip probe relaxation as explanations for the enhanced resolution that resolves these intermolecular force lines. Our study aims to compute ab initio real-space images of intermolecular interactions.
Maps are important to engineer nanomaterials in applications ranging from photovoltaics to sensing and therapeutics. Wavelengths (\(\lambda\)) near-IR probe electronic transitions in materials, providing information regarding band gap and defects while light in mid-IR probes vibrational transitions and processes.

Forces between the nc-AFM tip and specimen. We simulate images of planar organic molecules with two different approaches: 1) with a chemically inert tip and 2) with a CO functionalized tip. We find dramatic differences in the resulting images, which are consistent with recent experimental work.

Our work is supported by the DOE under DOE/DE-FG02-06ER46286 and by the Welch Foundation under grant F-1837. Computational resources were provided by NERSC and XSEDE.

Photo Thermal Induced Resonance (PTIR) is a novel technique that circumvents light diffraction by employing an AFM tip as a local detector for measuring light absorption with \(\lambda\)-independent nanoscale resolution. Our PTIR setup combines an AFM microscope with three lasers providing \(\lambda\)-tunability from 500 nm to 1600 nm continuously. The AFM tip transduces locally the sample thermal expansion induced by light absorption into large cantilever oscillations. Local absorption spectra (for electronic, vibrational, or functional) and maps are obtained recording the amplitude of the tip deflection as a function of \(\lambda\) and position, respectively. The working principles of the PTIR technique will be described first, and nano-patterned polymer samples will be used to evaluate its lateral resolution, sensitivity, and linearity. Results show that the PTIR signal intensity is proportional to the local absorbed energy suggesting applicability of this technique for quantitative chemical analysis at nanoscale, at least for thin (less than 1000 nm thick) samples. Additionally, a \(\lambda\)-independent resolution of 20 nm is demonstrated through the work of the talk. In the second part of the talk, PTIR will be applied to image the dark plasmonic resonance of gold asymmetric split ring resonators (A-SRRs) in the mid-IR. Additionally, the chemically-specific PTIR signal will be used to map the near-field absorption enhancement of PMMA coated A-SRRs, revealing hot-spots with enhancement factors up to \(\approx 30\). PTIR has broad applicability; recent examples from my lab include the characterization of chemically heterogeneous domains in metal-organic frameworks crystals and solar cells materials.

NC-AFM identification of different aluminum atoms on \(\text{Al}_2\text{O}_3/\text{NiAl}(110)\) surface was supported by APVV-0207-11 and VEGA (2/0007/12) projects.

Improving Nano-MRI Spatial Resolution with Phase Multiplexing was supported by National Basic Research Programs of China, National Science Foundation of China.

Direct visualization of concerted proton tunneling in a water nanocluster was supported by National Basic Research Programs of China, National Science Foundation of China.

Connecting the Tips of a Millikelvin Dual-Tip STM was supported by National Basic Research Programs of China, National Science Foundation of China.

Asymmetric superconducting quantum interference devices for suppression of phase diffusion in small Josephson junctions was supported by National Basic Research Programs of China, National Science Foundation of China.

Connecting the Tips of a Millikelvin Dual-Tip STM is a novel technique that recombinates, spectrally-separated, local electron tunneling and thermal expansion to measure the sample chemical potential with \(\lambda\)-independent nanoscale resolution. Our PTIR setup combines an AFM microscope with three lasers providing \(\lambda\)-tunability from 500 nm to 1600 nm continuously. The AFM tip transduces locally the sample thermal expansion induced by light absorption into large cantilever oscillations. Local absorption spectra (for electronic, vibrational, or functional) and maps are obtained recording the amplitude of the tip deflection as a function of \(\lambda\) and position, respectively. The working principles of the PTIR technique will be described first, and nano-patterned polymer samples will be used to evaluate its lateral resolution, sensitivity, and linearity. Results show that the PTIR signal intensity is proportional to the local absorbed energy suggesting applicability of this technique for quantitative chemical analysis at nanoscale, at least for thin (less than 1000 nm thick) samples. Additionally, a \(\lambda\)-independent resolution of 20 nm is demonstrated through the work of the talk. In the second part of the talk, PTIR will be applied to image the dark plasmonic resonance of gold asymmetric split ring resonators (A-SRRs) in the mid-IR. Additionally, the chemically-specific PTIR signal will be used to map the near-field absorption enhancement of PMMA coated A-SRRs, revealing hot-spots with enhancement factors up to \(\approx 30\). PTIR has broad applicability; recent examples from my lab include the characterization of chemically heterogeneous domains in metal-organic frameworks crystals and solar cells materials.

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Nano-MRI Spatial Resolution with Phase Multiplexing was supported by National Basic Research Programs of China, National Science Foundation of China.
10:36AM A21.00012 Kelvin probe force microscopy: imaging open-circuit voltage in optoelectronic devices. ELIZABETH TENNYSON, Materials Science and Engineering, Univ. of Maryland, JOSEPH GARRETT, Physics, Univ. of Maryland, JESSE FRANTZ, JASON MYERS, U.S. Naval Research Laboratory, ROBEL BEKELE, University Research Foundation, JASBINDER SANGHERA, U.S. Naval Research Laboratory, JEREMY MUNDAY, Electrical and Computer Engineering, Univ. of Maryland, MARINA LEITE, Materials Science and Engineering, Univ. of Maryland — Scanning probe microscopy has been successfully implemented to probe the electrical characteristics of optoelectronic devices. Currently, a method that directly correlates measured signals to device performance is missing. We implement illuminated Kelvin probe force microscopy (KPFM) to spatially resolve the open-circuit voltage of optoelectronics with nanoscale resolution, 5 orders of magnitude better than previous methods. In illuminated-KPFM, the surface photovoltage, is the difference between the contact potential difference under illumination and in the dark, and proportional to the Fermi level splitting. We apply our imaging method to a variety of solar cells and find that the open-circuit voltage in some materials varies locally by >0.2 V, suggesting the spatial variation of non-radiative recombination strongly affects performance. A detailed examination of possible topography pick-up was excluded by measuring samples with modified surface morphology and considering the tip-sample separation dependence of the signal. This novel metrology enables new insights into the loss mechanisms that hinder solar cells and provides a new platform to image device performance with nanoscale resolution.

10:48AM A21.00013 A method for correcting out-of-plane, fast time scale positional drift in atomic force microscopy1 . JOHN P. WHEELER, PARDEEP S. BANWAIT, ISAAC D. ROHRER, GREG A. HAMILTON, KELLY A. SHAW, MICHAEL C. LEOPOLD, MATTHEW L. TRAWICK, University of Richmond — We describe a method for correcting atomic force microscopy images that have been affected by random fluctuations (fast time scale positional drift) in measurements along the axis perpendicular to the sample plane. These fluctuations, typically manifested as random horizontal streaks or bands across the image, have several sources, including electrostatic charging and the transfer of material between the sample and the tip. Our correction method involves scanning a second, partial image after each full image scan, and applying an offset correction to each individual scan line in both images in order to minimize the statistical discrepancy between them. This method supersedes the widely used “flattening” algorithm, which can destroy valid height information and can create additional image artifacts.

8:00AM A22.00001 Gapped collective modes in quantum solids, DANIEL AROVAS, University of California - San Diego, SNIR GAZIT, ASSA AUERBACH, HELOISE NONNE, DANIEL PODOLSKY, Technion - Israel Institute of Technology — The harmonic theory of crystals predicts that the excitation spectrum of a Bravais lattice, i.e. a mono-atomic crystal structure, consists solely of gapless acoustic phonons. Surprisingly, an inelastic Neutron scattering experiment of solid He4 BCC phase has uncovered a zero momentum gapped excitation [1]. Motivated by the large zero point motion in the BCC phase, we describe the crystal through a phenomenological effective Ginzburg-Landau field theory of a charge density wave order parameter. We find that the excitation spectrum contains gapped modes which correspond to fluctuations of the charge density wave order parameter amplitude. We characterize the modes according to their symmetry and compute their visibility in Neutron scattering experiments. To further validate our results, we calculate the scalar susceptibility by means of an ab-initio quantum Monte Carlo simulation. We find a gapped resonance in good agreement with the experimental measurements. Our results motivate future studies of the excitation spectrum of quantum solids. [1] T. Markovich, E. Polturak, J. Bossy, and E. Farhi, Phys. Rev. Lett. 88, 195301 (2002)

8:12AM A22.00002 Strong-coupling and the stability of crystalline order in superfluid 3He films1 . JOSHUA WIMAN, J. A. SAULS, Northwestern University — In a film of thickness D, weak-coupling theory for p-wave, spin-triplet pairing predicts a “stripe” phase that spontaneously breaks translational symmetry in the plane of the film[2]. NMR on superfluid 3He confined in a slab has so far failed to detect any signature of the stripe phase, and the A-B transition is observed at lower temperatures than predicted by weak-coupling theory[2]. We report calculations of the phase diagram for 3He films based on Ginzburg-Landau (GL) theory that includes strong-coupling effects via experimentally estimated β parameters[3]. At low pressures GL theory predicts the A-stripe phase transition, for small D, to be significantly suppressed compared to weak-coupling. For large D, the stripe transition is eliminated in favor of an A-B transition at lower temperatures than in weak-coupling. At higher pressures the stripe phase is predicted to be stable only at very low temperatures, outside the expected applicability of the strong-coupling GL theory. Our results suggest that the discrepancy between experiment and weak-coupling theory likely results from strong-coupling effects.

8:24AM A22.00003 Is there a stable commensurate solid phase in the second 4He layer on graphite? — path integral Monte Carlo study, JEONGHWAN AHN, HOOKYUNG LEE, YONGKYUNG KWON, KonKuk Univ — Existence of a stable commensurate structure in the second 4He layer on graphite has been a subject of intensive experimental and theoretical studies because of its implication in the possible realization of two-dimensional supersolidity. Earlier path-integral Monte Carlo (PIMC) calculations of Pierce and Manousakis predicted a stable C_{17} commensurate structure above the first-layer 4He atoms fixed at triangular lattice sites [1], but Corboz et al. later showed that no commensurate phase was stable when quantum dynamics of the first-layer 4He atoms was incorporated in the PIMC calculations [2]. On the other hand, recent heat capacity measurements of Nakamura et al. provided a strong evidence for a commensurate solid in the second 4He layer over an extended density range [3]. Motivated by this, we have performed new PIMC calculations for the second helium layer on graphite. Unlike previous PIMC calculations where a laterally-averaged one-dimensional substrate potential was used, we here employ an anisotropic 4He-graphite potential described by a sum of the 4He-C pair potentials. With this fully-corrected substrate potential we make more accurate description of quantum dynamics of the first-layer 4He atoms and analyze its effects on the phase diagram of the second layer.

1Supported by NSF Grant DMR-1106315.

8:36AM A22.00004 High temperature superfluidity in a commensurate phase of adsorbed \(^{4}\text{He}\)

RAINIA OLSEN, Oak Ridge National Laboratory — It is well known that a substrate can have a significant effect on the phase diagram of adsorbed atoms. For instance, \(^{4}\text{He}\) adsorbed on graphene forms a solid structure commensurate (aligned) with the substrate which has a density much smaller than the density of bulk \(^{4}\text{He}\). This occurs because the underlying periodic potential stabilizes the solid by opening an energy gap between the commensurate solid and the longest wavelength lattice excitations which would otherwise change the structure. Here we report calculations of superfluidity for \(^{4}\text{He}\) in a periodic potential with variable lattice spacing, using a Bogoliubov transformation to calculate the energy spectrum of the excitations. We find a gap in energy between the superfluid state and the longest wavelength excitations. When this superfluid energy gap is large enough, there should be few excitations even at temperatures above the lambda point, where superfluidity is not observed in the bulk. This occurs only when the lattice spacing of the substrate corresponds to the lattice spacing of bulk \(^{4}\text{He}\). In contrast, when the substrate periodicity is too large, as is the case with graphene, a classical commensurate solid is expected instead. We discuss other possible materials.

8:48AM A22.00005 Dislocation structure and mobility in hcp \(^{4}\text{He}\)

MAURICE DE KONING, EDGAR JOSUÉ LANDINEZ BORDA, UNICAMP-Univ de Campinas, WEI CAI, Stanford University — We present results of Path-integral Monte Carlo simulations of the basal-plane screw dislocation in hcp \(^{4}\text{He}\) at temperatures below 1K. First, our results show that, due to the extremely low stacking-fault energy, its core is widely extended, dissociating into a pair of Shockley partials separated by a ribbon of stacking-fault. Second, our findings suggest that the stress required to initiate dislocation motion is different from zero and of the order of 0.1 bar. Finally, we discuss the role of \(^{3}\text{He}\) impurities.

9:00AM A22.00006 Shear modulus of solid \(^{3}\text{He}\) in the bcc and hcp phases

JOHN BEAMISH, ZHIGANG CHENG, FABIEN SOURIS, University of Alberta — The shear modulus of solid hcp \(^{4}\text{He}\) decreases significantly at temperatures above 100 mK [1, 2]. This is due to dislocations which are localized when pinned by \(^{4}\text{He}\) impurities at low temperature but become mobile when \(^{3}\text{He}\) impurities “evaporate” at high temperature. The unpinned dislocations move freely in the basal plane of the hcp structure. This produces anisotropic and extraordinarily large softening of the shear elastic constant C_{44}, an effect referred to as “giant plasticity” [2]. Previous measurements [3] on solid \(^{3}\text{He}\) showed similar shear modulus changes in the hcp phase but not in the bcc phase. Here, we report new shear modulus measurements in both the bcc and hcp phases. These show a similar shear modulus anomaly in the bcc phase, indicating that dislocation softening is not unique to hcp phase of helium. We compare our results for bcc and hcp \(^{4}\text{He}\) to those \(^{4}\text{He}\), and discuss the roles that lattice structure and quantum statistics play in dislocation motion and impurity pinning.


Research supported by NSERC Canada

9:12AM A22.00007 Impact of dislocations on the structure of solid helium

HANS LAUTER, Oak Ridge National Lab, JOHN GOODKIND, USCD San Diego, KENNETH HERWIG, Oak Ridge National Lab, ECKHARD KROTSCHECK, University at Buffalo, EFIM KATS, Institut Laue Langevin, ANDREY PODLEŞNYAK, ANDREI SAVICI, DIALLO SOULEYMANE, JUSTIN CAREMICHAEL, Oak Ridge National Lab — Uncommon phonon spectra were obtained from solid helium below 1.3K and at pressures near 30 bar. Rapid cooling using the blocked capillary method created stressed solid helium in non-equilibrium state. Using inelastic neutron scattering, we disclosed the absence of Bragg-scattering combined with the presence of a phonon-gap, a phenomenon revealing the absence of long-range crystalline order. The energy of the gap is close to the value of a thermal activation energy measured by ultrasonic attenuation in unstrained solid \(^{4}\text{He}\) crystals. The dispersion of the phonons shows point-like intensities interpreted as signature of finite-edge length dislocations. The range and shape of the strain field perpendicular to the dislocation line was identified discerning excitations related to the fluttering mechanism [2]. These findings give new input to the discussion of a dislocation network in view of the shear modulus in distorted solid \(^{4}\text{He}\) [3, 4].


This work was supported by the Scientific User Facilities Division, BES, DOE

9:24AM A22.00008 Interaction of ultrasound and torsional oscillation in solid \(^{4}\text{He}\)

IZUMI IWASA, Kanagawa University, Kanagawa Japan, JOHN GOODKIND. Department of Physics, University of California San Diego, La Jolla, CA 92093, HARRY KOJIMA, Serin Physics Laboratory, Rutgers University, Piscataway, NJ — A new cell for studying ultrasound (10 MHz) propagation and torsional oscillation (1013 Hz) in solid \(^{4}\text{He}\) was constructed. Improvements were made in the design of the spacer for the quartz transducers and the diameter of the torsion rod containing helium fill hole to reduce the effects of the shear modulus of the solid \(^{4}\text{He}\) sample on the torsional oscillator response. Sudden shifts in both the sound propagation velocity and attenuation are observed below 100 mK. The detailed response depends on the ultrasound excitation level and thermal history. Increase in torsional oscillator frequency is observed at nearly the same temperature as where the sound propagation velocity shifts occur. At temperatures below 50 mK, changes in the ultrasound excitation level induce changes in the torsional oscillator frequency. Interpretation of these results in terms of He-3 impurity being trapped on dislocation lines will be discussed.

NSF grant DMR-1005325.

9:36AM A22.00009 Frequency-dependent Study of Ultrapure Solid \(^{4}\text{He}\) by Using Rigid Double-pendulum Torsional Oscillator

JAEWON CHOI, JAEHO SHIN, EUNSEONG KIM, Korea Advanced Institute of Science and Technology — The physical origin of the period drop found in the torsional oscillator (TO) containing solid \(^{4}\text{He}\) was previously interpreted as the appearance of supersolidity[4]. The current consensus is that the increase in the shear modulus leads to the period anomaly. Further studies show that the stiffening effect in TO can be simplified if a TO is not properly design in TO. High purity solid \(^{4}\text{He}\) sample (0.6ppb) was grown by the blocked capillary method. The resonant period of TO starts to decrease from the empty cell data at 80mK. The ratio of the resonant period changes to the total mass loading are \(3.8 \times 10^{-5}\) and \(2.6 \times 10^{-4}\) for 1st and 2nd mode, respectively. Unlike recent experiment[1] we could not found a frequency-independent period drop. The upper bound for the putative supersolid fraction is less than \(4 \times 10^{-6}\). The dissipation peak accompanied with the period drop was also analyzed with Cole-Cole plot and \(\omega \tau\) plot. We conclude that major contribution for the anomalous TO responses comes from the elastic effect.

10:00AM A22.00011 Mass Superflux in Solid Helium: Dependence on Temperature, Density and $^3$He Impurity Concentration, YEGOR VEKHOV, ROBERT HALLOCK, Univ. of Mass. - Amherst — The mass flux, $F$, induced to flow through solid $^4$He by means chemical potential differences imposed by the fountain effect in the range $25.6 < \rho < 26.4$ bar rises with falling temperature below 650 mK. At a lower temperature, $T_\text{d}$, the flux drops sharply. The behavior of the flux above $T_\text{d}$ is consistent with the presence of a bosonic Luttinger liquid. We report a study $F$ as a function of $^3$He concentration, $\chi$ (0.17 – 220) ppm, and explore the effect of level of $^3$He impurities on $T_\text{d}$. We find a strong reversible reduction of the flux, typically complete within a few mK. We find that $T_\text{d}$ is an increasing function of $\chi$ and the $T_\text{d}(\chi)$ dependence differs somewhat from the predictions for bulk phase separation. It is possible that the cores of edge dislocations carry the flux. In such a case the flux may be extinguished by the decoration of the cores or dislocation intersections by $^4$He.

1Work supported by NSF DMR 12-05217.

10:12AM A22.00012 Mass Superflux in Solid Helium: What Limits the Flux? $^1$, ROBERT HALLOCK, YEGOR VEKHOV, Univ. of Mass. - Amherst — The thermo-mechanical effect in superfluid helium is used to create a chemical potential difference, $\Delta \mu$, across a superfluid-filled vertical Vycor rod. This rod separates a bulk liquid superfluid helium reservoir, $R_1$, on the top of the Vycor at $T_1 = 1.46 – 1.51$ K and solid hcp $^4$He on the bottom at $T_\text{C} = 0.1 – 0.8$ K. Two in situ capacitance pressure gauges, $C_1$ and $C_2$, are placed at the ends of the horizontal cylindrical solid helium sample (1.84 cm$^3$, 25.9 – 26.4 bar) and located at different distances from the position of the Vycor rod in the solid helium, 10 and 31 mm, respectively. A $T_\text{d}$ decrease/increase changes $\Delta \mu$ and leads to a solid helium pressure increase/decrease detected by both $C_1$s. The rate of pressure change is slower at the further gauge, $C_2$, than at the nearer one, $C_1$. This behavior is interpreted as due to the presence of a mass flux bottleneck inside the solid helium sample. We believe, e.g. in the case of a $T_\text{d}$ decrease, that helium atoms emerge from the Vycor rod, perhaps migrate along the superfluid core of edge dislocations in solid helium and adsorb on them. This is the so-called "syringe-effect" or superclimb of edge dislocations. The dependence on temperature will be discussed.

1Work supported by NSF DMR 12-05217.

10:24AM A22.00013 Quantum Plasticity and Supersolid Response in Helium-4$^1$, ANATOLY KUKLOV, Department of Physics & Engineering, College of Staten Island, CUÑY, LODE POLLET, Department of Physics, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, University of Munich, NIKOLAY PROKOF'EV, BORIS SVISTUNOV, Department of Physics, University of Massachusetts, Amherst — We argue that the three key phenomena recently observed in solid $^4$He — mass supertransport, anomalous isochoric compressibility (syringe effect), and giant plasticity—are closely related to each other: 1) the characteristics of an interconnected network of tilted quantum-rough gliding and superclimbing dislocations. Such roughness is guaranteed, on one hand, by tilting of dislocations in Peierls barrier, and, on the other, by fast tunneling of kinks and jogs. Quantum rough gliding or superclimbing dislocation features 1D quantum liquid of kinks or jogs, respectively. As immediate implications of this connection several predictions follow: In the absence of $^3$He impurities, the syringe effect and giant plasticity persist down to $T = 0$; the dynamical low-frequency syringe and giant-plasticity responses are dispersionless; and similarly to giant plasticity but without direct relationship to the supertransport along the dislocation cores, $^3$He impurities should suppress the syringe effect partially or completely at appropriately low temperatures.

1This work was supported by the National Science Foundation under the grants PHY-1314469 and PHY-1314735, and by FP7/ Marie-Curie Grant No. 621918 and FP7/ERC Starting Grant No. 306897.

10:36AM A22.00014 Helium-4 superfluid density; action-at-a-distance effects $^1$, STEPHEN R.D. THOMSON, FRANCIS M. GASPARINI, The State University of New York at Buffalo — We report results from experiments with $^4$He confined in two concentric 277 nm thick planar regions that are connected across a ring which forms a thin film weak link 33 nm thick. Measurements of the superfluid fraction within rings of varying widths have shown that the planar regions affect the film in the ring over distances much longer than the correlation length $\xi$. These results are analogous to those reported for a different geometry of both the specific heat and superfluid fraction [1]. To investigate the wide dependence of this proximity effect we have performed measurements with rings that are 8, 17, 40 and 100 $\mu$m wide. We will discuss our method of measurement and a possible mechanism for the long range action-at-a-distance effect suggested in [2] for the 2D Ising system.


1This work was supported by the NSF grant DMR-1101189 and utilized The Cornell Nanoscale Science and Technology Facility, Project No. 526-94.

10:48AM A22.00015 Mass transport in micrometer size solid $^4$He $^1$, ARIEL HAZIOT, DUK YOUNG KIM, MOSES CHAN, The Pennsylvania State University — We have studied the transport of $^4$He atoms through a thin solid $^4$He slab of $\sim$50 $\mu$m thick sandwiched between two superfluid ‘electrodes’ of liquid helium filled Vycor rods. The geometry of the experiment is similar to the configuration used by Hallock and collaborators at the University of Mass [1,2] however the thickness of our solid sample is about 8000 times thinner than the UMmass solid sample. The observed mass flow through the solid slab shows the characteristic of a superflow and the rate is more than a 1000 times higher than the UMass experiment. The mass flow rate decreases strongly with the pressure to vanish around 31 bar and it shows an hysteresis loop as a function of pressure. In contrast to the UMass experiment, the mass flow rate in our experiment decreases weakly and smoothly with increasing temperature between 30 mK and 1.2 K. In addition, we found no dependence on the $^3$He concentration from 3 ppm to 1%.


$^1$Fundings provided by NSERC Canada and by ERC (AdG 247258-SUPERSOLID)
8:00AM A23.00001 Vertical Transport in Ferroelectric/Superconductor Heterostructures\(^1\),
LAURA BEGON-LOURS, JUAN TRASTOY, ROZENN BERNARD, ERIC JACQUET, CECILE CARRETERO, KARIM BOUZEHOUANE, STEPHANE FUSIL, VINCENT GARCIA, STEPHANE XAVIER, STEPHANIE GIROD, CYRILE DERANLOT, MANUEL BIBES, AGNES BARTHELEMY, JAVIER E. VILLEGAS, Unite Mixte de Physique CNRS/Thales, France — We study electric field-effects in superconducting films by measuring vertical transport in ferroelectric/superconductor heterostructures. These are based on ultrathin (4 to 8 nm thick) BiFeO\(_3\)-Mn grown on YBa\(_2\)Cu\(_3\)O\(_7\) by pulsed laser deposition. Nanoscale contacts are defined on the BiFeO\(_3\) via a series of nanofabrication steps which include e-beam lithography, metal deposition (Nb or Co capped with Pt) and lift-off. Conductive-tip atomic force microscopy and piezoresponse force microscopy are used to characterize the transport across the ferroelectric barrier as a function of its polarization (up/down). The observed electro-resistance, measured at various temperatures, allows studying the different electric-field screening in the normal and superconducting states.

\(^1\)Work supported by DIM Oxymore.

8:12AM A23.00002 Two-dimensional simulations of the superconducting proximity in superconductor-semiconductor junctions, VICTOR CHUA, University of Illinois at Urbana-Champaign, MICHAEL VISSERS, The National Institute of Standards and Technology (NIST), STEPHANIE A. LAW, University of Delaware, SMITHA VISHVESHWARA, JAMES N. ECKSTEIN, University of Illinois at Urbana-Champaign — We simulate the consequences of the superconducting proximity effect on the DC current response of a semiconductor-superconductor proximity device within the quasiclassical formalism in the diffusively disordered limit. The device is modeled on in-situ fabricated NS junctions of superconducting Nb films on metallic doped InAs films, with electrical terminals placed in an N-S-N T-junction configuration. Due to the non-collinear configuration of this three terminal device, a theoretical model based on coupled two dimensional spectral and distributional Usadel equations was constructed and numerically solved using Finite-Elements methods. In the regime of high junction conductance, our numerical results demonstrate strong temperature and spatial dependencies of the proximity induced modifications to spectral and transport properties. Such characteristics deviate strongly from usual tunnel junction behavior and aspects of this have been observed in prior experiments[arXiv:1402.6055].

8:24AM A23.00003 STM/STS on proximity-coupled superconducting graphene\(^1\), MAOZ OVADIA, YU JI, JENNIFER HOFFMAN, Harvard University, JOEL I-JAN WANG, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — Graphene in good electrical contact with a superconductor has been observed to have an enhanced proximity effect. Application of a magnetic field is expected to generate an Abrikosov lattice of superconducting vortices, each containing Andreev bound states in its core. With our versatile, homebuilt, low temperature scanning tunneling force microscope (STM/SFM), we investigate the electronic properties of graphene on superconducting NbSe\(_2\) in a magnetic field and search for signatures of these vortex core states.

\(^1\)This work was supported by the STC Center for Integrated Quantum Materials, NSF Grant No. DMR-1231319

8:36AM A23.00004 Closing the gap in the Andreev spectrum in a three-terminal superconducting junction, CIPRIAN PADURARIU, RÉGIS MELIN, Institut Néel CNRS, Grenoble, France, THIBAULT JONCKHEERE, JÉRÔME RECH, THIERRY MARTIN, Centre de Physique Théorique CNRS, Marseille, France, DENIS FEINBERG, Institut Néel CNRS, Grenoble, France, BENOÎT DOUCOT, Laboratoire de Physique Théorique et Hautes Energies CNRS. Paris, France, YULI NAZAROV, Kavli Institute of Nanoscience, TU Delft, The Netherlands — Quasiclassical circuit theory \(^1\) is used to investigate transport in a mesoscopic junction with three superconducting terminals. Our study reveals the closing of the gap in the Andreev spectrum for a wide range of phase-biases and transparencies, in agreement with previous work \(^2\). In this regime a superconducting current flows in the junction, while the proximity mini-gap is closed. The corresponding parameter region is studied systematically, both analytically in the low transparency limit and numerically. We provide a microscopic explanation for the closing of the gap in terms of multiple pair processes that correlate the superconducting currents flowing between different pairs of terminals \(^3\). We show that multi-terminal superconducting junctions provide unique opportunities for applications in quantum devices based on Josephson and/or Majorana physics.

\(^1\)Yu. V. Nazarov, Superlattices Microstruct. 25, 1221-1231 (1999).

8:48AM A23.00005 Proximity Effects in Superconductor–Graphene Junctions\(^1\), FABIAN A. CUEL-LAR, DAVID PERCONE, MARIE-BLANDINE MARTIN, BRUNO DLIBAK, MAELIS PIQUEMAIL, ROZENN BERNARD, JUAN TRASTOY, CONSTANCE MOREAU-LUCHAIRE, PIERRE SENEOR, JAVIER E. VILLEGAS, Unite Mixte de Physique and Universite Paris-Sud, Palaiseau, France, PIRAN KIDAMBI, STEPHAN HOFMANN, JOHN ROBERTSON, Department of Engineering, University of Cambridge, Cambridge, United Kingdom — Superconducting proximity effects are of particular interest in graphene: because of its band structure, an unconventional (specular) Andreev reflection is expected \(^1\). In this context, high-Tc superconductor-graphene junctions are especially attractive. In these, the size of the superconducting energy-gap may exceed the graphene doping inhomogeneities around the Dirac point, which should favor the observation of the specular Andreev reflection. Yet, the fabrication of high-Tc superconductor-graphene junctions is challenging: the usual growth and lithography processes in both materials are incompatible. We report here on a fabrication method that allow us to fabricate planar cuprate superconductor-graphene junctions, which we characterize via conductance spectroscopy. We analyze the features in the conductance spectra as a function of graphene doping, and discuss them in the framework of the Andreev reflection. \(^1\)C. W. J. Beenakker. Phys. Rev. Lett. 97, 067007 (2006)

\(^1\)work supported by Labex Nanosaclay

9:00AM A23.00006 ABSTRACT WITHDRAWN —

9:12AM A23.00007 ABSTRACT WITHDRAWN —
9:24AM A23.00008 AC measurements of the superconducting proximity effect in metal nanowires, RUSSELL LKKE, JOONAS GOVENIUS, KUAN YEN TAN, MIKKO MÖTTÖNEN, QCD Labs, COMP Centre of Excellence, Department of Applied Physics, Aalto University School of Science, PO Box 13500, FI-00076 Aalto, Finland — We quantitatively probe the admittance of diffusive superconductor/nanowire/superconductor (SNS) weak links. Measurements are performed from 0.4 GHz to 12.8 GHz which includes regimes above and below the predicted characteristic energy scale for the superconducting proximity effect. Each device consists of a flux-biased SNS SQUID chain where N is a gold-palladium nanowire. The chain has strong capacitive coupling to a multimode microwave resonator. Measurements of the resonance frequency and quality factor for each resonator mode reveal the dissipative and reactive parts of the admittance of the SNS SQUID chain. The measurement results are valuable because they provide a direct test for theories of non-equilibrium superconductivity in SNS weak links and because AC measurements have only recently been reported in the literature. The data presented is also crucial for understanding losses in microwave circuits that employ SNS weak links, including nanobolometers. References: [1] P. Virtanen et al. Phys. Rev. B 83, 144514 (2011), [2] F. Kos et al. Phys. Rev. B 87, 174521 (2013), [3] B. Dassonville et al. Phys. Rev. Lett. 110, 217001 (2013). [4] J. Govenius et al. Phys. Rev. B 90, 064505 (2014)

9:36AM A23.00009 Cascading Proximity Effect and Singlet-Triplet Mixing in Rotating Magnetization Junctions, ANDREAS BILL, California State University Long Beach, CA 90840-9505, THOMAS E. BAKER, University of California, Irvine, CA 92697, ADAM RICHE-HALFORD, University of Washington, Seattle, WA 98195 — The proximity of a superconductor to an inhomogeneous magnetic material induces singlet and triplet pair correlations in the hybrid structure. The amount of each component and their presence deep in the magnetic material strongly depends on the magnetic inhomogeneity. We present a comparative study of pair correlations in a diffusive magnetic Josephson junction involving a multilayer with misaligned magnetization, a cosine-type helical structure and a more flexible and realistic domain wall of an exchange spring. Using the cascading effect we demonstrate that the three systems induce qualitatively different mixtures of correlations. In particular, we show that misaligned and continuously rotating magnetizations do not display the same physical state. Analyzing the Gor’kov functions we find that so-called short range singlet correlations can be found deep in the magnetic material and compete with triplet correlations giving rise to the so-called singlet-triplet 0 – π transition.

1We gratefully acknowledge support from the National Science Foundation (DMR-1309341). TEB graciously thanks the support of the UC Irvine Achievement Rewards for College Scientists Fellowship.

9:48AM A23.00010 Spin-transfer torque effect in nanopillar superconducting-magnetic hybrid Josephson junctions, BURM BAEK, WILLIAM RIPPARD, MATTHEW PUFALL, SAMUEL BENZ, STEPHEN RUSSEK, HORST ROGALLA, PAUL DRESSELHAUS, National Institute of Standards and Technology, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY TEAM — We have developed single nanopillar Josephson junctions with pseudo-spin-valve barriers with a feature size 50 nm or larger. We observed changes in Josephson critical current depending on the magnetization state of the barrier (parallel or anti-parallel) through the superconductor-ferromagnet proximity effect. The magnetization states of the pseudo-spin-valve barriers could also be switched with applied bias currents which is consistent with the spin-transfer torque effect in room-temperature spin valve devices. Our results demonstrate devices that combine superconducting and spintronic functions promising for a nanoscale cryogenic memory technology.

10:00AM A23.00011 Josephson Interference due to Orbital States in Nanowire Proximity Effect Junctions, KAVEH GHARAVI, GREGORY HOLLOWAY, JONATHAN BAUGH, Institute for Quantum Computing, University of Waterloo — The Josephson effect in a nanowire-based superconductor-normal-superconductor (SNS) junction is studied theoretically and experimentally, focusing on the effects of nanoscale confinement on the current-phase relationship of the junction. An axial external magnetic field is applied. The theory of a previously unstudied type of Josephson interference is described, based on the coupling between the axial flux and N-section Andreev quasiparticles (continuum states or bound states) occupying subbands of non-zero orbital angular momentum. The Bogoliubov-de Gennes equations are solved while considering the transverse subbands in the N-section, yielding energy-versus-phase curves that are shifted in phase in the presence of the flux. A similar phase shift is observed in the continuum current of the junction. An intuitive, semi-classical version of the theory is presented. The critical current $I_c$ of the junction is numerically calculated, and shown to oscillate versus the axial flux. Experimental observations of the oscillations of $I_c$ in an Nb-InAs nanowire-Nb junction are reported. It is shown that the observed oscillations can be described by the semi-classical picture. The scope and applicability of the theory to experimental devices is discussed.

2This work was supported by NSERC, Ontario Ministry for Research and Innovation, Canada Foundation for Innovation, and Industry Canada.

Monday, March 2, 2015 8:00AM - 10:36AM – Session A26 DCP: Focus Session: Non-Adiabatic Dynamics: New Insights from Experiment and Theory –

8:00AM A26.00001 Representing Adiabatic Potential Energy Surfaces Coupled by Conical Intersections in their Full Dimensionality Using Coupled Quasi-Diabatic States, DAVID YARKONY, Johns Hopkins University — The construction of fit single state potential energy surfaces (PESs), analytic representations of ab initio electronic energies and energy gradients, is now well established. These single state PESs, which are essential for accurate quantum dynamics and have found wide application in more approximate quasi-classical treatments, have revolutionized adiabatic dynamics. The situation for nonadiabatic processes involving dissociative and large amplitude motion is less sanguine. In these cases, compared to single electronic state dynamics, both the electronic structure data and the representation are more challenging to determine. We describe the recent development and applications of algorithms that enable description of multiple adiabatic electronic potential energy surfaces coupled by conical intersections in their full dimensionality using coupled quasi-diabatic states. These representations are demonstrably quasi-diabatic, provide accurate representations of conical intersection seams and can smooth out the discontinuities in electronic structure energies due to changing active orbital spaces that routinely afflict global multistate representations.

8:48AM A26.00003 Non-adiabatic dynamics of reactions of O(1D) with Xe, CO, NO2, and CO2 from crossed atomic and molecular beam experiments. KRISTIE BOERING, University of California, Berkeley — Reactions of the first excited state of atomic oxygen, O(1D), with small molecules such as CO, NO2, and CO2 continue to be of interest in aeronomy and atmospheric chemistry, thus providing additional motivation to understand the dynamics of these reactions and how well they are predicted by theory. In collaboration with Prof. Jim Lin of the Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan, we have studied the dynamics of quenching and non-quenching reactions between O(1D) and various small molecules using a universal crossed atomic and molecular beam apparatus. New experimental results for the dynamics of quenching of O(1D) by Xe and CO will be presented and compared with previous results for NO2 (K.A. Mar, A.L. Van Wynyarden, C.-W. Liang, Y.T. Lee, J.J. Lin, K.A. Boering, J. Chem. Phys., 137, 044302, doi: 10.1063/1.4736567, 2012) and CO2 (M.J. Perri, A.L. Van Wynyarden, K.A. Boering, J.J. Lin, and Y.T. Lee, J. Chem. Phys., 119(16), 8213-8216, 2003; M.J. Perri, A.L. Van Wynyarden, J.J. Lin, Y.T. Lee, and K.A. Boering, J. Phys. Chem. A, 108(39), 7995-8001, doi: 10.1021/jp0458545, 2004). Among the most intriguing of the new results are for quenching of O(1D) by Xe, for which marked oscillations in the differential cross sections were observed for the O(1P) and Xe products. The shape and relative phase of the oscillatory structure depended strongly on collision energy. This behavior is likely due to the quantum nature of the collision dynamics, caused by interferences among multiple curve crossing pathways accessible during electronic quenching, known as Stueckelberg oscillations.

9:24AM A26.00004 Light, Molecules, Action: Broadband UV-visible transient absorption studies of excited state dynamics in photoactive molecules. ROSEANNE SENSION, Departments of Chemistry and Physics, Univ of Michigan - Ann Arbor — Broadband UV-visible transient absorption spectroscopy provides a powerful tool for the investigation of the dynamics of electronically excited molecules in the condensed phase. It is now possible to obtain transient spectra on a routine basis spanning the range from <300 nm to >800 nm with femtosecond time resolution. We have used this method to study the excited state dynamics and internal conversion of a range of molecular systems with potential application as optically powered molecular devices. The cyclohexadiene ring-opening reaction is the basis of a class of important optical switches and of the biological synthesis of vitamin D3. The ring-opening reaction is ultrafast, occurring on a picosecond to subpicosecond timescale depending on the substituents around the ring. These have a significant influence on the dynamics and electronic structure of the electronically excited molecule. The results of a series of transient absorption studies as a function of chromophore substitution and environment will be presented. The cis-trans isomerization of polynene molecules, especially substituted stilbenes, provides another important class of functional molecular transformations. Again the excited state dynamics can be ultrafast with photochemistry controlled by details of the curve crossings and conical intersections. Finally the photochemistry of the even more complex set of cobalamin chromophores with a photoactivable C-Co bond has been proposed as a tool for spatio-temporal control of molecule delivery including drug delivery. Broadband transient absorption spectroscopy has been used to investigate the ultrafast electronic dynamics of a range of cobalamin compounds with comparison to detailed theoretical calculations. The results of these studies will be presented.

10:00AM A26.00005 Long-lived complexes in the F + H2O and F + CH3OH Hydrogen Abstraction Reactions. ROBERT CONTINETTI, Univ of California - San Diego — Extending our recent study of the benchmark four-atom F·H2O system [1], we have now studied the dissociative photodetachment (DPD) of the seven-atom F·(CH3OH) cluster as well. The energetics of this system dictate that DPD only occurs to the HF + OCH3+ e− product channel on the neutral potential energy surface resulting in diagonal banding in the photoelectron-photofragment coincidence spectrum consistent with resolved HF vibrational excitation in the products. Evidence for photodetachment to long-lived (μs) van der Waals complexes (FH···OCH3) was also observed, as in the F·H2O system. The metastable states involved in F·H2O are best described as vibrational Feshbach resonances, and the energetics and dynamics of the metastable complexes in the two systems will be examined. This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under award number DE-FG03-98ER14679.

10:12AM A26.00006 Non-adiabatic dynamics in the detachment continuum of radical anions. JAN VERLET, Durham University — Using photoelectron (PE) spectroscopy at a range of photon energies above the detachment threshold of a radical anion, the dynamics of resonances can be identified by the appearance of various channels. These include: (i) direct and prompt autodetachment, which appears in the PE spectrum as a peak that increases in intensity as the photon energy is shifted to lower kinetic energy and typically does not shift with photon energy; and (ii) thermionic emission from the radical anion ground state which appears as an exponential decay at low very low kinetic energy. Using time-resolved PE spectroscopy, the non-adiabatic dynamics leading to the formation of the ground state anion can be monitored in real time. In some cases, these dynamics occur on timescales that vastly out-compete autodetachment, even at energies of 3 eV above the neutral. The methodology has been applied to a number of quinone-related molecules and provides insights into how electron capture can lead to stable anions, which is of relevance in switches and of the biological synthesis of previtamin D3. The ring-opening reaction is ultrafast, occurring on a picosecond to subpicosecond timescale depending on the substituents around the ring. These have a significant influence on the dynamics and electronic structure of the electronically excited molecule. The results of a series of transient absorption studies as a function of chromophore substitution and environment will be presented. The cis-trans isomerization of polynene molecules, especially substituted stilbenes, provides another important class of functional molecular transformations. Again the excited state dynamics can be ultrafast with photochemistry controlled by details of the curve crossings and conical intersections. Finally the photochemistry of the even more complex set of cobalamin chromophores with a photoactivable C-Co bond has been proposed as a tool for spatio-temporal control of molecule delivery including drug delivery. Broadband transient absorption spectroscopy has been used to investigate the ultrafast electronic dynamics of a range of cobalamin compounds with comparison to detailed theoretical calculations. The results of these studies will be presented.

10:24AM A26.00007 Photofragment vector correlations and rotational distributions from ozone dissociation at 266 and 248 nm. MICHELLE WARTER, WEI WEI, SIMON NORTH, Texas A&M University — Ozone photolysis is very important in the atmosphere and has been studied by many people, but there are still mysteries involved in O3 dissociation. Velocity-Max-Planck imaging experiments on O3 dissociation at 266 and 248 nm have been performed to reveal these mysteries. The even odd population alternations of the O2 rotational distribution and the vector correlations have been studied to determine if there is a dynamical effect on the odd state depletion.

Monday, March 2, 2015 8:00AM - 10:48AM
Session A27 DCP: Focus Session: Emerging Ultrafast Technologies

204B - Andrei Tokmakoff, University of Chicago
these features, we investigate the quantum-coherent interaction between the ultrashort electron pulse and the optical near-field of an illuminated nanostructure.

Finally, further applications and prospects of ultrafast electron imaging, diffraction and spectroscopy using nanoscale field emitters will be discussed. Finally, an update on our new results in coupling ultrafast lasers with TERS. This last topic illuminates a path forward toward the goal of understanding chemistry at the space-time limit.

8:36AM A27.00002 Coherent two-dimensional infrared microscopy, CARLOS BAIZ, DENISE SCHACH, ANDREI TOKMAKOFF, Univ of Chicago — We developed ultrafast 2D IR spectral microscopy, a new technique to measure spatially-resolved 2D infrared spectra and vibrational dynamics with diffraction-limited spatial resolution and femtosecond time resolution. The key enabling development consists of a new geometry where all three IR pulses propagate fully collinearly through an all-reflective IR microscope. A combination of polarization, chopping, and phase-cycling isolates the 2D IR signal by removing all unwanted signal and interference contributions. The single-beam collinear geometry enables us to implement 2D IR in three configurations: transmission, reflectance, and ATR. In terms of sensitivity, the 6 micron focus size produces an 8-fold enhancement of the signal compared to focusing with standard parabolic mirrors. These methods open up new possibilities for imaging proteins in cells, lipid membranes, or vesicles, as well as performing surface-sensitive studies on biological systems.

8:48AM A27.00003 Mapping the nanoscale energetic landscape in conductive polymer films with spatially super-resolved exciton dynamics, NAOMI GINSBERG, Univ of California - Berkeley — The migration of Frenkel excitons, tightly-bound electron-hole pairs, in polymeric organic semiconducting films is critical to the efficiency of bulk heterojunction solar cells. While these materials exhibit a high degree of structural heterogeneity on the nanoscale, traditional measurements of exciton diffusion lengths are performed on bulk samples. Since both the characteristic length scales of structural heterogeneity and the reported bulk diffusion lengths are smaller than the optical diffraction limit, we adapt far-field super-resolution fluorescence imaging to uncover the correlations between the structural and energetic landscapes that the excitons explore.

9:24AM A27.00004 Ultrafast electron microscopy and diffraction with laser-driven field emitters, CLAUS ROPERS, University of Goettingen — Ultrafast structural dynamics in solids and nanostructures can be investigated by an increasing number of sophisticated electron and x-ray diffraction techniques. Electrons are particularly suited for this purpose, exhibiting high scattering cross-sections and allowing for beam control by versatile electrostatic or magnetic lens systems. The capabilities of time-resolved electron imaging techniques critically depend on the employed source of laser-driven ultrashort electron pulses. Nanoscopic sources offer exceptional possibilities for the generation of electron probe pulses with very short durations and high spatial beam coherence. In this talk, I will discuss recent progress in the development of ultrafast electron microscopy and diffraction based on nanoscopic photocathodes. In particular, we implemented ultrafast low-energy electron diffraction (ULEED) and ultrafast transmission electron microscopy (UTEM) driven by nonlinear photoemission from field emission tips. ULEED enables the study of structural changes with high temporal resolution and ultimate surface sensitivity, at sub-keV electron energies. As a first application of this technique, we studied the structural phase transition in a stripe-like polymer superstructure on freestanding monolayer graphene. An advanced UTEM instrument was realized by custom modifications of a standard transmission electron microscope, leading to electron focal spot sizes in the microscope's sample plane of about 10 nm and electron pulse durations of less than 700 fs. Utilizing these features, we investigate the quantum-coherent interaction between the ultrashort electron pulse and the optical near-field of an illuminated nanostructure. Finally, further applications and prospects of ultrafast electron imaging, diffraction and spectroscopy using nanoscale field emitters will be discussed.
8:00AM A28.00001 Magnetic droplets and dynamical skyrmions, JOHAN AKERMAN, University of Gothenburg — Nanocontact spin-torque oscillators (NC-STOs) provide an excellent environment for studying nano-magnetic phenomena such as localized and propagating auto-oscillatory spin wave (SW) modes. The recent experimental observation of magnetic droplet solitons in NC-STOs with perpendicular magnetic anisotropy (PMA) free layers [1], and the numerical [2] and experimental [3] demonstrations of spin transfer torque (STT) nucleated skyrmions in similar magnetic thin films add two interesting and useful nanoscale magnetic objects. Due to the competition between exchange, anisotropy, and, in the case of skyrmions, the Dzyaloshinskii-Moriya interaction (DMI), the droplet and the skyrmion are extremely compact, on the order of 10-100 nm. One of the main differences between a magnetic dissipative droplet soliton and a skyrmion is that the former is a dynamical object with all its spins precessing around an effective field and stabilized by STT, exchange, and PMA, while the latter has static spins and an internal structure stabilized by DMI, exchange, and PMA. The dissipative droplet is furthermore a non-topological soliton, while the skyrmion is topologically protected. In this work I will report on our most recent droplet experiments, including droplet collapse at very high fields, droplets excited in nano-wire based NC-STOs, and studies of the field-current droplet nucleation boundary. I will also demonstrate numerically and analytically that STT driven precession can stabilize so-called dynamical skyrmions even in the absence of DMI, and I will describe their very promising properties in detail. From a more fundamental perspective, precession is hence a third independent possibility to stabilize a skyrmion, without the need for the conventional stabilization from either dipolar energy or DMI.


8:36AM A28.00002 Physical Mechanisms and Limits of Skyrmions for Information Processing and Storage, GEN YIN, ROGER LAKE, Department of Electrical Engineering, UC Riverside, CHIA-LING CHIEN, JIADONG ZANG, Department of Physics and Astronomy, Johns Hopkins University — Magnetic Skyrmions have been proposed for applications in future information storage because of their small size, their stability and their facial movement with low current. For such purposes the ability to create single Skyrmions is required and an understanding of the process of Skyrmion creation and decay is highly desirable. Here we numerically show that the location and the moment of Skyrmion creation or annihilation can be precisely controlled by a nano second unpolarized current pulse. To analyze the microscopic process we employ a lattice version of the topological charge on a tight-binding 2D plate. It provides a clear picture of the spin trajectories and orientations that locally trigger a topological transition, and it reviews the topological origin of a Skyrmion’s stability at finite temperatures. The robustness and experimental feasibility of the proposed mechanism are numerically examined.

8:48AM A28.00003 Electrical transport in three-dimensional cubic Skyrmion crystal, XIAO-XIAO ZHANG, Univ of Tokyo, NAOTO NAGAOSA, Univ of Tokyo and RIKEN CEMS — Two-dimensional magnetic Skyrmions have been well confirmed via various experimental techniques in the bulk or on epitaxial thin films. Besides, a topologically nontrivial three-dimensional cubic Skyrmion crystal in the bulk, which is essentially a hedgehog-antihedgehog pair texture predicted theoretically, has also been tentatively observed. Equipped with a sophisticated spectral analysis program, we adopt Matsubara Green’s function technique to study electrical transport, especially diagonal conductivity, in such system. We consider conduction electrons interacting with spinwaves via the strong Hund’s rule coupling, wherein fluctuation of monopolar emergent electromagnetic field exits within adiabatic approximation. We describe in detail the influence of temperature and Skyrmion number on both dc and ac conductivities. Possible deviation from Fermi liquid behavior will also be discussed.

9:00AM A28.00004 Statics and dynamics of zero field stable skyrmions in magnetic thin layers, NIKOLAI S. KISELEV, IAS1, Forschungszentrum Jülich, Germany, CHANGHOON HEO, IMM, Radboud University Nijmegen, Netherlands, ASHIS KUMAR NANDY, IAS1, Forschungszentrum Jülich, Germany, THEO RASING, IMM, Radboud University Nijmegen, Netherlands, STEFAN BLÜGEL, IAS1, PG1, Forschungszentrum Jülich, Germany — We present a comprehensive theoretical study of the statics and dynamics of magnetic skyrmions stabilized in zero magnetic field. The essential energy contributions for the stability of such magnetic skyrmions are the Dzyaloshinskii-Moriya interaction (DMI) and the uniaxial anisotropy. We define a finite range of the strength of these parameters corresponding to the stability of isolated skyrmions at zero magnetic field. Within this range there are two metastable Skyrmion solutions characterized by opposite polarity and opposite topological charge. Such skyrmions can lead to conceptually new approaches in data storage provided by field or current induced switching between two of such skyrmion states. We discuss in detail various aspects of the problem connected with the switching between two skyrmion states driven by an applied magnetic field pulse, including the role of magnetic pulse width, intensity and direction. The role of damping and dependencies on magnetic layer thickness, size and shape are also discussed. Presented results are obtained by the method of stochastic spin dynamics simulation applied to an extended Heisenberg model for localized magnetic spins.

9:12AM A28.00005 Collective Transport Properties of Driven Skyrmions with Random Disorder, DIPANJAN RAY, CYNTHIA OLSON REICHHARDT, CHARLES REICHHARDT, Los Alamos National Laboratory — We use particle-based simulations to examine the static and driven collective phases of skyrmions interacting with random quenched disorder. We show that non-dissipative effects due to the Magnus term reduce the depinning threshold and strongly affect the skyrmion motion and the nature of the dynamic phases. The quenched disorder causes the Hall angle to become drive-dependent in the moving skyrmion phase, while different flow regimes produce distinct signatures in the transport curves. For weak disorder, the skyrmions form a pinned crystal and depin elastically, while for strong disorder the system forms a pinned amorphous state that depins plastically. We discuss in detail the influence of temperature and Skyrmion number on both dc and ac conductivities. Possible deviation from Fermi liquid behavior will also be discussed.

9:24AM A28.00006 Dynamics of monopole-like excitation in chiral magnets under a current drive, SHI-ZENG LIN, AVADH SAXENA, Theoretical Division, Los Alamos National Laboratory — Skyrmions in chiral magnets are hedgehog-like spin textures, which wrap the sphere once. Skyrmion lines in metallic chiral magnets produce an emergent magnetic field that couples to the orbital motion of the conduction electrons. The inflow and outflow of this field around a closed surface is not necessary equal, i.e. the divergence of this field is not necessary zero, and thus it allows for the existence of emergent monopoles. One example is a finite segment of a skyrmion line inside crystal. The two ends of the segment produce a monopole and antimonopole, which are connected by lines of the emergent magnetic flux. Here we study the monopole dynamics induced by an electric current injected in the chiral magnet. We reveal that skyrmion segments are nucleated via the creation of monopoles and antimonopoles. Then these segments merge to form longer skyrmion lines via annihilation of monopoles and antimonopoles. Finally these skyrmion lines span the whole system, where all monopoles and antimonopoles disappear. The skyrmion lines are destroyed via the proliferation of monopoles and antimonopoles. We also propose to create the monopoles in a controlled way by applying current to surfaces. The existence of monopoles can be inferred from transport or imaging measurements.

This work was carried out under the auspices of the NNSA of the US DOE at LANL under Contract No. DE-AC52-06NA25396, and was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.
9:36AM A28.00007 Detection of helical spin structures by magnetotransport 1, ALI C. BASARAN, Univ of California - San Diego, RAFAEL MORALES, Univ of the Basque Country, STEFAN GUENON, Eberhard-Karls-Universitat Tubingen, IVAN K. SCHULLER, Univ of California - San Diego — We have developed a method which allows determining the magnetic helicity in thin films by magnetotransport measurements. A helical spin configuration occurs during magnetization reversal in exchange coupled Ni/FeF 2 heterostructures. Both longitudinal and transverse components of the magnetization are concurrently detected using magnetotransport through a lithographically patterned cross junction. Small angle deviations around the well-defined unidirectional anisotropy axis reveal the change in the helicity of in-depth spin configuration. The simulations obtained using an incomplete domain wall model are in excellent agreement with the experimental data. Thus, we show that the complex spin formations in nanomagnetic systems can be studied with a lab based, well known, and rather simple experimental technique.

1 Research supported by the Department of Energy’s Office of Basic Energy Science, DMR under grant DE FG03 87ER-45332. R.M. acknowledges funding from EU FP7-IRSES-2012 318901, MINECO FIS2013-45469 and MECID CAS12/00241.

9:48AM A28.00008 Micromagnetic modeling of skyrmion injection in an inhomogeneous geometry 1. OLLE HEINONEN, WANJUN JIANG, SUZANNE TE VELTHUIS, AXEL HOFFMANN, Argonne Natl Lab — Magnetic systems with broken inversion symmetry can support skyrmion structures stabilized by the Dzyaloshinskii-Moriya interaction (DMI). This can be realized in thin magnetic films, such as CoFe, on a substrate with appreciable spin-orbit interactions, e.g., Ta or Pt. Recent works have explored the creation and manipulations in such thin films using spin transfer torque or domain wall injection, which is challenging. We recently demonstrated that an inhomogeneous spin-Hall current can efficiently create and inject skyrmions, which can then be manipulated and transported. Based on this observation we will here present micromagnetic modeling of the injection dynamics of skyrmions in a geometry similar to the ones used experimentally. For small current densities, the system will inject meandering stripes that will arrange themselves along equipotential lines. For large enough current densities, a domain wall forms in the narrow part of the system and much complicated dynamical structures are sprayed into the wider part of the system. When the driving current is subsequently turned off, these structures coalesce into skyrmions. A key ingredient here is the inhomogeneous spin-Hall torque resulting from the geometry of the system.

1 This work was financially supported by the Department of Energy, Office of Science, Materials Sciences and Engineering Division.

10:00AM A28.00009 Annihilation of skyrmions by spin wave in crossbar geometry 1, YIZHOU LIU, Department of Electrical and Computer Engineering, University of California Riverside, JIAODONG ZANG, Department of Physics and Astronomy, Johns Hopkins University, ROGER LAKE, Department of Electrical and Computer Engineering, University of California Riverside — Magnetic Skyrmions are possible candidates for future information storage applications due to their small size and topological protection. Understanding of the creation and annihilation process is necessary for developing a Skyrmion-based technology. We theoretically study the annihilation process within a crossbar geometry. By micromagnetic simulation, we find the annihilation of a single Skyrmion can be achieved by injecting a spin wave. The influence of a defect in this system is also discussed. Our method could be applied to individually address arrays of Skyrmions in a memory architecture.

1 This work was supported by the National Science Foundation under Grant No. ECCS-1408168.

10:12AM A28.00010 Magnetization pumping and dynamics in a uniform Dzyaloshinskii-Moriya magnet, ALEXEY KOVALEV, UTKAN GÜNÖRDÜ, University of Nebraska-Lincoln — We formulate a phenomenological description of thin ferromagnetic layers with inversion asymmetry where the long-wavelength magnetic dynamics experiences magnon current-induced torques and leads to magnon-motive forces. We first construct a phenomenological theory based on irreversible thermodynamics, taking into account the symmetries of the system. Furthermore, we confirm that these effects originate from Dzyaloshinskii-Moriya interactions from the analysis based on the stochastic Landau-Lifshitz-Gilbert equation. Our phenomenological results can be generalized to other systems such as pyrochlore crystals and chiral magnets. Possible applications include spin current generation, magnetization reversal and magnonic cooling.

10:24AM A28.00011 Current-Driven Dynamics of Skyrmions Stabilized in MnSi Nanowires Revealed by Topological Hall Effect 1, DONG LIANG, JOHN DEGRAVE, MATTHEW STOLT, Department of Chemistry, University of Wisconsin-Madison, YOSHINORI TOKURA, RIKEN Center for Emergent Matter Science, SONG JIN, Department of Chemistry, University of Wisconsin-Madison — Skyrmions, novel topologically stable spin vortices, hold promise for next-generation high-density magnetic storage technologies due to their nanoscale domains and ultralow energy consumption. One-dimensional (1D) nanowires are ideal hosts for skyrmions since they not only serve as a natural platform for magnetic racetrack memory devices but also can potentially stabilize skyrmions. We use the topological Hall effect (THE) to study the phase stability and current-driven dynamics of the skyrmions in MnSi nanowires. The THE was observed in an extended magnetic field-temperature window (15 to 30 K), suggesting stabilization of skyrmion phase in nanowires compared with the bulk (27 to 29.5 K). Furthermore, we study skyrmion dynamics in this extended skyrmion phase region and found that under the high current-density of 10 10−10 10−9 Am−2 enabled by nanowire geometry, the THE decreases with increasing current densities, which demonstrates the current-driven motion of skyrmions generating the emergent electric field. These results open up the exploration of nanowires as an attractive platform for investigating skyrmion physics in 1D systems and exploiting skyrmions in magnetic storage concepts.

1 This work is supported by US National Science Foundation (ECCS-1231916) and JSPS Grant-in-Aid for Scientific Research No. 24224000.

10:36AM A28.00012 Towards Skyrmions: Magnetic and electrical properties of Mn 2−xRh xSn Heusler compounds, KUMARI GAURAV RANA, MPI for Chemical Physics of Solids, Dresden, Germany and MPI of Microstructure Physics, Halle, Germany, E. BENEDIKT, MPI for Chemical Physics of Solids, Dresden, Germany, O. MESHCHERIAKOVA, MPI for Chemical Physics of Solids, Dresden, Germany and MPI of Microstructure Physics, Halle, Germany. A. KÖHLER, D. EBKE, C. FELSER, MPI for Chemical Physics of Solids, Dresden, Germany — A variety of possible ground states and tunable magnetic and electronic properties makes Mn 2−xRh xSn one of the most relevant materials for spintronic devices. Mn 2−xRh xSn, a non-centrosymmetric tetragonal Heusler with enhanced spin-orbit coupling, is recently found to possess a strong spin canting of its magnetic sublattices and the found strong Dzyaloshinskii-Moriya exchange encourages studies of Skyrmions in this promising Heusler compound. We report on the evolution of magnetic and electronic properties of ordered Mn 2−xRh xSn films grown on single crystalline MgO (100) substrates using DC co-sputtering. For tetragonally ordered films, a curie temperature of up to 281 K and coercive field of up to 630 Oe (out of plane) is obtained. However, an in-plane component sets in for temperatures below 100 K. The structural ordering for the films grown at different substrate temperatures influences the magnetic as well as the electronic properties. The exchange energies, magneto-transport properties, Hall effect will be discussed. Our work gives an insight to tailor the properties of Mn 2−xRh xSn films and highlights it as a potential candidate for future spintronic devices.

This work was supported by the National Science Foundation under Grant No. ECCS-1231916 and JSPS Grant-in-Aid for Scientific Research No. 24224000.
10:48AM A28.00013 Large non-collinearity and spin-reorientation in the novel Mn$_2$RhSn Heusler magnet. — O. MESHCHERIUKOVA, S. CHADOV, A. NAYAK, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, U.K. ROESSLE, Institute for Theoretical Solid State Physics, Leibniz Institute for Solid State and Materials Research, Dresden, Germany, J. KUEBELER, Institute of Solid State Physics, Technical University of Darmstadt, Darmstadt, Germany, G. ANDRE, Laboratoire Leon Brillouin, CEA-CNRS Saclay, Gif-sur-Yvette, France, A.A. TSIRLIN, National Institute of Chemical Physics and Biophysics, Akadeemia tee 23, 12618 Tallinn, Estonia, C. FELSER, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — Heusler compounds is a large class of materials, which exhibits diverse fundamental phenomena, together with the possibility of the specific tailoring for various engineering tasks. Present work discusses the magnetic noncollinearity in the family of noncentrosymmetric Mn$_2$-based Heusler compounds. According to the experimental and theoretical results, Mn$_2$YZ Heusler family is suspected to provide promising candidates for the formation of the skyrmion lattice. The work is focused on Mn$_2$RhSn bulk polycrystalline sample, which serves as a prototype. It crystallizes in the tetragonal noncentrosymmetric structure (No. 119 I4/mcm), which enables the anisotropic DM coupling. Additional short-range modulation, induced by the competing nearest and next-nearest interplane Heisenberg exchange, is suppressed above the 80 K. This allows to develop the long-range modulations in the ideal ferrimagnetic structure within the $ab$ crystallographic planes.

Monday, March 2, 2015 8:00AM - 11:00AM –
Session A29 GMAG DMP: Focus Session: Antiferromagnets on Triangular Lattices 206A -
Alexander Chernyshev, University of California, Irvine

8:00AM A29.00001 Magnetostriiction to 100T in SrCu$_2$(BO$_3$)$_2$: magnetic pantograph effect and tuning of $J'/J$ ratio. — M. JAIME, NHMF-LLNL, A. SAUL, CINaM/CNRS, CEE/MIT, G. RADTKE, IMPMC/CNRS, M.B. SALAMON, Physics, UT Dallas, H.A. DABKOWSKA, McMaster Univ. — The magnetostriiction of the frustrated spin dimer system SrCu$_2$(BO$_3$)$_2$ was measured in pulsed high magnetic fields with an optical fiber Bragg grating technique. Both longitudinal (c-axis) and transverse (ab-plane) magnetostriiction were obtained to be $H = 60T$ for $H // c$-axis, observing a reduction of the unit cell volume as the sample is magnetized past the 1/3 saturation magnetization plateau. Modest changes in the lattice parameters, when combined with existing elastic neutron scattering data, suggest significant changes in the Cu-O-Cu bond angles (superexchange) through a pantograph effect as the sample is driven into highly polarized magnetic states. Supportive computations reveal an increase of the ratio of intra- to inter-dimer exchange integrals ($J'/J$) with a decrease in the Cu-O-Cu angle, and the concomitant drop in unit cell volume. These results impact our reading of existing predictions for the (H,T) phase diagram, and predictions for the effect of hydrostatic pressures on the ground state.

8:12AM A29.00002 Theory of lattice response to external magnetic field in SrCu$_2$(BO$_3$)$_2$: magnetostriiction driven by pantograph effect. — ANDRES SAUL, CINaM/CNRS, CEE/MIT and UMI/CNRS-MIT, GUILLAUME RADTKE, IMPMC/CNRS and Univ Paris 06, MARCELO JAIME, National High Magnetic Field Laboratory, Los Alamos National Laboratory, MYRON SALAMON, Department of Physics, The University of Texas at Dallas, HANNA DABKOWSKA, McMaster Univ. — Recent magnetostriiction experiments have shown that the macroscopic physical dimensions of the Shastry-Sutherland compound SrCu$_2$(BO$_3$)$_2$ change with the applied magnetic field mimicking the same complex behavior observed in the magnetization. Using Density Functional based methods we find that the driving force behind the magnetostriiction coupling is the Cu-O-Cu superexchange angle which, thanks to the orthogonal Cu$^{2+}$ dimers acting as pantographs, can shrink significantly (0.44%) with minute (0.01%) variations in the lattice parameters. The consequence is a reduction of the order of ~10% in the antiferromagnetic intra-dimer exchange integral J, sufficient to compensate the elastic energy loss in the deformation.

8:24AM A29.00003 NMR in Pulsed Magnetic Fields on the Orthogonal Shastry-Sutherland spin system SrCu$_2$(BO$_3$)$_2$: magnetostriiction driven by pantograph effect. — RAIVO STERN, NICPB, JONAS KOHLRAUTZ, Uni-Leipzig, HANNES KÜHNE, LIZ GREENE, JOCHEN WOSNITZA, EMFL-HLD, JÜGEN HAASE, Uni-Leipzig — SrCu$_2$(BO$_3$)$_2$ is a quasi-two-dimensional spin system consisting of Cu$^{2+}$ ions which form orthogonal spin singlet dimers, also known as the Shastry-Sutherland lattice, in the ground state. Though this system has been studied extensively using a variety of techniques to probe the spin triplet excitations, including recent magnetostriiction measurements over 100T, microscopic techniques, such as nuclear magnetic resonance (NMR), could provide further insight into the spin excitations and spin-coupling mechanisms. We demonstrate the feasibility of performing NMR on real physical system in pulsed magnets. We present $^{11}$B NMR spectra measured in pulsed magnetic fields up to 53 T, and compare those with prior results obtained in static magnetic fields. Herewith we prove the efficacy of this technique and then extend to higher fields to fully explore the spin structure of the 1/3 plateau.

$^1$Support by EMFL, DFG, EETag (EML+ & PUT210).

8:36AM A29.00004 Identifying topological order in the Shastry-Sutherland model via entanglement entropy. — DAVID RONQULLIO, MICHAEL PETERSON, Cal State Univ- Long Beach — It is known that for a topologically ordered state the area law for the entanglement entropy shows a negative universal additive constant contribution, $-\gamma$, called the topological entanglement entropy. We theoretically study the entanglement entropy of the two-dimensional Shastry-Sutherland quantum antiferromagnet using exact diagonalization on clusters of 16 and 24 spins, utilizing the Kitaev-Preskill construction [A. Kitaev and J. Preskill, Phys. Rev. Lett. 96, 110404 (2006)]. We extract a finite topological term, $-\gamma$, in the region of bond-strength parameter space corresponding to high geometrical frustration. Thus, we provide strong evidence for the existence of an exotic topological ordered state and shed light on the nature of this model’s strongly frustrated, and long controversial, intermediate phase.

$^1$We acknowledge California State University Long Beach Office of Research and Sponsored Programs. Published as Phys. Rev. B 90, 201108(R) (2014).

8:48AM A29.00005 Magnetic vortex crystals in frustrated 3D Mott insulators. — ZHENTAO WANG, Department of Physics and Astronomy, Rice University, YOSHITOMO KAMIYA, ITHIS Research Group and Condensed Matter Theory Laboratory, RIKEN, ANDRIY NEVIDOMSKYY, Department of Physics and Astronomy, Rice University, CRISTIAN BATISTA, Theoretical Division, T-4 and CNSL, Los Alamos National Laboratory — Topological spin textures, such as skyrmions, are of great interest to the field of spintronics and usually arise due to the interplay of Dzyaloshinskii-Moriya and exchange couplings. By contrast, using the BCC and FCC lattices as examples, here we demonstrate that frustrated spin exchange interactions alone can produce topological vortex crystals near the magnetic field-induced saturation transition of 3D bulk Mott insulators. Because of the magnetic frustration, the magnon spectrum of the high-field fully polarized state has multiple degenerate minima at different Q-vectors. This quantum paramagnet becomes gapless and goes through a Bose-Einstein condensation at the saturation field (quantum critical point). In this limit, we apply the dilute boson gas approximation to study the rich topological structures produced due to multi-Q condensation. We find that the vortex crystal phases span sizable regions in the phase diagrams of frustrated 3D Mott insulators with isotropic Heisenberg interactions, and are further stabilized by exchange anisotropies. Vortex strings emerge in the direction of the magnetic field and, depending on the distributions of the condensed modes, can form different exotic patterns.
9:00AM A29.00006 Magnetic phase diagram of the S=1/2 triangular-lattice antiferromagnet Ba$_3$CoSb$_2$O$_9$\cite{1}, YOSHITOMO KAMIYA, RIKEN, CRISTIAN BATISTA, Los Alamos National Laboratory — To explain the recently reported magnetic phase diagram of the spin-1/2 triangular-lattice compound Ba$_3$CoSb$_2$O$_9$ [1-3], we present a semiclassical mean-field theory for the easy-plane XXZ model on the stacked (pentagonal-lattice with a small inter-layer coupling. Quantum effects are incorporated by deriving effective interactions from the linear spin-wave analysis of the two-dimensional model. This analysis reproduces the main experimental observations, such as the 1/3-magnetization plateau (B |c/3, a cusp near 1/3 of the saturated moment (B |c), and a small step anomaly in the high field regime. The predicted spin configurations are compared against the NMR measurements on this compound. This work was done in collaboration with G. Koutroulakis (Los Alamos), T. Zhou (UCLA), J. D. Thompson (Los Alamos), H. D. Zhou (Univ. of Tennessee), and S. E. Brown (UCLA).


Y.K. acknowledges financial support from the RIKEN ITHES Project.

9:12AM A29.00007 Exotic magnetism on the quasi-FCC lattices of the d$^3$ double perovskites La$_2$NaBO$_6$ (B' = Ru, Os)\cite{2}, ADAM ACZEL, Quantum Condensed Matter Division, Oak Ridge National Laboratory — B-site ordered double perovskites with quantum spins S = 1/2 (d$^3$) and S = 1 (d$^4$) on the B' site have attracted a great deal of recent interest, due to the possibility of studying 4d and 5d magnetism combined with magnetic frustration on the face-centered-cubic (FCC) lattice. There has been less focus on d$^3$ systems, as they are generally expected to behave more classically and yield simple, commensurate magnetic ground states. In contrast, we find evidence for long-range and short-range (ξ = 70 A at 4 K) incommensurate magnetic order on the quasi-FCC lattices of the monoclinic double perovskites La$_2$NaRuO$_6$ and La$_2$NaOsO$_6$, respectively. Incommensurate magnetic order on the FCC lattice has not been predicted by mean field theory, but may arise via a delicate balance of inequivalent nearest neighbor and next nearest neighbor exchange interactions. Furthermore, in the Ru system with long-range order, inelastic neutron scattering reveals a spin gap Δ = 2.75 meV. Magnetic anisotropy is generally minimized in the more familiar octahedrally-coordinated 3d$^3$ systems, so the large gap observed for La$_2$NaRuO$_6$ may result from the significantly enhanced value of spin-orbit coupling in this 4d$^3$ material.


9:48AM A29.00008 The incommensurate-commensurate phase transition of anisotropic XXZ model on the triangular lattice, XUEFENG ZHANG, SHI-JIE HU, AXEL PELSTER, SEBASTIAN EGGERT, Univ Kaiserslautern — We investigate the XXZ model on the triangular lattice with anisotropic ferromagnetic xy coupling and antiferromagnetic z coupling. In previous studies, an incommensurate supersolid phase was found when introducing anisotropy of interactions in different directions. However, the mechanism of the incommensurate phase is still unknown. In the strong coupling regime where interactions in the z direction are larger than in the xy plane, we found that quantum fluctuation of domain wall excitations can reduce the energy and cause the incommensurate order. By using quantum Monte Carlo simulations, we confirmed our theoretical analysis and found that the number of domain walls and the incommensurate k-vector monotonically increase with the anisotropy. The physics is dimensionally reduced to 1d.

10:00AM A29.00009 Spin phonon induced magnetic soft mode in triangular antiferromagnet h-RMnO$_3$, JOOSUNG OH, MANH DUC LE, HASUNG SIM, JE-GEUN PARK, Center for Correlated Electron Systems, Institute for Basic Science & Department of Physics and Astronomy, Seoul National University, T.G. PERRING, ISIS Facility, STFC Rutherford Appleton Laboratory — The relief of geometrical magnetic frustration by spin-lattice coupling is an extensively studied subject: For example, theory shows that in triangular lattice antiferromagnets, the spin-phonon coupling can stabilize a collinear magnet order over the non-collinear 120° order. We report inelastic neutron scattering measurements on the triangular lattice antiferromagnets (Y/Lu)MnO$_3$, showing evidence of magnon-phonon hybridization at the Brillouin zone boundary. Furthermore, a magnetic soft mode is observed at lower energy at the same momentum transfer. The exchange striction model within the linear approximation qualitatively explains the observed features while the 1/S expansion calculation shows that a third of the observed softening is caused by magnon-magnon interactions. Our results demonstrate how the spin-phonon coupling and quantum effect cooperatively develops the roton-like minimum in triangular lattice antiferromagnets with a 120° structure.

10:12AM A29.00010 Magnetic phase diagram and multiferroicity of Ba$_3$MnNb$_2$O$_9$: A spin-triangular lattice antiferromagnet with weak easy-axis anisotropy\cite{3}, M. LEE, E.S. CHOI, Natl High Magnetic Field Lab, X. HUANG, Southeast University, Nanjing, China, J. MA, C.R. DELA CRUZ, M. MATSUDA, W. TIAN, Oak Ridge Natl Lab, TN, USA, Z.L. DUN, University of Tennessee, TN, USA, S. DONG, Southeast University, Nanjing, China, H.D. ZHOU, University of Tennessee, TN, USA — We have performed magnetic, electric, thermal, and neutron powder diffraction (NPD) experiments as well as density functional theory (DFT) calculations on Ba$_3$MnNb$_2$O$_9$. All results suggest that Ba$_3$MnNb$_2$O$_9$ is a spin-1/2 triangular lattice antiferromagnet (TLAF) with weak easy-axis anisotropy. At zero field, we observed a narrow two-step transition at $T_{k1} = 3.4$ K and $T_{k2} = 3.0$ K. The neutron diffraction measurement and the DFT calculation indicate a 120° spin structure in the ab plane with out-of-plane canting at low temperatures. With increasing magnetic field, the 120° spin structure evolves into up-up-down (udd) and oblique phase showing successive magnetic phase transitions, which fits well to the theoretical prediction for the 2D Heisenberg TLAF with classical spins. Multiferroicity is observed when the spins are not collinear but suppressed in the udd and the oblique phase. We discuss the results in comparison with our previous works on its sister compounds with small spins, Ba$_3$NiNb$_2$O$_9$ ($S = 1$) (J. Hwang et al., Phys. Rev. Lett. 109, 257205 (2012) and Ba$_3$CoNb$_2$O$_9$ ($S = \frac{3}{2}$) (M. Lee et al., Phys. Rev. B 89, 104420 (2014)).


1NIMHL is supported by NSF, the state of Florida and US DOE. ORNL HFIR was sponsored by U. S. DOE.

10:24AM A29.00011 Indirect RIXS study of bimagnon excitations in triangular-lattice quantum Heisenberg antiferromagnet\cite{4}, TRINANJAN DATTA, Georgia Regents University, CHENG LUO, ZHENGE HUANG, DAO-XIN YAO, Sun Yat-Sen University — Bimagnon correlations in triangular-lattice quantum Heisenberg antiferromagnet can be probed by the resonant inelastic X-ray scattering (RIXS) technique. Utilizing an interacting spin wave theory within the Bethe-Salpeter approximation scheme, we compute the K-edge indirect RIXS spectra for the nearest neighbor Heisenberg model with a general S for the entire magnetic Brillouin zone. The non-collinear spin arrangement in the triangular lattice geometry supports the intrinsic spontaneous single-magnon decay or recombination. Based on our calculation, we find that the RIXS spectra display a peak at the antiferromagnetic wave vector (4π/3, 0) corresponding to the triangular lattice, which is in contrast to the square lattice case. The major contribution to the RIXS spectra originates from the decay vertices arising from the three-magnon interaction terms, with the quartic interaction contributions subduced. Our results indicate that the spontaneous decay and recombination of magnons inherent to the triangular lattice model can be observed in the RIXS spectra without a disintegration.

10:36AM A29.00012 Stripes and antiphase boundaries in CaFe$_2$O$_4$\(^1\), CHRIS STOCK, Univ of Edinburgh, EFRAIN RODRIGUEZ, University of Maryland, MARK GREEN, Kent University, NARA LEE, S.-W. CHEONG, Rutgers University — We report on the magnetic structure and spin dynamics in CaFe$_2$O$_4$ based upon an orthorhombic structure \[1\]. The magnetic structure consists of two competing magnetic phases based upon stripes of S=5/2 Fe$^{3+}$ ions. The magnetic dynamics illustrate that the coupling is primarily two dimensional. On application of a magnetic field, antiphase magnetic boundaries can be introduced into the lattice and frozen in at low temperatures. We investigate the structure and dynamics of these domains using polarized and unpolarized neutron scattering and discuss how the triangular geometry allow these localized defects to be energetically favorable.  

\(^{1}\)Carnegie Trust for the Universities of Scotland, Royal Society, and EPSRC

10:48AM A29.00013 Anomalous weak ferromagnetism in \(R_{1-x}Y_xB_4\) \((R=\text{Sm, Gd, Tb, Dy, Ho, Er})\), B.Y. KANG, MYUNGUK SONG, B.K. CHO, School of Materials Science and Engineering, Gwangju Institute of Science and Technology (GIST), Korea, J.Y. KIM, Research Institute of Industrial Science & Technology, Korea — Since the report of magnetic properties of rare earth tetraborides, \(R_{1-x}Y_xB_4\) compounds have received a great attention over last decades because it shows various interesting magnetic ground states depending on rare-earth elements. \(R_{1-x}Y_xB_4\) exhibits antiferromagnetic ordering at low temperature and is classified as the Shastry-Sutherland lattice, which is a geometrically frustrated system. In this system, the disturbance of a delicate balance can lead to new electronic and magnetic states. In this study, single crystals of \(R_{1-x}Y_xB_4\) \((R=\text{Sm, Gd, Tb, Dy, Ho, Er})\), \((x=0, 0.1, 0.2, 0.3, 0.35, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1)\) were synthesized using the high-temperature AI solution growth method. Interestingly, weak ferromagnetism was found to emerge at the Neel temperature for the Y-doped single crystals of \(R_{1-x}Y_xB_4\). The magnitude of spontaneous magnetic moment was found to be correlated with the Y substitution ratio, which have maximum value at about 30% of Y-concentration. The weak ferromagnetism reveals also a strong magnetic anisotropy depending on rare-earth elements. The observed data indicate that the weak ferromagnetism is not due to an individual atomic effect but a systematic bulk effect. The exotic antiferromagnetic properties will be discussed in detail in terms of yttrium substitution and magnetic and geometrical structures.

Monday, March 2, 2015 8:00AM - 11:00AM –
Session A30 GMAG DMP: Focus Session: Nanomagnetic Devices I
206B - Alexander Khitun, University of California, Riverside

8:00AM A30.00001 Magnonic Holographic Memory\(^1\), ALEXANDER KHITUN, University of California Riverside, ALEXANDER KOZHEVNIKOV, Kotel’nikov Institute of Radioengineering and Electronics of Russian Academy of Sciences, Saratov Branch, FREDERICK GERTZ, University of California Riverside, YURI FILIMONOV, Kotel’nikov Institute of Radioengineering and Electronics of Russian Academy of Sciences, Saratov Branch — Collective oscillation of spins in magnetic lattice known as spin waves (magnons) possess relatively long coherence length at room temperature, which makes it possible to build sub-micrometer scale holographic devices similar to the devices developed in optics. In this work, we present a prototype 2-bit magnonic holographic memory. The memory consists of the double-cross waveguide structure made of \(Y_{x}Fe_{2}(FeO)_{13}\) with magnets placed on the top of waveguide junctions. Information is encoded in the orientation of the magnets, while the read-out is accomplished by the spin waves generated by the micro-antennas placed on the edges of the waveguides. The interference pattern produced by multiple spin waves makes it possible to build a unique holographic image of the magnetic structure and recognize the state of the each magnet. The development of magnonic holographic devices opens a new horizon for building scalable holographic devices compatible with conventional electronic devices.

\(^{1}\)This work was supported in part by the FAME Center, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA and by the National Science Foundation under the NEB2020 Grant ECCS-1124714.

8:12AM A30.00002 Calculating a parameter space to smoothly transport magnetically-trapped suspended superparamagnetic microbeads with electric-field domain wall control\(^1\), BRENDA MCLELLAN, New York University Polytechnic School of Engineering, MARK NOWAKOWSKI, JEFFREY BOKOR, University of California, Berkeley, CHENG-YEN LIANG, JOSHUA HOCKEL, KYLE WETZLAR, SCOTT KELLER, HYUNMIN SOHN, GREGORY CARMAN, University of California, Los Angeles, ANTHONY YOUNG, ANDREW DORAN, MATTHEW MARCUS, Advanced Light Source, Lawrence Berkeley National Laboratory, MATHIAS KLAUI, Institute of Physics, University of Mainz, 55128 Mainz, Germany, ROBERT CANDLER, University of California, Los Angeles, California NanoSystems Institute, Los Angeles, CA — We demonstrate the capture and electrically-driven piecewise transport of superparamagnetic microbeads trapped in a magnetostatic potential energy well produced by the magnetic domain walls of Ni micromirrors on a [Pb(Mg$_{1/3}$Nb$_{2/3}$)O$_3$]$_{66}$-[PbTiO$_3$]$_{34}$ (PMN-PT) substrate. Here I present micromagnetic simulations that illustrate the formation of field-initialized domain walls in Ni micromirrors and calculate the approximate force of attraction experienced by superparamagnetic microbeads near the domain walls. This force is estimated as a function of the ring geometry, bead diameter, and distance from the domain wall, and provides an upper bound for the strain-mediated, electrically-induced domain wall velocity that can be implemented to smoothly transport coupled microbeads within a fluidic environment. These results provide an initial estimate for important technological parameters and set a foundation for the optimization of this microfluidic magnetic control scheme. H. Sohn, M. Nowakowski, et al. submitted, 2014.

\(^{1}\)Supported by ESS and TANMS.

8:24AM A30.00003 Stochastic simulations of switching error in magneto elastic and spin-Hall effect based switching of nanomagnetic devices\(^1\), MD MAMUN AL-RASHID, SUPRIYO BANDYOPADHYAY, JAYASIMHA ATULASIMHA, Virginia Commonwealth University — Switching of single domain multiferroic nanomagnets with electrically generated mechanical strain \[1\] and with spin torque due to spin current generated via the giant spin Hall effect \[2\] are two promising energy-efficient methods to switch nanomagnets in magnetic computing devices. However, switching of nanomagnets is always error-prone at room temperature owing to the effect of thermal noise. In this work, we model the strain-based and spin-Hall-effect-based switching of nanomagnetic devices using stochastic Landau-Lifshitz-Gilbert (LLG) equation and present a quantitative comparison in terms of switching time, reliability and energy dissipation.  

\(^{1}\)This work is supported by the US National Science Foundation under the SHF-Small grant CCF-1216614, CAREER grant CCF-1253370, NEB 2020 grant ECCS-1124714 and SRC under NRI Task 2203.001.
8:36AM A30.0004 Preliminary experiments on SAW based magnetization switching of nanomagnets\textsuperscript{1}. VIMAL SAMPATH, NOEL D’SOUZA, SUPRIYOGO BANDYOPADHYAY, JAYASIMHA ATULASIMHA, Virginia Commonwealth University — Magnetization rotation in micron-sized ferromagnetic elements, using Surface Acoustic Waves (SAW), has been demonstrated experimentally \textsuperscript{1} while the use of SAW to lower the energy dissipation in switching of nanomagnets with spin transfer torque has been studied theoretically \textsuperscript{2}. Furthermore, SAW can be used to “Bennett clock” an array of nanomagnets in nanomagnetic logic without requiring lithographic contacts to individual nanomagnets \textsuperscript{3}. We report preliminary experiments on use of SAW to switch magnetostrictive Co nanomagnets grown on bulk 128 Y-cut lithium niobate. Switching is studied by imaging the nanomagnets’ magnetic states with Magnetic Force Microscopy (MFM) before and after the SAW waves interact with them. Switching of single, isolated nanomagnets of various sizes, and dipole coupled nanomagnets implementing a Boolean NOT gate, is studied.

\textsuperscript{1}This work is supported by the US National Science Foundation under the SHF-Small grant CCF-1216614.
\textsuperscript{2}CAREER grant CCF-1253370. NEB 2020 grant ECCS-1124714 and SRC under NRI Task 2203.001

8:48AM A30.0005 Magneto-elastic artificial neurons with extremely low energy dissipation\textsuperscript{1}. AYAN K. BISWAS, MD MAMUN AL-RASHID, JAYASIMHA ATULASIMHA, SUPRIYOGO BANDYOPADHYAY, Virginia Commonwealth University — We present a detailed analysis of artificial step transfer function neurons and binary weight synapses implemented with magneto-tunneling junctions whose soft layers are magnetostrictive nanomagnets switched with voltage generated mechanical strain. These devices are more energy-efficient than CMOS-based neurons or so-called spin neurons that are based on magnets switched with spin-polarized current \textsuperscript{1}. We studied their switching dynamics using stochastic Landau-Lifshitz-Gilbert simulations for two different geometries (elliptical and cylindrical) of the magnetostrictive nanomagnet. Our study revealed that while the step transition (firing) of the magnetic neuron is always very sharp at 0 K, the threshold is significantly broadened at room temperature, regardless of geometry and regardless of whether the magnetic neuron is switched with strain or spin-polarized current. While this could preclude some applications, the extreme energy-efficiency of these neurons makes them nearly ideal for use in certain types of neuromorphic computation. \textsuperscript{1}M. Sharad, et al., IEEE Trans. Nanotechnol., 11, 843 (2012).

This work is supported by the NSF under grant ECCS-1124714 and CCF-1216614.

9:00AM A30.0006 Three dimensional magnetic abacus memory \textsuperscript{1}. SHILEI ZHANG, Oxford University, JINGYAN ZHANG, University of Science and Technology Beijing, ALEXANDER BAKER, University of Oxford, SHOUGUO WANG, Chinese Academy of Science, GUANGHUA YU, University of Science and Technology Beijing, THORSTEN HESJEDAL, University of Oxford — Stacking nonvolatile memory cells into a three-dimensional matrix represents a powerful solution for the future of magnetic memory \textsuperscript{1,2}. However, it is technologically challenging to access the individual data in the storage medium if large numbers of bits are stacked on top of each other. Here we introduce a new type of multilevel, nonvolatile magnetic memory concept, the magnetic abacus \textsuperscript{3}. Instead of storing information in individual magnetic layers, thereby having to read out each magnetic layer separately, the magnetic abacus adopts a new encoding scheme which envisions a classical abacus with the beads operated by electron spins. It is inspired by the idea of second quantization, dealing with the memory state of the entire stack simultaneously. Direct read operations are implemented by measuring the artificially engineered 'quantized' Hall voltage \textsuperscript{4}, representing a count of the spin-up and spin-down layers in the stack. This concept of 'second quantization of memory' realizes the 3D memory architecture with superior reading and operation efficiency, thus is a promising approach for future nonvolatile magnetic random access memory. \textsuperscript{1}Parkin, S. S. P. et al. Science 320, 190 (2008). \textsuperscript{2}Lavrijsen, R. et al. Nature 493, 647 (2013). \textsuperscript{3}Zhang, S. L. et al. Sci. Rep. 4, 6109 (2014). \textsuperscript{4}Zhang, S. L. et al. Sci. Rep. 3, 2087 (2013).

9:12AM A30.0007 Controlling Magnetization using Spin Orbit Torque \textsuperscript{1}. SAYEEF SALAHUDDIN, EECS, UC Berkeley — Recently it has been shown that spin orbit coupling (SOC) and/or broken inversion symmetry in vertical heterostructures can generate accumulation of spins when a current is flowing through them. In doing so, it can exert a torque on an adjacent magnet \textsuperscript{1,2}. Indeed, high Z metals (Ta, Pt, W, etc.) with strong SOC have been used to inject spin currents into adjacent ferromagnetic layers and thereby to induce magnetic switching, oscillation, domain wall movement etc. SOC physics promises to significantly reduce the required current for current induced magnetic switching for next generation data-storage applications. In this presentation we shall discuss some of our recent work on SOC induced control of magnets with perpendicular magnetic anisotropy (PMA). A current flowing in-plane present interesting symmetry problems with respect to a PMA magnet. We shall discuss how these symmetry relations can be utilized for switching of and domain wall movement in the PMA magnets \textsuperscript{3}. In addition to storage applications, we shall also discuss possibility of exploiting SOC for spintronic logic applications \textsuperscript{4}.

\textsuperscript{3}D. Bhownik, et al., Deterministic Domain Wall Motion Orthogonal To Current Flow Due To Spin Orbit Torque, arXiv:1407.6137v1

9:48AM A30.0008 Bridging amount of spin-glasses over ferromagnetic/antiferromagnetic thin films and bit-cell dispersion of exchange bias in corresponding TA-MRAM devices \textsuperscript{1}. KAMIL AKMALDINOV, Spintec/Crocus Technology, CLARISSE DUCRUET, JEREMY ALVAREZ-HERAULT, Crocus Technology, VINCENT BALTZ, Spintec, SPIN-TEC TEAM\textsuperscript{2} — For thermally-assisted magnetic random access memories (TA-MRAM), lowering bit-cells dispersions of exchange bias is necessary. In this study, we prove that spin-glass-like phases (SG) spread over the ferromagnetic/antiferromagnetic (F/AF) storage layer are the main cause of such distributions once the film is nanofabricated into a device. In particular, we show that the less the SG, the lower the bit-cell dispersion. More precisely, the amount of SG was varied from sample to sample by sputtering various AFS: IrMn, FeMn and their alloys \textsuperscript{1}. Blocking temperature distributions were measured to quantify the amount of SG at the wafer level \textsuperscript{2}. The wafers were then patterned to obtain 1kb devices and all the cells were tested electrically. Finally, the resulting loop shift cumulative distribution functions accounting for the bit-cell dispersions were correlated to the initial amount of SG. In addition to bridging the gap between fundamental SG and a technological application, we also demonstrated that blocking temperature distributions are a versatile method to qualify TA-MRAM production batches before processing \textsuperscript{3}.


\textsuperscript{1}Univ. Grenoble-Alpes/CNRS/INAC-CEA, 38000 Grenoble, France
\textsuperscript{2}38000 Grenoble, France
10:00AM A30.00009 Electromechanical Switching of the Magnetization in Nanomagnets¹.
REEM JAAFAAR, City University of New York - LaGuardia Community College, EUGENE CHUDNOVSKY, City University of New York - Lehman College — We demonstrate the possibility of switching the magnetization by a mechanical kick generated by, e.g., a pulse of the electric field applied to a multiferroic nanoparticle or to a piezoelectric coupled to a magnetic particle that is free to rotate. The effect is based upon the observation that the mechanical rotation is equivalent to the magnetic field in the coordinate frame of the particle. This removes the symmetry argument on the way of reversing the magnetic moment by the electric field as the latter is used to generate rotation which provides the effective magnetic field acting on the magnetic moment. Analytical and numerical results will be reported.

¹This research was funded by DARPA MESO.

10:12AM A30.00010 Strain-induced Electric Field Switching of Magnetic Anisotropy in Ferromagnetic/Ferroelectric Interface¹.
Milwaukee — Magnetism induced by an external electric field (e-field) has received much attention as a potential approach for controlling magnetism at the nano-scale with the promise of ultra-low energy power consumption. Here, the electric field as the latter is used to generate rotation which provides the effective magnetic field acting on the magnetic moment.

¹This work was supported by NSF Grant No. ERCTANMS- 1160504.

10:24AM A30.00011 Strain control of magnetization in TbFe₂.
DORJKHUU, Department of Physics, Incheon National University, South Korea, P. V. ONG, TSEVELMAA, N. KIOUSSIS, Department of Physics and Astronomy, California State University Northridge, USA — Magnetostriuctive materials change their shape upon application of strain and can be used as actuators and sensors. In this work, we perform a computational analysis of a highly magnetostriuctive compound, TbFe₂, to understand how the lattice and magnetization couple. We use Density Functional Theory (DFT) to investigate the magnitude and direction of the metallic moment as a function of pressure. The localized nature of Tb e-electrons classify this compound as “strongly-correlated” and necessitate the simultaneous use of spin-orbit coupling to treat magnetostriction and the DFT methodology to capture the physics of the e-electrons. Although, the energy scales involved in spin-lattice interactions are extremely small, we were able to correctly reproduce the correct magnetic ground state and the experimentally observed ferrimagnetic coupling between Tb and Fe atoms in TbFe₂. The easy axis in TbFe₂ points along one of its body diagonals, which makes the shape of the crystal rhombohedral. Switching of magnetization between the easy axes requires the magnetization to pass through one of the [100] directions. In our study we show that by applying isotropic strain on TbFe₂ crystal, we can decrease the energy barrier between [111] and [100] magnetization directions of the crystal.

10:36AM A30.00012 Spin Optodynamics in Magnetic Solids¹.
TIANYU LIU, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa, XUFENG ZHANG, HONG X. TANG, Department of Electrical Engineering, Yale University, MICHAEL E. FLATTÉ, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa — Coherent couplings between cavity photons and spin ensembles, such as cold atoms [1] and nanomagnets [2], have been studied theoretically before. By virtue of magneto-optic interactions, we propose here to use a photonic cavity made of magnetic crystal to study the intrinsic coupling rate (Γ) that describes the effect of a single photon on the cavity. Cavity bistability due to multistatic magnetization is identified, and with clever choosing of driving fields, one can realize coherent amplification/damping of spin-wave amplitudes, which is superior than the incoherent methods, such as the one using spin transfer torque. Our theory has great potential in developing all optical control of magnonics.

¹This work was supported by DARPA MESO.

10:48AM A30.00013 Electric-field-induced modification in Curie temperature of Co monolayer on Pt (111).
KOHI NAKAMURA, MIKITO OBA, TORU AKIYAMA, TOMONORI ITO, Mie Univ, MICHAEL WEINERT, University of Wisconsin-Milwaukee — Magnetism induced by an external electric field (E-field) has received much attention as a potential approach for controlling magnetism at the nano-scale with the promise of ultra-low energy power consumption. Here, the E-field-induced modification of the Curie temperature for a prototypical transition-metal thin layer of a Co monolayer on Pt(111) is investigated by first-principles calculations by using the full-potential linearized augmented plane wave method that treats spin-spiral structures in an E-field. An applied E-field modifies the magnon (spin-spiral formation) energies by a few meV, which leads to a modification of the exchange pair interaction parameters within the classical Heisenberg model. With inclusion of the spin-orbit coupling (SOC), the magnetocrystalline anisotropy and the Dzyaloshinskii-Moriya interaction are obtained by the second variation SOC method. An E-field-induced modification of the Curie temperature is demonstrated by Monte Carlo simulations, in which a change in the exchange interaction is found to play a key role.

Monday, March 2, 2015 8:00AM - 11:00AM — Session A31 GMAG DMP: Focus Session: Molecular Magnets
207A - Christopher Landee, Clark University
8:00AM A31.00001 Photocontrol of Magnetism above 77 K in Nanoscaled Heterostructures of Cyanometallate Coordination Networks: Mechanism and Limits1. MARK W. MEISEL, Department of Physics and NHMFL, University of Florida — Using nanometer-sized heterostructures of cyanometallate coordination networks, specifically core@shell nanoparticles of CoFe@Cr2-PBA (PBA = Prussian blue analogues), irradiation by white light at 80 K modifies the magnetic response, and these changes remain intact and persist without continued irradiation to nominally 125 K. Preliminary pressure studies indicate the photoinduced changes can be maintained up to 200 K, the transition temperature of the ferromagnetic Cr2-PBA component. The effect, which we first reported up to 70 K, arises from thermally induced interface strain, which is relaxed by irradiation of the photactive constituent, CoFe-PBA. The ferromagnetic domains in the strained interface region are affected and generate the persistent changes of the magnetism. Our understanding of this photo-magnetostructural mechanism enabled us to extend the phenomenon to include photoactive spin-crossover systems2 and other ferromagnetic PBAs. The potential path to higher temperatures will be sketched.

1Presentation coauthored with Daniel R. Talham, UF Chemistry, and supported by the NSF via DMR-1405439 (DRT), DMR-1202033 (MWM), and DMR-1157490 (NHMFL), and by the UF Division of Sponsored Research.

8:36AM A31.00002 Single Crystal Neutron Diffraction Study of Organic Multiferroic (Nd1.2[FeCl3(D2)3])1. WEI TIAN, HUIBO CAO, JIAQIANG YAN, BRYAN CHAKOUMAKOS, BRIAN SALES, JAIME FERNANDEZ-BACA, Oak Ridge National Laboratory — (NH4)2[FeCl3(H2O)] is a new organic multiferroic that exhibits intriguing magnetic/multiferroic behavior as a function of temperature and applied magnetic field. Unlike its counterpart compounds where NH4 group is replaced by K, Cs, and Rb, [(NH3)2[FeCl3(H2O)] is the only system that undergoes two successive magnetic transitions accompanied by pronounced spontaneous electric polarization. Large deuterated (Nd1.2[FeCl3(D2)3]) single crystals were grown and characterized by specific heat and magnetization measurements showing no significant effects due to deuteration. Here we report single crystal neutron diffraction results that reveal an incommensurate antiferromagnetic order below Tc ∼ 7.3 K with a propagation vector of (0 0 0.77). Higher harmonic Bragg peaks were observed indicate “squaring up” behavior upon further cooling. At 1.5 K, a field induced incommensurate-to-commensurate transition was also observed by applying magnetic field along the a-axis.

8:48AM A31.00003 Slow relaxation of the magnetization in an Isostructural series of Zinc-lanthanide complexes: an integrated EPR and AC susceptibility study, ASMA AMJAD, INSTM Research Unit - LAMM Dipartimento di Chimica “U. Schiff,” Università di Firenze, Sesto Fiorentino(FI), Italy, AUGUSTIN MADALAN, MARIUS ANDRUH, University of Bucharest, Faculty of Chemistry, Inorganic Chemistry Laboratory, Bucharest, Romania, ANDREA CANESCHI, LORENZO SORACE, INSTM Research Unit - LAMM Dipartimento di Chimica “U. Schiff,” Università di Firenze, Sesto Fiorentino(FI), Italy. UNIVERSITY OF BUCHAREST, FACULTY OF CHEMISTRY, INORGANIC CHEMISTRY LABORATORY, BUCHAREST, ROMANIA COLLABORATION — Lanthanide based molecular complexes have shown potential to behave as single molecule magnets proficient to function above cryogenic temperatures. In this work we explore the dynamics of one such family, [Zn(LH)2Ln](NO3)2·6H2O – (Ln = Nd3+, Dy3+, Tb3+, Ho3+, Er3+, Yb3+). The series has a single lanthanide ion as a magnetic center in a low symmetry environment; the dynamics and energy landscape of the series is explored using X-band EPR, AC and DC susceptibility over a range of temperature, field and frequency. DC magnetic data show βX value consistent with expected behavior. EPR spectra for Er3+ and Yb3+ complexes shows EPR spectra typical for easy-plane and quasi-isotropic systems respectively, thus explaining the lack of out of phase susceptibility even in an external applied field. However, Dy3+ derivative show slow relaxation of the magnetization in zero field up to 15 K and is, accordingly EPR silent.

9:00AM A31.00004 Controlled Under Pressure: Understanding Spin Orbit Coupling and Exchange Anisotropy in Organic Magnets1. STEPHEN HILL, Florida State University and NHMFL, Tallahassee, FL32310 — The application of high pressure in the study of molecule-based materials has gained considerable interest, in part due to their high compressibilities, but also because the relevant electronic/magnetic degrees of freedom are often very sensitive to pressure. For example, small changes in the coordination environment around a magnetic transition metal ion can produce quite dramatic variations in both the on-site spin-orbit anisotropy as well as the exchange interactions between such ions when assembled into clusters or 3D networks. This has spurred the development of sophisticated spectroscopic tools that can be integrated with high-pressure instrumentation. The study of magnetic structure/property relations requires not only precise crystallographic data, but also detailed spectroscopic information concerning the unpaired electrons that give rise to the magnetic properties. This invited talk will begin with a brief description of the development and application of methods enabling EPR studies of oriented single-crystal samples subjected to hydrostatic pressures of up to 3.5 GPa. After an introductory example, the remainder of the talk will focus on a family of heavy atom organic radical ferromagnets (containing S and Se heteroatoms) that hold records for both the highest transition temperature and coercivity (for organic magnets). The latter is the result of an unexpectedly high magnetic anisotropy, attributable to spin-orbit-mediated exchange (hopping) processes. Ferromagnetic resonance (FMR) measurements reveal a continuous increase in the magnetic anisotropy with increasing pressure in the all Se compound, in excellent agreement with ab initio calculations based on the known pressure-dependence of its structure. The large value of anisotropic exchange terms in this heavy atom organic ferromagnet emphasizes the important role of spin-orbit coupling in a wide range of organic magnets where this effect is usually considered to be small.

1This work was supported by the NSERC (Canada) and the US NSF (DMR-1309463 and CHE-0924374).
2Work performed in collaboration with K. Thirunavukkuarasu (NHMFL), S. M. Winter (Waterloo), C. C. Beedle (NHMFL), A. E. Kovalev (NHMFL), R. T. Oakley (Waterloo).
6Thirunavukkuarasu et al., submitted (2014).
9:36AM A31.00005 Realization of Long-Term Air Stability in the Organic Magnet Vanadium Tetracyanoethylene\textsuperscript{1}  
IAN FRONING, MEGAN HARBERTS, YU LU, HOWARD YU, ARTHUR J. EPSTEIN, EZEKIEL JOHNSTON-HALPERIN,  
Ohio State Univ - Columbus — The organic ferromagnet vanadium tetracyanoethylene (VTCNE)\textsubscript{2} has potential uses in both microwave electronics and spintronics due to the combination of high temperature magnetic ordering (TC \geq 600 K), extremely sharp ferromagnetic resonance (peak to peak linewidth of 1 G), and low-temperature conformal deposition via chemical vapor deposition (CVD; deposition temperature of 50 C), but air-sensitivity leads to the complete degradation of the films within 2 hours under ambient conditions. We have encapsulated thin films of VTCNE\textsubscript{2} using a UV-cured epoxy that increases film lifetime to over 700 hours as measured by the remanent magnetization. The saturation magnetization and Curie temperature decay more slowly than the remanence, and the coercivity is unchanged after 340 hours of air exposure. Fourier transform infrared spectroscopy (FTIR) shows that the epoxy does not react with the film, and magnetometry measurements show that the epoxy does not impact bulk magnetic properties. This encapsulation strategy enables experimental protocols and investigations that were not previously possible for air-sensitive samples and points the way toward the development of practical applications for this promising organic-based magnetic material.

\textsuperscript{1}Supported by NSF grant DMR 1207243, and the NanoSystems Laboratory at the Ohio State University

9:48AM A31.00006 Photomagnetic and structural studies of Prussian blue analogue CoFe@CoCr core@shell heterostructures\textsuperscript{1}  
P.A. QUINTERO, T.V. BRINZARI, M.W. MEISEL, Dept. of Physics and NHMFL, Univ. of Florida, O.N. RISSET, M.J. ANDRUS, D.R. TALHAM, Dept. of Chemistry, Univ. of Florida, M.W. LUFASO, Dept. of Chemistry, Univ. of North Florida — The photomagnetic and structural properties of core@shell nanostructures of Prussian blue analogues, Rb\textsubscript{0.24}CoFe(CN)\textsubscript{6}O\textsubscript{0.74}K\textsubscript{0.10}CoCr(CN)\textsubscript{6}O\textsubscript{0.70} \cdot nH\textsubscript{2}O, with different shell thicknesses have been studied as a function of temperature and under white light irradiation\textsuperscript{2} The nature of the charge transfer induced spin transition (CTIST) of the core was affected by the presence of the shell. Specifically, while a continuous and hysteretic CTIST was observed in the bare cores, a discontinuous and non-hysteretic behavior was observed for the core@shell systems. In addition, the core@shell nanoparticles show light-induced magnetization changes radically different from the bare cores. These changes were modeled as a combination of the expected light-induced magnetism change in the cores and a modification of the magnetism in a region of the shell close to the interface, where the depth of the modified region was found to be about 25 nm for all shell thicknesses investigated.

\textsuperscript{1}Supported by the NSF via DMR-1202033 (MMW), DMR-1405439 (DRT), and DMR-1157490 (NHMFL).

10:00AM A31.00007 Separation of a molecular electronic configuration transition from the spin-crossover transition  
XIN ZHANG, SAU MU, University of Nebraska-Lincoln, JIA CHEN, Columbia University, GILLESCHI CHASTANET, DARO NATHALIE, JEAN-FRANCOIS LERTARD, TATIANA PALAMARCIUC, PATRICK ROSA, Université de Bordeaux, JING LIU, DARIO ARENA, GEORGE STELBINSKY, Brookhaven National Laboratory, BOHDAN KUNDYS, BERNARD DOUDIN, Université Louis Pasteur Strasbourg, PETER A. DOWBEN, University of Nebraska-Lincoln — We have investigated the unoccupied electronic structure of several molecular spin crossover systems including [Fe(H\textsubscript{2}B(pz)\textsubscript{2})\textsubscript{2}(bipy)]\textsuperscript{2+}, [Fe(H\textsubscript{2}B(pz)\textsubscript{2})\textsubscript{2}(phen)],[Fe(PM-Aza)\textsubscript{2}(NCS)\textsubscript{2} and [Fe(phen)\textsubscript{2}(NCS)\textsubscript{2}] by inverse photoemission (IPES) and X-ray absorption spectroscopy (XAS). The XAS clearly shows the change of iron L\textsubscript{2} edge spectra, typically associated with thermal induced spin crossover, occurring at temperatures well below the temperatures of the spin crossover transition. This suggests a change in the electronic structure configuration occurring separately from the spin ordering from a low spin to high spin state. These results may be significant to understand the observations that indicate that the spin crossover transition, and certainly the unoccupied electronic structure, is influenced by electric field. In some respects, these results for the molecular spin crossover transition resemble the separation of the charge ordering transition from the ferromagnetic transition in the manganites.

10:12AM A31.00008 Changes in the unoccupied electronic structure of [Fe(H\textsubscript{2}B(pz)\textsubscript{2})\textsubscript{2}(bipy)]\textsuperscript{2+} thin films  
YANG LIU, XIN ZHANG, SUMIT BENIWAL, AXEL ENDERS, Univ of Nebraska - Lincoln, PATRICK ROSA, JEAN-FRANCOIS LERTARD, TATIANA PALAMARCIUC, Université de Bordeaux, JING LIU, DARIO ARENA, National Synchrotron Light Source, BERNARD DOUDIN, Université Louis Pasteur Strasbourg, PETER A. DOWBEN, Univ of Nebraska - Lincoln, GROUPE DES SCIENCES MOLECULAIRES, UNIVERSITE DE BORDEAUX COLLABORATION, BROOKHAVEN NATIONAL LABORATORY, NATIONAL SYNCHROTRON LIGHT SOURCE COLLABORATION, INSTITUT DE PHYSIQUE APPLIQUE DU PHYSIQUE ET CHIMIE DES MATIEREAUX DE STRASBOURG, UNIVERSITE LOUIS COLLABORATION — We have investigated the unoccupied electronic structure of ultra thin films of the spin crossover [Fe(H\textsubscript{2}B(pz)\textsubscript{2})\textsubscript{2}(bipy)] complex (with H\textsubscript{2}B(pz)\textsubscript{2} =bis(hydrido)bis(1H-pyrazol-1-yl)borate and bipy = 2,2'-bipyridine) deposited on Au(111) by inverse photoemission (IPES) and X-ray absorption spectroscopy (XAS). The XAS clearly shows the changes of iron L\textsubscript{2} edge spectra typically associated with thermal induced spin crossover and found to be very consistent with the changed of the lowest unoccupied molecular orbitals seen in inverse photoemission with temperature. A band gap of 2-3 eV is deduced from combined UPS and IPES measurements of the films on Au substrates. The shift of the unoccupied density of states seen in inverse photoemission and XAS, with temperature, differs little from the molecular powder suggesting little influence of the substrate. We suggested that the ordering of this spin-crossover molecule on the gold substrate, may lead to a small anisotropy energy, for the molecular high spin state.

10:24AM A31.00009 Spin-lattice interactions as revealed by the pressure-temperature phase diagram of Co[N(CN)\textsubscript{2}]\textsubscript{2}  
JANICE MUSFELDT, Univ of Tennessee, Knoxville, T. V. BRINZARI, K. R. O’NEAL, P. CHEN, University of Tennessee, J. A. SCHLEUTER, Argonne National Laboratory, J. L. MANSON, Eastern Washington University, A. P. LITVINCHUK, University of Houston, Z. LIU, Carnegie Institute — We combined diamond anvil cell techniques, synchrotron-based infrared and Raman spectroscopies, and complementary lattice dynamics calculations to investigate spin-lattice coupling and the magnetic crossover mechanism in the molecule-based quantum magnet Co[N(CN)\textsubscript{2}]\textsubscript{2}. These findings along with prior magnetic properties work were brought together to create a pressure-temperature phase diagram in which the second-order structural boundaries converge on key areas of activity involving the spin state, exposing how the pressure-induced local lattice distortions trigger the ferromagnetic to antiferromagnetic crossover transition. Similar triggering events may take place in other materials.

\textsuperscript{1}We thank the NSF and PRF for support of this work.
10:36AM A31.00010 Observation of the interplay between Photoinduced Magnetisation and Pressure Induced Electron Transfer in Cobalt Hexacyanoferrare Prussian Blue Analogue1, M.K. PEHRAH, M.F. DUMONT, M.W. MEISEL, Dept. of Physics and NHMFL, Univ. of Florida, C.H. LI, D.R. TALHAM, Dept. of Chemistry, Univ. of Florida — The Prussian blue analogue K₃[CoFe(CN)₆]·nH₂O (CoFe-PBA) has been studied in both its light and dark states as a function of pressure up to 2.23 GPa. The material is known to undergo photoinduced magnetization (PIM) where irradiation leads to an increase in magnetization. On the other hand, application of pressure results in a pressure induced electron transfer (PIET) where a decrease in magnetization is observed. Both phenomena involve a spin transition between the low spin (S = 0) and the high spin (S = 2) states, and our work encompasses the application of both light and pressure to study the interplay between these two external stimuli. Our magnetic results indicate the suppression of the PIM at 2.23 GPa, but below this pressure, the coexistence of PIET and PIM is observed. Furthermore, in high temperature region, we observe a increase in the temperature at which the charge transfer induced spin transition (CTST) occurs.

1Supported by NSF DMR-105581 and DMR-1405439 (DRT), DMR-1202033 (WWM), and DMR-1157490 (NHMFL).

10:48AM A31.00011 A fully first-principles approach to the Molecular Kondo problem, MARIA SORIANO, Univ Autonoma de Madrid, DAVID JACKOB, Max Planck Institute of Microstructure Physics, JUAN JOSÉ PALACIOS, Univ Autonoma de Madrid, ATOMELIX TEAM — There has been a great effort in recent years to understand the emerging Kondo-like resonances in different magnetic molecules such as MnPC. Theoretical approaches based on atomic models have proven to be very useful for the study of this phenomenon when the magnetic moment is essentially localized on a magnetic atom [1,2]. Nevertheless the Kondo effect can arise in pure carbon-based systems as has been demonstrated experimentally in fullerences and carbon nanotubes [3,4]. In this communication we present a multiorbital Anderson model where the orbitals are not atomic but molecular orbitals. This model is fully obtained from Density Functional Theory calculation in combination with Green’s functions methodologies [5,6]. Standard impurity solver techniques are used to solve the model which is applied to fullerenes and other nanographene structures [7].

1 A. Ströbele et. al. Phys. Rev. Lett. 109, 147202 (2012);
2 D. Jacob et. al. Phys. Rev. B 88, 134417 (2013);
4 P. Jarillo-Herrero et. al. Nature 434, 484. (2005);
5 ANT.G03. www.alacant.dfa.ua.es;
6 D. Jacob et. al. Phys. Rev. B 82, 195115 (2010);

Monday, March 2, 2015 8:00AM - 11:00AM — Session A32 GMAG DMP: Focus Session: Magnetic Oxide Films. Surface and Interface Effects

8:00AM A32.00001 New chemical and magnetic structure at the domain walls of an epitaxial oxide, SAEDEEH FAROKHIPOOR, University of Groningen, Netherlands, C. MAGEN, Universidad de Zaragoza, Spain, S. VENKATESAN, Universitat Munchen, Germany, J. INIGUEZ, ICMAB-CSIC, Spain, C.J.M DAUMONT, D. RUBI, University of Groningen, Netherlands, E. SNOECK, CEMES - CNRS, France, M. MOSTOVOY, C. DE GRAAF, University of Groningen, Netherlands, A. MULLER, M. DOBLINGER, C. SCHEU, Universitat Munchen, Germany, B. NOHEDA, University of Groningen, Netherlands — Domain walls (DWs) in multiferroic thin films are nanoscale regions presenting different properties compared to the adjacent domains. This distinct behavior originates from the broken crystal symmetry and intense strain gradients around the walls. Therefore, engineering and controlling the properties of DWs in different types of functional materials, in particular in complex oxides, can become a promising path to design and tailor novel electronic and spintronic devices. In TbMnO₃, an antiferromagnetic orthorhombic perovskite in bulk form, ferroelastic DWs can also be achieved in a very controlled way, with densities that increase inversely proportional to the film thickness, such that for the thinnest films, the volume fraction of DWs can be as much as 25% of the total film volume. These DWs, display a net magnetic moment that originates in an unique chemical environment, a novel Mn coordination has been locally synthesized due to the local stress present at the DWs. We believe that this method can be applied more generally to obtain embedded 2D ferromagnetic sheets of interest in electronics and spintronics. S. Farokhipoor, et al., Nature (20 Nov.2014).

8:12AM A32.00002 The stoichiometry and Surface termination of La₂/₃Sr₁/₃MnO₃ film on SrTiO₃ (001) substrate *, LINA CHEN, ZHEN WANG, GAOMIN WANG, HANGWEN GUO, MOHAMMAD SAGHAYEZHIAN, E.W. PLUMMER, JIANDI ZHANG, Louisiana State Univ - Baton Rouge, JING TAO, LIJUN WU, YIMEI ZHU, Brookhaven National Laboratory — It has been observed that films of La₂/₃Sr₁/₃MnO₃ (LSMO) are insulating when the films are below a certain critical thickness. The nature of such thickness-driven metal-to-insulator transition is still under debate: is this an intrinsic (dimensional confinement) or an extrinsic (oxygen vacancies or change of stoichiometry) effect? We have investigated the thickness-dependent composition variation in the LSMO films on SrTiO₃ (001) by Low Energy Electron Diffraction (LEED), Angle-resolved XPS (ARXPS), and scanning transmission electron microscopy (STEM). Both ARXPS and STEM results show that the LSMO films prefer to terminated with (La/Sr)-O layer and exists a thickness-dependence of Sr vs La concentration ratio in the film as well as the Sr surface segregation, incorporated with the thickness, are used to solve the model which is in the Mo2O2 basal plane. These changes should have profound effect on the electronic and magnetic property, including the emergent insulating behavior in ultrathin films. * Supported by U.S. DOE under Grant No. DOE DE-SC0002136


10:48AM A32.00004 Exchange Bias and Unusual Initial Magnetization in Nanocrystalline Spinel Ferrite Thin Films¹, URUSA ALAAN, Stanford University, SREENIVASULU GOLLAPUDI, Oakland University, KIN MAN YU, Lawrence Berkeley National Laboratory, PADRAIC SIMPER, ELKE ARENHOLZ, Advanced Light Source, GOPALAN SRINIVASAN, Oakland University, YURI SUZUKI, Stanford University — We report on unconventional magnetic behavior in nanocrystalline (Mn,Zn,Fe)₂O₄ (MZO) thin films grown at room temperature. Structural studies show no secondary phases, yet these films are exchange biased, with magnetic hysteresis loops shifted by as much as ~ 200 Oe at 10 K after field-cooling. The samples can be “trained” so that successive magnetization loops exhibit reduced exchange bias. Shifts of the hysteresis loops exist even after cooling in zero field, indicating that the MZO is not externally biased. We attribute the exchange bias to disordered, grain-boundary-like regions that bias more ordered MZO. Annealing experiments that improved sample crystallinity decreased the exchange bias. Higher annealing temperatures resulted in reduced coercivities, higher magnetizations, and even the elimination of the exchange bias. Annealing also removed an unusual crossover of the initial magnetization curve outside of the saturated magnetization loop. This behavior has been seen in so-called “mictomagnetic” alloys. Using x-ray magnetic circular dichroism measurements, we have shown that cation disorder was reduced with annealing, and correlated the atypical initial magnetization with the degree of disorder.

1We gratefully acknowledge the National Science Foundation for funding this research.
9:12AM A32.00005 New features in electronic transport across the ferromagnetic transition in SrRuO3/Nb:STo3 devices. SAURABH ROY, Physics of Nanodevices, Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — SrRuO3 (SRO), a moderately correlated material system, exhibits unique structural and magnetoelectric properties at interfaces with other correlated oxides. Here we report on new features in electronic transport across a functional interface between SRO and Nb:STo3, a n-type semiconductor. We map the potential landscape across such an interface using a nanoscale transport probe and find it to be strongly influenced by differences in local substrate termination. A difference in Schottky barrier height of 0.19 eV for SRO grown on local TiO2 or StO substrate terminations is found. This difference is attributed to different metal-oxygen displacements of the first unit cell of SRO at the different terminations; further supported by High-Resolution Transmission-Electron-Microscopy studies and Density Functional Theory calculations. This strong correlation of structure with electronic transport at the interface is reflected in a concomitant decrease of hot electron attenuation length from 1.6 u.c. to 0.88 u.c. at -2.1 V with the onset of the ferromagnetic state. This is attributed to the increased buckling of Ru-O-Ru bonds in ferromagnetic SRO, highlighting the role of strong correlations at such interfaces.

9:24AM A32.00006 Controlling the dimensionality of the octahedra network in SrRuO3/STo3 superlattice, MINGQIANG GU, Northwestern University, QIYUN XIE, Nanjing University of Posts and Telecommunications, GUOPING ZHANG, Indiana State University, XIAOSHAN WU, Nanjing University — Two dimensional (2D) systems in perovskites have been widely investigated by designing superlattices. We propose a way to control the dimensionality of the octahedra network in perovskite superlattices by selecting different substrate orientation and superlattice periods. Lower dimensionality like one-dimension (1D) and zero-dimension (0D) can be achieved. Taking SrRuO3/STo3 as an example, we demonstrate that the 1D structure is in a 1D Ising state, which is paramagnetic, while the 0D structure is ferromagnetic insulator with fully saturated magnetic moment on the Ru sites. New phenomena in the magnetic and electronic properties are observed, including large strain response, half-metallicity, and orbital-selective quantum confinement effects.

9:36AM A32.00007 The surface study of ReFeO3 (Re=Lu, Yb) thin films by X-ray Photoemission Spectroscopy and Density Function Calculation, SHI CAO, TULA PAUDEL, KISHAN SINHA, XUANYUAN JIANG, Dept. of Physics and Astronomy, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, Nebraska 68588, USA, WENBIN WANG, Dept. of Physics, Fudan University, Shanghai, 200433, China, EVGENY TSYMBAL, XIAOSHAN XU, PETER DOWBEN, Dept. of Physics and Astronomy, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, Nebraska 68588, USA — The rare-earth ferrites, ReFeO3, may have a large magneto-electric response, with high surface/interface polarization, thus the surfaces are of considerable interest. We have characterized the surfaces of hexagonal ReFeO3 (Re= Lu, Yb) and orthorhombic LuFeO3 thin films by angle resolved X-ray photoemission spectroscopy (ARPES) and compared with density function theory (DFT). The surfaces will terminate in either Fe-O or Re-O depending on whether in the hexagonal or orthorhombic phase of the rare earth ferrite, but consistent with the expectations of DFT. The orthorhombic or hexagonal phases of these rare earth ferrites have the Fe in different crystal fields, which in turn affects the electronic properties of the Fe-O ligands. These changes in electronegativity are experimentally evident as differences in the Fe 2p core level photoemission system properties, notably leading to a decrease of the atomic magnetic moments.

10:00AM A32.00009 ABSTRACT WITHDRAWN
high-pressure shock waves into the sample, while 8 keV x-rays from LCLS was used to probe the target.

We compressed using 3 ns square pulses with total laser energy of 6 J per beam. A drive intensity of $3 \times 10^{12}$, MAXENCE GAUTHIER, LUKE FLETCHER, ALESSANDRA RAVASIO, SLAC National Accelerator Laboratory and deuterated plastic targets are very large at very early times decay occurs rapidly as propagation distance increases. Finally we will consider the prospects for using these data to obtain theoretical models of compressed matter and will discuss future plans for the study of hot and dense matter.

measure plasmons and to visualize the density and pressure evolution across melt lines by resolving correlations at distances comparable to atomic scales. Our theoretical models of compressed matter include shifts in the peak positions and changes in their crystal-field splitting, on moving from the bulk to the surface. Moreover, we observe these changes to extend several layers into the films rather than being restricted to the topmost layer. For example in a $\text{LaFeO}_3/(\text{SrFeO}_3)_m$ superlattice, we observe that the Fe oxidation state remains unchanged, a reversal in the intensity of the crystal-field split $I_{6g}$ and $I_{eg}$ peaks occurs over a length of 5 unit cells suggesting a shift from octahedral coordination in the bulk to tetrahedral coordination at the surface. Simultaneously acquired annular bright field and dark field images allow us to map the associated changes in their structure, such as cation displacements and changes in oxygen columns. We combine these results with density functional theory calculations to give a complete picture of surface reconstruction in the studied films including changes in the electronic, magnetic properties and its effect on the adsorption of $\text{CO}_2$ and $\text{H}_2\text{O}$ molecules that could point to routes to tune surface properties for water splitting and other applications.

In Extreme Conditions instrument at the Linac Coherent Light Source a world-unique experimental capability has become available to study the physics of hot and dense matter. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory — We have obtained pressure physics data from micron-thick tantalum films using our ultrafast laser shock platform. By measuring free surface velocity time histories at breakout, and shock wave arrival times at different film thicknesses, we have been able to estimate the dependence of peak and shock velocities on propagation distances and strain rates. We will show how elastic precursor shock waves depend on strain rate in the regime up to and above $10^9$ s$^{-1}$. We find that while elastic amplitudes are very large at very early times decay occurs rapidly as propagation distance increases. Finally we will consider the prospects for using these data to obtain the dynamic strength of tantalum at these very high strain rates. This work was supported by the NSF (DMR-1008791 and ECCS-1232275).

10:48AM A32.00013 Magnetic anomalies in self-assembled SrRuO3 - CoFe2O4 nanostructures studied by Raman spectroscopy . YI-CHUN CHEN, YEN-CHIN HUANG, CHIA-HSIEN CHIEN, Department of Physics, National Cheng Kung University, HENG-JUI LIU, YING-HAO CHU, Department of Materials Science and Engineering, National Chiao Tung University — Self-assembled nanostructures with high interface-to-volume ratio usually possess interesting physical properties through the coupling between neighboring materials. In complex-oxide nanomaterials, the interplay of spin charge, orbital, and lattice degrees of freedom especially provides various functionalities. Our recent study had shown photo-induced magnetization switching in a self-assembled system, CoFe2O4 (CFO)- SrRuO3(SRO), where the CFO nanopillars were embedded in the SRO matrix. Moreover, this system also has significant magnetoresistance behaviors. In this study, we used Raman spectroscopy to investigate the magnetic coupling mechanisms in CFO-SRO nanostructures. Compared to the pure CFO films, the CFO nano-pillars under out-of-plane compressive strain show a slightly increase of $\text{Al}_2\text{O}_3$/Al(Fe) intensity ratio, which corresponds to a migration of Co ions from O-site (oxygen octahedron) to T-site (oxygen tetrahedron). This behavior can be further tuned by external stimulus, such as magnetic fields and temperatures. A strong increase of $\text{Al}_2\text{O}_3$/Al(Fe) ratio together with a discontinuous Al2 frequency shift occur at the SRO magnetic transition temperature. This result confirms that the spin-orbital interaction in CFO can be modulated by the SRO magnetic transition.

Monday, March 2, 2015 8:00AM - 11:00AM — Session A34 DMP: Focus Session: Experimental Techniques and Results: Dynamic High-Pressure Physics 210A -

8:00AM A34.00001 Studying compressed matter physics at the Linac Coherent Light Source1, SIEGFRIED GLENZER, LUKE FLETCHER, SLAC National Accelerator Laboratory, HED SCIENCE, SLAC NATIONAL ACCELERATOR LABORATORY TEAM, LAWRENCE BERKELEY LABORATORY TEAM, LAWRENCE LIVERMORE NATIONAL LABORATORY TEAM — With the advent of the Matter in Extreme Conditions instrument at the Linac Coherent Light Source a world-unique experimental capability has become available to study the physics of dynamically compressed solids. Our new high-energy-density science program at SLAC is aimed to take advantage of x-ray pulses with the highest peak brightness available today. In a single shot, the x-ray beam delivers $10^{12}$ x-ray photons in 50 fs focused to a spot of order 1 µm. This capability allows us to measure plasmons and to visualize the density and pressure evolution across melt lines by resolving correlations at distances comparable to atomic scales. Our data allow direct determination of pressure for validating theoretical models for the thermodynamics at high pressure. We will show how LCLS data test our theoretical models of compressed matter and will discuss future plans for the study of hot and dense matter.

1This work was supported by DOE Office of Science, Fusion Energy Science under FWP 100182

8:12AM A34.00002 Elastic precursor shock waves in tantalum at very high strain rates. JONATHAN CROWHURST, MICHAEL ARMSTRONG, HARRY RADOUSKY. JOSEPH ZAUG, SEAN GATES, Lawrence Livermore National Laboratory — We have obtained data from micron-thick tantalum films using our ultrafast laser shock platform. By measuring free surface velocity time histories at breakout, and shock wave arrival times at different film thicknesses, we have been able to estimate the dependence of peak and shock velocities on propagation distances and strain rates. We will show how elastic precursor shock waves depend on strain rate in the regime up to and above $10^9$ s$^{-1}$. We find that while elastic amplitudes are very large at very early times decay occurs rapidly as propagation distance increases. Finally we will consider the prospects for using these data to obtain the dynamic strength of tantalum at these very high strain rates. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344 with Laboratory directed Research and Development funding (12ERD042).

8:24AM A34.00003 X-ray scattering measurements of laser-driven shock compressed plastic and deuterated plastic targets, MAXENCE GAUTHIER, LUKE FLETCHER, ALESSANDRA RAVASIO, SLAC National Accelerator Laboratory, TILO DÖPPNER, Lawrence Livermore National Laboratory, SIEGFRIED GLENZER, SLAC National Accelerator Laboratory, HED SCIENCE COLLABORATION — The study of materials under extreme conditions, i.e., high energy density, has gathered enormous scientific interest in various domains from inertial confinement fusion to planetary physics. The material response of plastic to shock and its behavior is important because of its common use as an ablative in inertial confinement fusion experiments. In this study, simultaneous measurements of spatially and x-ray temperature sensitive emission from laser-shock compressed plastic foils allow us to study the structural transition from a polymer to a liquid-like state. The 527 nm, 2 GW laser system available at the MEC station of the LCLS facility has been used to compress CH and CD foils using laser-driven shocks. 40 to 57 µm thick CH and CD targets were compressed using 3 ns square pulses with total laser energy of 6 J per beam. A drive intensity of $3 \times 10^{12}$ W/cm$^2$ on each irradiated surface was used to generate high-pressure shock waves into the sample, while 8 keV x-rays from LCLS was used to probe the target.
8:36AM A34.00004 Anguilarly resolved x-ray scattering measurements of shock and ramp compressed polycrysaalline diamond. M.J. MACDONALD, SLAC National Accelerator Lab, University of Michigan, L.B. FLETCHER, E.J. GAMBOA, M. GAUTHIER, H.J. LEE, E. GALTIER, SLAC National Accelerator Lab, A. RAVASIO, SLAC National Accelerator Lab, LULI, A. GELEON, SLAC National Accelerator Lab, Stanford University, S. HAMEL, Lawrence Livermore National Lab, J. VORBERGER, Max Plank Institute, D.O. GERICK, University of Warwick, Z. CHEN, University of Alberta, D. KRAUS, B. BARBREL, University of California Berkeley, S. FUNK, J.B. HASTINGS, S.H. GLENZER, SLAC National Accelerator Lab, HED SCIENCE COLLABORATION COLLABORATION — Direct measurements of the crystal structure of materials under shock and ramp compression has remained an interesting and at times challenging area of fundamental research, particularly in the area of high pressure matter. In this work we present the results from 102 experiments on polycrystalline diamond performed with table-top scale laser systems. Here we present results for ultrafast laser driven shock experiments using up to 500x more drive intensity than our previous experiments, as determined with XRD measurements, by Stevens et al. (Propellants Explos. Pyrotech. 33, 286 (2008)). A near perfect match between the two sets of data was observed. Moreover, we have observed the dynamic formation of hexagonal diamond by shock-compression of highly oriented graphite samples. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This work was supported SSAA program Contract No. DEFG52- 06NA26212.

8:48AM A34.00005 Equation of state measurements of shocked ammonia gas. JOHN LANG, DANA DATTELBAUM, PETER GOODWIN, JOSHUA COE, DANIEL GARCIA, Los Alamos National Laboratory — Ammonia is one of the constituents of the liquid phases of the outer planets. We here present results from a series of gas gun-driven plate impact experiments on NH₃ gas at elevated initial density. PDV and VISAR optical diagnostics were used to directly measure shock velocities and particle velocities in the shocked gas, used in quantifying the principal Hugoniot locus, and pressure and density of the shocked gas. Emission was measured using both 5-color pyrometry and streak spectroscopy, from which we estimated the temperature of the shocked gas. The pressure and density measurements were in good agreement with results from simulations using the SESAME EOS for NH₃, however the measured temperatures were found to be consistently lower than in the simulations, and lower than shocked atom gas species such as Ar.

9:00AM A34.00006 Extreme dynamic compression with a table top laser¹, MICHAEL ARMSTRONG, JONATHAN CROWHURST, HARRY RADOUSKY, JOSEPH ZAUG, Lawrence Livermore Natl Lab — Recently, it was shown that the energy required for laser driven dynamic compression experiments varies as the third power of the compression time, where the compression time must be larger than the equilibration time of the sample. Traditional dynamic compression experiments typically have drive times greater than 10 ns, but a wide range of materials equilibrate on substantially faster time scales, which should enable such materials to be compressed on much shorter time scales. So, for materials which equilibrate on a sub-nanosecond time scale, ultrafast dynamic compression has the potential to substantially reduce the laser energy required to obtain highly compressed states of matter. This has been demonstrated for sub-Mbar pressures with <100 µJ energy laser drive pulses, where the laser drive energy per unit density change is as much as 10³ smaller than longer time scale experiments. Although these results are promising, extreme pressures (up to 10 Mbar) have not yet been observed with tabletop scale laser systems. Here we present results for ultrafast laser driven shock experiments using up to 500x more drive intensity than our previous work, which, by conventional scaling, should result in dynamic pressures previously only accessible to facility scale inarts.

9:12AM A34.00007 Dynamics of the shock-induced transition from graphite to warm dense diamond and liquid carbon¹, D. KRAUS, B. BARBREL, UC Berkeley, S. FRYDRYCH, J. HELFRICH, G. SCHAUANN, TU Darmstadt, J. VORBERGER, Max Plank Institut fuer die Physik komplexer Systeme, Dresden, D.O. GERICK, University of Warwick, L.B. FLETCHER, M. GAUTHIER, S. GOEDE, E. GRANADOS, H.J. LEE, B. NAGLER, E. GAMBOA, A. RAVASIO, W. SCHUMAKER, SLAC National Accelerator Laboratory, T. DOEPPNER, B. BACHMANN, Lawrence Livermore National Laboratory, P. NEUMAYER, GSI Helmholtzzentrum fuer Schwerionenforschung, G. GREGORI, University of Oxford, M. ROTH, TU Darmstadt, S.H. GLENZER, SLAC National Accelerator Laboratory, R.W. FALCON, UC Berkeley — We present novel experimental observations of the ion structure in warm dense carbon at pressures from 20 to 220 GPa and temperatures of several thousand Kelvins. Our experiments employ x-ray sources at kilo-joule class laser facilities and at the Linac Coherent Light Source to perform spectrally and angularly resolved x-ray scattering from shock-compressed graphite samples. Using different types of graphite and varying drive laser intensity, we were able to probe conditions below and above the melting line, resolving the shock-induced graphite-to-diamond and graphite-to-liquid transitions on nanosecond time scale. Moreover, we have observed the dynamic formation of hexagonal diamond by shock-compression of highly oriented graphite samples.

9:24AM A34.00008 Quantitative Results from Shockless Compression Experiments on Solids to Multi-Megabar Pressure. JEAN-PAUL DAVIS, JUSTIN BROWN, MARCUS KNUDSON, RAYMOND LEMKE, Sandia Natl Labs — Quasi-isentropic, shockless ramp-wave experiments promise accurate equation-of-state (EOS) data in the solid phase at relatively low temperatures and multi-megabar pressures. In this range of pressure, isothermal diamond-anvil techniques have limited pressure accuracy due to reliance on theoretical EOSs of calibration standards, thus accurate quasi-isentropic compression data would help immensely in constraining EOS models. Multi-megabar shockless compression experiments using the Z Machine at Sandia as a magnetic drive with stringent limits continue to be performed on a number of solids. New developments will be presented in the design and analysis of these experiments, including topics such as 2-D and magneto-hydrodynamic (MHD) effects and the use of LiF windows. Results will be presented for tantalum and/or gold, with comparisons to independently developed EOS. A Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:36AM A34.00009 EOS determination through microscopy- interferometry measurements: A low symmetry energetic materials case study¹, ELISSAIOS STAVROU, JOSEPH ZAUG, JONATHAN CROWHURST, SORIN BASTEA, MIKE ARMSTRONG, Lawrence Livermore National Laboratory, Material Science Division — Measuring equation of state (EOS) of solid specimens under pressure usually involves the determination of the primitive cell volume using x-ray diffraction (XRD) measurements. However, in the case of low symmetry (e.g. triclinic) materials with twinning features and large primitive cells, this can be problematic and ambiguous. In order to address this issue we examine the possibility of a direct approach which is based on measuring the surface area and thickness with microscopy and optical interferometry respectively. To test the validity of this approach applied to a crystalline material, we first compared our results from Triamino-Trinitrobenzene (TATB, SG P-1) with the published SESAME EOS for NH₃, however the measured temperatures were found to be consistently lower than in the simulations, and lower than shocked atom gas species such as Ar.

¹This work was performed by the U.S. Department of Energy jointly by Lawrence Livermore National Laboratory; Contract DE-AC52-07NA27344.
9:48AM A34.00010 Pressure-induced antiferrodistortive phase transition in SrTiO3: common scaling of soft-mode with pressure and temperature, SHIHWANG WENG, National Synchrotron Radiation Research Center, RUQING XU, Advanced Photon Source, Argonne National Laboratory, XINYUE FANG, Department of Physics, University of Illinois at Urbana-Champaign, AYMAN SAID, BOGDAN LEU, YANG DING, HAWOONG HONG, Advanced Photon Source, Argonne National Laboratory, PETER ABBAMONTE, Department of Physics, University of Illinois at Urbana-Champaign, S.-L. CHANG, National Synchrotron Radiation Research Center, T.-C. CHIANG, Department of Physics, University of Illinois at Urbana-Champaign — We report a study of the pressure-induced antiferrodistortive cubic-to-tetragonal phase transition in strontium titanate (SrTiO3) at ambient temperature. High-resolution inelastic X-ray scattering measurements reveal the softening of a phonon mode (R20) at the Brillouin zone boundary; a lattice distortion sets in at a critical pressure of 9.5 GPa, which corresponds to a critical volume reduction of 5.3%. Prior studies have shown that phonon softening and ensuing lattice distortion can be induced under ambient pressure by lowering the sample temperature through a critical temperature of 105 K. The relationship between the two phase transitions is clarified by comparing the powers laws of the pressure and temperature dependences of the softening behavior and by first-principles calculations of the energetics of the system.

10:00AM A34.00011 A new uniaxial strain measurement technique for improved strain homogeneity, MARK BARBER, University of St Andrews, CLIFFORD HICKS, Max Planck Institute for Chemical Physics of Solids, STEPHEN EDKINS, DANIEL BRODSKY, University of St Andrews, ANDREW MACKENZIE, Max Planck Institute for Chemical Physics of Solids — Response to uniaxial distortion can be a powerful probe of the electronic properties of a solid. However, it is not a very commonly applied technique, chiefly because of the technical challenges of obtaining good strain homogeneity while applying significant pressures. In typical uniaxial pressure measurements, thin and wide samples are clamped between two anvil. Our approach uses a different, easier technique: cutting the sample into a long, narrow bar, and securing its two ends with epoxy across a vice. We have already demonstrated this technique with measurements on Sr2RuO4. Here we explain the details of this technique and by using finite element simulations present the guidelines (readily achievable in experiments) that need to be followed in order to achieve high strain homogeneity.

10:12AM A34.00012 Calorimetry at high-pressure using high-frequency Joule-heating, ZACHARY GEBALLE, VIKTOR STRUZHJKIN, Carnegie Geophysical Lab — Calorimetric measurements of materials at 1 to 100 GPa of pressure would provide intriguing tests of condensed matter theories, sensitive probes of chemical reactions during high-pressure synthesis, and useful inputs for models of the Earth’s interior. We present the design and first results of quantitative heat capacity measurements at >10 GPa of pressure. High-frequency AC voltage heats a small metal strip pressed between diamond anvils, creating temperature oscillations whose amplitudes are determined from the higher harmonics of voltage. Thermal models show that frequencies >100 kHz are required to contain heat in the ng-mass samples, while electrical models show that frequencies >100 MHz are not practical. Our experimental results show that the heat of iron and nickel can indeed be measured at high pressures in diamond anvil cells, paving the way for studies of the energetics of a wide-variety of entropy-driven phase changes at high pressure.

10:24AM A34.00013 High pressure, high magnetic field dilatometry experiment applied to strongly correlated electron systems1, AUDREY GROCKOWIAK, DAVID GRAF, WILLIAM CONIGLIO, JU-HYUN PARK, TIMOTHY MURPHY, SCOTT HANNAHS, STANLEY TOZER, NHMFL-Florida State University — Standard dilatometry techniques including capacitance measurements [1] have been developed and used for low temperature and high magnetic field measurements, but do not permit the use of high pressures. Following the experimental development of [2], we present a setup coupling Fiber Bragg Gratings (FBG) with pressure cells to map the whole magnetic field-pressure-temperature phase space of various systems as actinides and pnictides. FBG dilatometry measurements permit to achieve a resolution of ΔL/L ≈ 3.10⁻⁷ making it the most sensitive dilatometry technique. “Mini-me” piston cylinder cells developed at the NHMFL permit us to reach a pressure of 3 GPa, and their compact size allows them to be used in highly constrained sample volume of a portable dilution refrigerator, giving us the ability to do high pressure dilatometry studies in any high magnetic field facility at temperatures as low as 25 mK. We will present the setup along with preliminary results obtained on diverse test samples.


1 NSF DMR-1157490, State of Florida, DOE NNSA SSAA DE-NA00019

10:36AM A34.00014 Metallic carbon at high pressure and low temperature, KATSUYA SHIMIZU, MAEDA KOKI, MASAFUMI SAKATA, KYOKUGEN, Osaka University, MUTSUUKI MURAKAMI, KANEKA Co., KYOKUGEN TEAM, KANEKA TEAM — Graphite shows phase transition into hexagonal diamond by an application of pressure at room temperature. We have studied the pressure-induced phase transition to hexagonal or cubic diamond with Raman spectroscopy and resistance measurements using highly crystallized graphite films prepared by heat treatment of carbonized polyimide films. Inhomogeneous resistivity between current direction along ab-plane and c-axis was found to unite by squeezing at low temperature.

10:48AM A34.00015 The influence of moisture content on the shock compression responses of brittle granular materials, KUN XUE, Beijing Institute of Technology — The irreversible energy-absorbing compaction processes of shocked particle layers change with the moisture content. The shock wave interaction with dry and wet granular layers is experimentally investigated to elucidate the moisture effects on the energy distribution in the brittle granular layers. It is found that the frictional and breakage dissipation combined as the plastic dissipation of the granular layers is increasingly mitigated by the increasing moisture content. The higher strain rate in the shock loaded wet granular layer leads to an increased number of debris as predicted by the theoretical analysis. Nevertheless the inter-particle moisture effectively lubricates the enhanced particle friction arising from the intensive particle rearrangement concomitant with the greater degree of particle breakage. As a result, the efficiency of the momentum transfer in the wet granular layer is significantly improved manifested by the much larger particle kinetic energy. Meanwhile the particle breakage mode transits from the corner grinding to the shear cleavage with moisture content as revealed by the SEM image of the recovered grains from shock wave experiments.

Monday, March 2, 2015 8:00AM - 10:48AM – Session A35 DAMOP: Low-Dimensional and Non-Equilibrium Physics in Quantum Gases 210B
- David Pekker, University of Pittsburgh
8:00AM A35.00001 Non-equilibrium dynamics of an impurity in the one-dimensional Bose gas
NEIL ROBINSON, ROBERT KONIK, Brookhaven National Lab — In recent years, the out-of-equilibrium dynamics of interacting many-body quantum systems have attracted much attention. Integrable quantum models have played an important role in understanding the role of local conservation laws in the relaxation of observables, explaining unusual experimental observations in the one-component Bose gas [1]. We study the non-equilibrium dynamics of “impurity” wave packets containing a single boson propagating in the one-component Bose gas. Utilizing the integrability of the multi-component Lieb-Liniger model and recent results from the algebraic Bethe ansatz [2], we compute the time-evolution of the density profile of the “impurity” in the cases where the bosons is of the same or different species as the background gas. Our method, based upon numerically solving the Bethe ansatz equations and evaluating the Lehmann spectral representation for local observables, allows us to reach long times with high numerical precision. By comparing results from the two-component Lieb-Liniger model to the one-component Bose gas we can comment on the role of distinguishability of impurities in integrable models.


8:12AM A35.00002 Quench dynamics of one-dimensional interacting bosons in a disordered potential: Elastic dephasing and critical speeding-up of thermalization1, MARCO TAVORA, New York Univ NYU, ACHIM ROSCH, University of Cologne, ADITI MITRA, New York Univ NYU — The dynamics of interacting bosons in one dimension following the sudden switching on of a weak disordered potential is investigated. On time scales before quasiparticles scatter (prethermalized regime), the dephasing from random elastic forward scattering causes all correlations to decay exponentially fast, but the system remains far from thermal equilibrium. For longer times, the combined effect of disorder and interactions gives rise to inelastic scattering and to thermalization. A novel quantum kinetic equation accounting for both disorder and interactions is employed to study the dynamics. Thermalization turns out to be most effective close to the superfluid-Bose glass critical point where nonlinearities become more and more important. The numerically obtained thermalization times are found to agree well with analytic estimates.

1Supported by NSF DMR 1303177

8:24AM A35.00003 Thermalisation of a quantum system from first principles, GREGOIRE ITHIER, Department of Physics, Royal Holloway, FLORENT BENAYCH-GEORGES, MAP5 Université Paris Descartes — How does a quantum system reach thermodynamical equilibrium? Answering such a question from first principles is, perhaps surprisingly, still an open issue (Popescu Nat. Phys. 2006, Goldstein PRL 2006, Genway PRL 2013). We present here a new model comprising an arbitrary quantum system interacting with a large arbitrary quantum environment, both initially prepared in a quantum pure state. We then demonstrate that thermalisation is an emergent property of the unitary evolution under a Schrödinger equation of this large composite system. The key conceptual tool of our method is the phenomenon of “measure concentration” appearing with functions defined on large dimension Hilbert spaces, a phenomenon which cancels out any effect of the microscopic structure of interaction Hamiltonians. Using our model, we first characterize the transient evolution or decoherence of the system and show its universal character. We then focus on the stationary regime and recover the canonical state well known from statistical thermodynamics. This finding leads us to propose an alternative and more general definition of the canonical partition function, that includes, among other things, the possibility of describing partial thermalisation.

8:36AM A35.00004 ABSTRACT WITHDRAWN

8:48AM A35.00005 Relaxation and thermalization in the one-dimensional Bose-Hubbard model: A case study for the interaction quantum quench from the atomic limit2, FABIAN HEIDRICH-MEISSNER, LODE POLLET, STEFAN SORG, LEV VDIMAR, LMU Munich — We study the relaxation dynamics and thermalization in the one-dimensional Bose-Hubbard model induced by a global interaction quench. Specifically, we start from an initial state that has exactly one boson per site and is the ground state of a system with infinitely strong repulsive interactions at unit filling [1]. The same interaction quench was realized in a recent experiment [2]. Using exact diagonalization and the density-matrix renormalization-group method, we compute the time dependence of such observables as the multiparticle occupancy and the momentum distribution function. We discuss our numerical results in the framework of the eigenstate thermalization hypothesis and we observe that the microcanonical ensemble describes the time averages of many observables reasonably well for small and intermediate interaction strength. Moreover, the diagonal and the canonical ensembles are practically identical for our initial conditions already on the level of their respective energy distributions for small interaction strengths.

[1] Sorg et al., PRA 90, 033606 (2014)

1Supported by the DFG through FOR 801 and the Alexander von Humboldt foundation.

9:00AM A35.00006 Measuring time-dependent Greens Functions of strongly correlated gases in optical lattices3, ADRIAN KANTIAN, DQMP, University of Geneva, ULRICH SCHOLLWOECK, Department für Physik, LMU München, THIERRY GIAMARCHI, DQMP, University of Geneva — Recent advances in single-site addressing [1] in optical-lattice confined strongly correlated ultracold gases promise to deliver entirely new capabilities for these systems to serve as quantum simulators. We show how these advances may be employed to design in-situ measurements of both local and nonlocal time-dependent Greens functions as well as higher-order correlators. Using analytics side-by-side with time-dependent DMRG we quantify the practically available resolutions of these schemes - which can be applied for practically any 1D and 2D system of lattice-confined ultracold atoms - for several examples of interest, such as the mobile impurity problem [2] and the superfluid-Mott insulator transition.


3This work was supported in part by the Swiss NSF under Division II.

9:12AM A35.00007 Entanglement entropy scaling laws and eigenstate thermalization in free fermion systems4, HSIN-HUA LAI, Natl High Magnetic Field Lab, KUN YANG, Natl High Magnetic Field Lab and Florida State University — We demonstrate that the entanglement entropy area law for free fermion ground states and the corresponding volume law for highly excited states are related by a position-momentum duality, thus of the same origin. For a typical excited state in the thermodynamic limit, we further show that the reduced density matrix of a subsystem approaches thermal density matrix, provided the subsystem’s linear size is small compared to that of the whole system in all directions. This provides an explicit example of eigenstate thermalization, and reveals how statistical physics emerges from a single eigenstate by tracing out a large number of degrees of freedom.

4This research is supported by the National Science Foundation through grant No. DMR-1004545.
9:24AM A35.00008 Particle partition entanglement of Luttinger liquids

C.M. HERDMAN, University of Waterloo, ADRIAN DEL MAESTRO, University of Vermont — We consider the Rényi entanglement entropy of a Luttinger liquid under a particle bipartition. Using Luttinger liquid theory, we demonstrate that the leading finite-size scaling of the second Rényi particle entanglement entropy is logarithmic in the system-size with a prefactor that is the inverse Luttinger parameter. While higher order corrections depend on the short distance physics, the leading order scaling depends only on the sole dimensionless parameter that characterizes the low energy physics; this contrasts with the leading entanglement entropy scaling under a spatial bipartition, for which the scaling coefficient is universal and independent of the Luttinger parameter. Additionally, using quantum Monte Carlo calculations, we explicitly confirm the Luttinger liquid theory scaling for the Lieb-Liniger model of delta function interacting bosons in the one-dimensional spatial continuum; we find that the scaling coefficient of the 2nd Rényi particle entropy of the ground state of the Lieb-Liniger model agrees with the Luttinger parameter determined from the Bethe ansatz.

9:36AM A35.00009 ABSTRACT WITHDRAWN

9:48AM A35.00010 ABSTRACT MOVED TO Y35.00008

10:00AM A35.00011 2D Superexchange mediated magnetization dynamics in an optical lattice

R.C. BROWN, Joint Quantum Institute, NIST & UMD, R. WYLLIE, Joint Quantum Institute, NIST & UMD; GTRI, S.B. KOLLER, E.A. GOLDSCHMIDT, M. FOSS-FEIG, J.V. PORTO, Joint Quantum Institute, NIST & UMD — The competition of magnetic exchange interactions and tunneling underlies many complex quantum phenomena observed in real materials. We study non-equilibrium magnetization dynamics in an extended 2D system by loading effective spin-1/2 bosons into a spin-dependent optical lattice, and we use the lattice to separately control the resonance conditions for tunneling and superexchange. After preparing a non-equilibrium anti-ferromagnetically ordered state, we quench the lattice to its final configuration, and observe relaxation dynamics governed by two well-separated rates. These rates scale with the underlying Hamiltonian parameters associated with superexchange and tunneling. Remarkably, with tunneling off-resonantly suppressed, we are able to observe superexchange dominated dynamics over two orders of magnitude in magnetic coupling strength, despite the presence of vacancies. In this regime, the measured timescales are in agreement with simple theoretical estimates, but the detailed dynamics of this 2D, strongly correlated, and far-from-equilibrium quantum system remain out of reach of current computational techniques.

1This work was partially supported by the AROs atomtronics MURI, and NIST. M.F.P. and E.A.G. acknowledge support from the National Research Council Research Associateship program.

10:12AM A35.00012 Sound-induced vortex interactions in a zero temperature two-dimensional superfluid

PIOTR SUROWKA, ANDREW LUCAS, Harvard University — Recent experimental work on two-dimensional turbulent superfluids have increased the importance of resolving fundamental theoretical questions about the nature of superfluid turbulence in two dimensions. Crucial to this task is a proper understanding of the effective dynamics of vortices in the superfluid. We present a systematic calculation of the effective action of $N > 1$ superfluid vortices, assuming that the underlying continuum action is the Gross-Pitaevskii action. Our calculation is valid at next-to-leading order in the ratio of the vortex core size to intervortex spacing, and so takes into account the leading-order dressing of superfluid vortices by sound. We are able to exactly determine the action for a pair of vortices and we find that it demonstrates no instability to annihilation. This is suggestive that the inverse cascade picture of classical turbulence is qualitatively correct for a turbulent zero temperature superfluid.

2W. J. Kwon et al., arXiv:1403.4658.

10:24AM A35.00013 Decay of hydrodynamic modes in dilute Bose-Einstein condensates

ERICH GUST, LINDA REICHL, Univ of Texas, Austin, Center for Complex Quantum Systems — We present the results of Bogoliubov mean field theory [1] applied to the hydrodynamic modes in a dilute Bose-Einstein condensate. The condensate has six hydrodynamic modes, two of which are decaying shear modes related to the viscosity, and two pairs of sound modes which undergo an avoided crossing as the equilibrium temperature is varied [2]. The two pairs of sound modes decay at very different rates, except in the neighborhood of the avoided crossing, where the identity of the longest-lived mode switches. The predicted speed and lifetime of the longest-lived sound mode are consistent with recent experimental observations on sound in an $^87$Rb Bose-Einstein condensate. The strong dependence of the decay rates on temperature implies a possible new method for determining the temperature of Bose-Einstein condensates. [1] L. E. Reichl and Erich D. Gust, Phys. Rev. A 88, 053603 (2013) [2] Erich D. Gust and L. E. Reichl, Phys. Rev. A, 90, 043615 (2014)

The authors wish to thank the Robert A. Welch Foundation Grant No. F-1051 for support of this work.

10:36AM A35.00014 ABSTRACT WITHDRAWN

Monday, March 2, 2015 8:00AM - 10:48AM —
Session A36 DAMOP: Interacting Fermi Gases I

8:00AM A36.00001 Dynamical instabilities and transient short-range order in the fermionic Hubbard model

JOHANNES BAUER, Harvard University, MEHRTASH BABADI, California Institute of Technology, EUGENE DEMLER, Harvard University — We study the dynamics of magnetic correlations in the half-filled fermionic Hubbard model following a fast ramp of the repulsive interaction. We use Schwinger-Keldysh self-consistent one-loop perturbation theory to investigate the evolution of single-particle Green’s functions and solve the non-equilibrium Bethe-Salpeter equation to study the dynamics of magnetic correlations. This approach gives us new insights into the interplay between single-particle relaxation dynamics and the growth of antiferromagnetic correlations. Depending on the ramping time and the final value of the interaction, we find different dynamical behavior which we illustrate using a dynamical phase diagram. Of particular interest is the emergence of a transient short-range ordered regime characterized by the strong initial growth of antiferromagnetic correlations followed by a decay of correlations upon thermalization. The discussed phenomena can be probed in experiments with ultracold atoms in optical lattices.

8:12AM A36.00002 Polarization induced phase separation and re-entrant transition of two component lattice fermions in one dimension

THEJA DESILVA, Georgia Regents University — By investigating the compressibility of one dimensional lattice fermions at various filling factors, we study phase separation and re-entrant transition within the framework of Bethe ansatz method. We model the system by repulsive Hubbard model and calculate compressibility as functions of polarization for arbitrary values of chemical potential, temperature, and interaction strength. For filling factors $0 < n < 1$, the compressibility is a non-monotonic function of polarization at all thermodynamic parameters. The compressibility reveals phase transition into phase separated state for both low and intermediate temperatures, as well as intermediate interactions as one increases the polarization. For certain filling factors, we find re-entrant transition into the mixed phase at a higher polarization.
8:24AM A36.00003 Size and shape of Mott regions for fermionic atoms in a two-dimensional optical lattice, TIAGO MENDES SANTOS, THEREZA PAIVA, RAIMUNDO R. DOS SANTOS, Federal University of Rio de Janeiro (UFRJ) — We investigate the harmonic-trap control of size and shape of Mott regions in the Fermi Hubbard model on a square optical lattice. The use of Lanczos diagonalization on clusters with twisted boundary conditions, followed by an average over 50-80 samples, drastically reduce finite-size effects in some ground state properties; calculations in the grand canonical ensemble together with a local-density approximation (LDA) allow us to simulate the radial density distribution. We have found that as the trap closes, the atomic cloud goes from a metallic state, to a Mott core, and to a Mott ring; the coverage of Mott atoms reaches a maximum at the core-ring transition. A “phase diagram” in terms of an effective density and the on-site repulsion is proposed, as a guide to maximize the Mott coverage. We also predict that the usual experimentally accessible quantities, the global compressibility and the average double occupancy (rather, its density derivative) display detectable signatures of the core-ring transition. Some spin correlation functions are also calculated, and predict the existence Néel ordering within Mott cores and rings.

8:36AM A36.00004 Ground-state properties of spin-imbalanced Fermions in three-dimensional optical lattices, PETER ROSENBERG, SIMONE CHIESA, SHIWEI ZHANG, College of William and Mary — The past two decades have seen remarkable progress in cold atom physics. Novel experimental techniques have made it possible to simulate many condensed matter models. One system that has received considerable focus is ultra-cold atoms in an optical lattice with unequal populations of two hyperfine states. This system is an ideal candidate for the experimental realization of the elusive Fulde-Ferrell-Larkin-Ovchinnikov phase. We investigate the phase diagram of this system using Hartree-Fock-Bogoliubov theory. Detailed numerical calculations are performed to determine the ground-state properties systematically for different values of density, spin polarization and interaction strength. We first consider the high density and low polarization regime, in which the effect of the optical lattice is most evident. We then proceed to the low density and high polarization regime where the effects of the underlying lattice are less significant and the system begins to resemble a continuum Fermi gas. We explore the effects of density, polarization and interaction on the character of the phases in each regime and highlight the qualitative differences between the two regimes.

8:48AM A36.00005 Spin-balanced Fulde-Ferrell superfluids in driven fermionic optical lattices, ZHEN ZHENG, The University of Texas at Dallas; University of Science and Technology of China, CHUNLEI QU, The University of Texas at Dallas, XUBO ZOU, University of Science and Technology of China, ZOU, College of William and Mary — We study a two-leg fermionic Hubbard ladder model with a state-dependent hopping. We find that, contrarily to the case without a state-dependent hopping, for which the system has a superfluid nature regardless of the sign of the interaction at incommensurate filling, in the presence of such a hopping a spin-triplet superfluid, spin- density wave and charge-density wave phases emerge. We examine our results in the light of periodically-driven optical lattices in cold atoms, and give protocols allowing to realize the spin-triplet superfluid elusive in the cold atoms.

9:00AM A36.00006 Two-leg fermionic Hubbard model with a state-dependent hopping, SHUN UCHINO, THIERRY GIAMARCHI, DQMP, University of Geneva — We study a two-leg fermionic Hubbard ladder model with a state-dependent hopping. We find that, contrarily to the case without a state-dependent hopping, for which the system has a superfluid nature regardless of the sign of the interaction at incommensurate filling, in the presence of such a hopping a spin-triplet superfluid, spin- density wave and charge-density wave phases emerge. We examine our results in the light of periodically-driven optical lattices in cold atoms, and give protocols allowing to realize the spin-triplet superfluid elusive in the cold atoms.

9:12AM A36.00007 Attractive Hofstadter-Hubbard model with imbalanced chemical and vector potentials, MENDERES ISKIN, Koc University - Istanbul — We study the interplay between the Hofstadter butterfly, strong interactions and Zeeman field within the mean-field Bogoliubov-de Gennes theory in real space, and explore the ground states of the attractive single-band Hofstadter-Hubbard Hamiltonian on a square lattice, including the exotic possibility of imbalanced vector potentials. We find that the cooperation between the vector potential and superfluid order breaks the spatial symmetry of the system, and gives rise to stripe-ordered Fulde-Ferrell-Larkin-Ovchinnikov (FFLO)-like superfluid and supersolid phases that can be distinguished and characterised according to their coexisting pair-density (PDW), charge-density (CDW) and spin-density (SDW) wave orders. We also discuss confined systems and comment on the likelihood of observing such stripe-ordered phases by loading neutral atomic Fermi gases on laser-induced optical lattices under laser-generated artificial gauge fields.

9:24AM A36.00008 Induced p-wave Superfluidity in Imbalanced Fermi Gases in a Synthetic Gauge Field, HERON CALDAS, Universidade Federal de Sao Joao del Rei, Sao Joao del Rei, Brazil, MUCIO CONTINENTINO, Centro Brasileiro de Pesquisas Físicas, Rio de Janeiro, Brazil — We study pairing formation and the appearance of induced spin-triplet p-wave superfluidity in dilute three-dimensional imbalanced Fermi gases in the presence of a uniform non-Abelian gauge field. This gauge field generates a synthetic Rashba-type spin-orbit interaction which has remarkable consequences in the induced p-wave pairing gaps. Without the synthetic gauge field, the p-wave pairing occurs in one of the components due to the induced (second-order) interaction via an exchange of density fluctuations in the other component. We show that this p-wave superfluid gap induced by density fluctuations is greatly enhanced due to the Rashba-type spin-orbit coupling.

9:36AM A36.00009 The Realization of 3D Weyl Semimetal Phase in Optical lattice and its Detection, WEN-YU HE, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China, SHI-ZHONG ZHANG, Department of Physics and Center of Theoretical and Computational Physics, The University of Hong Kong, Hong Kong, China, KAM TUEN LAW, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China — We describe a method to realize 3D Weyl semimetal phase in multilayer-coupled honeycomb optical lattices, with energy offset between the sublattices turned on. Two Raman beams are utilized to assist coupling between neighbor sites and generate synthetic magnetic flux both vertically and horizontally. Both one and two pairs of Weyl points can be achieved by tuning the unconventional interlayer coupling strength and the detuning in the Raman processes. We demonstrate that the detection of the emergence of Weyl points can be done through measuring the Landau Zener transitions of atoms from the lower occupied bands to the upper unoccupied bands.
9:48AM A36.00010 Nambu-Goldstone modes of an ultracold $^6\text{Li} - ^{40}\text{K}$ mixture in an optical lattice. ZLATKO KOINOV, Department of Physics and Astronomy, University of Texas at San Antonio, San Antonio, TX 78249, SHANNA PAHL, RAFAEL MENDOZA, Department of Physics and Astronomy, University of Texas at San Antonio, San Antonio, USA — A low-energy theory of the Nambu-Goldstone excitation spectrum and the corresponding speed of sound of an interacting Fermi mixture of Lithium-6 and Potassium-40 atoms in a two-dimensional optical lattice at finite temperatures with the Fulde-Ferrell order parameter is presented. We assume that the interacting fermions are in a sufficiently deep periodic lattice potential described by the Hubbard Hamiltonian. The discussion is restricted to the BCS side of the Feshbach resonance where the Fermi atoms exhibit superfluidity. The quartic on-site Hubbard interaction is decoupled via a Hubbard-Stratonovich transformation. The numerical solution of the Bethe-Salpeter equation in the generalized random phase approximation shows that the two-species Fermi gas has a superfluid phase revealed by two roton-like minima in the composite collective-mode energy. At some values of polarization, interacting strength and temperature, the dispersion relation of the Nambu-Goldstone excitation $\omega(Q)$ initially bends upward as the quasimomentum $Q$ increases before bending over. Due to this anomalous dispersion one long-wavelength phonon can decay into another one by absorbing a second phonon (Landau damping), or one phonon can decay into two others (the Beliaev damping).

10:00AM A36.00011 Unusual robust phase coherence in a coupled boson-fermion system. MACIEJ MASKA, Institute of Physics, University of Silesia, NANDINI TRIVEDI, The Ohio State University — We consider a coupled boson-fermion model in two dimensions, that describes itinerant fermions hybridizing with localized bosons composed of pairs of tightly bound opposite-spin fermions. We trace out the fermionic degrees of freedom and perform a Monte Carlo simulation for the effective classical Hamiltonian of boson phases. We find that the fermions not only generate an effective long-range temperature-dependent boson-boson coupling that generates a finite phase stiffness, but remarkably the phase stiffness is considerably more robust than that described by the XY model. Our analysis further shows that the inter-vortex interaction in the effective model is a power law rather than logarithmic as in the XY model. As one of the possible explanations for this persistent phase stiffness we consider the long range Berry phases carried by the itinerant fermions. Our results are relevant for resonance superfluids in the BCS-BEC crossover regime and also certain aspects of the high temperature superconductivity.

10:12AM A36.00012 Shear viscosity to entropy density ratios and implications for (im)perfect fluidity in Fermionic and Bosonic superfluids. RUFUS BOYACK, James Franck Institute, University of Chicago, Chicago, IL, HAO GUO, Department of Physics, Southeast University, Nanjing 211189, China, K. LEVIN, James Franck Institute, University of Chicago, Chicago, IL — Recent experiments on both unitary Fermi gases and high temperature superconductors (arxiv:1410.4835 [cond-mat.quant-gas], arxiv:1409.5820 [cond-mat.str-el]) have led to renewed interest in near perfect fluidity in condensed matter systems. This is quantified by studying the ratio of shear viscosity to entropy density. In this talk we present calculations of this ratio in homogeneous bosonic and fermionic superfluids, with the latter ranging from BCS to BEC. While the shear viscosity exhibits a power law (for bosons) or exponential suppression (for fermions), a similar dependence is found for the respective entropy densities. As a result, strict BCS and (true) bosonic superfluids have an analogous viscosity to entropy density ratio, behaving linearly with temperature times the (T-dependent) dissipation rate; this is characteristic of imperfect fluidity in weakly coupled fluids. This is contrasted with the behavior of fermions at unitarity which we argue is a consequence of additional terms in the entropy density thereby leading to more perfect fluidity. (arXiv:1407.7572v1 [cond-mat.quant-gas])

10:24AM A36.00013 Odd frequency Bosonic and Fermionic condensate. ALEXANDER BALATSKY, Los Alamos Natl Lab, Nordita — We introduce the concept of the odd-frequency Bose-Einstein Condensate (BEC), characterized by the odd frequency/time two-boson expectation value. To illustrate the concept of odd frequency BEC we present simple classification of pair boson condensates that explicitly permits this state. We point qualitative differences of odd-frequency BEC with conventional BEC and introduce the order parameter and wave function for the odd-frequency BEC [1]. This step extends the classification of the odd frequency states typically discussed in the context of odd frequency fermion pairing [2].


1Work supported by US DOE BES E304 and KAW.

10:36AM A36.00014 Vortex Dynamics in Atomic BECs: Some Recent Developments. PANAYOTIS KEVREKIDIS, UMass, Amherst — In the present work, we will briefly discuss a series of recent experiments by a number of groups enabling the examination of a small number of vortices (including ones of different charges) in atomic BECs. We will use a particle method to try to understand the dynamics of these vortices, in the appropriate limits. We will also briefly demonstrate a so-called generating function method that allows to connect the problem of identifying vortex centers to the theory of classical orthogonal (such as Hermite) polynomials. This formalism will be shown to be quite useful in identifying vortex polygons and other complex vortex patterns. Time permitting, generalizations to 3D settings and vortex rings will be briefly touched upon.

Monday, March 2, 2015 8:00AM - 11:00AM — Session A37 GQI: Focus Session: Semiconductor Qubits - Single Donors 212A - Bruce Kane, Laboratory for Physical Sciences

8:00AM A37.00001 Entanglement of an Electron-Nuclear Spin Pair in $^{28}\text{Si}$. STEPHANIE SIMMONS, CQ2T, Electrical Engineering Department, UNSW, Australia — Single-shot, single spin readout allows for strong projective quantum measurements which are used for Bell inequality violations, teleportation, error correction, and many other quantum codes. Very recently, strong projective measurements have become available using a long-lived electron-nuclear donor spin pair in silicon-$^{28}$. Here we demonstrate Bell/CHSH inequality violations, a proven entanglement witness, using this two spin system. A Bell inequality violation of 2.7(1) conclusively demonstrates on-demand two-spin entanglement, and the $>99\%$ detection efficiency simultaneously closes the detection loophole for this system. Furthermore, we improve upon the destructive electron measurement approach by mapping all electron detection efficiency onto the nuclear spin for high-fidelity quantum non-demolition (QND) measurement. Lastly, we complement the Bell inequality entanglement witness with full two-qubit state tomography complete with QND measurement. Preliminary results confirm a highly entangled state, yielding a fidelity of 99(2)\%, concurrence of 0.8(0), and a partial transpose negativity result of 0.46(4). Together these results demonstrate, within a single experiment, the very high initialisation ($>97\%$), estimated control ($>98\%$) and measurement ($>99.9\%$) fidelities in this two-qubit system.
8:36AM A37.00002 Local electrical control of a single-atom spin qubit in a continuous microwave field ¹, ANDREA MORELLO, ARNE LAUCHT, JUHA MUHONEN, FAHD MOHIYADDIN, RACHPON KALRA, JUAN DEHOLLAIN, SOLOMON FREER, FAY HUDDSON, MENNO VELDHORST, ANDREW DZURAK, UNSW Australia, KOHEI ITOH, Keio University, JEFFREY MCCALLUM, DAVID JAMIESON, University of Melbourne, ANDREA MORELLO, UNSW Australia — Local coherence times and fast manipulation are two desirable qualities of a qubit that for many systems are mutually incompatible. Storing quantum information in an ancillary qubit, i.e. a ‘quantum memory’, is a strategy to address this issue. It is a advantageous property of donor impurities in silicon to have qubits of both qualities in a single lattice site. Here we demonstrate storage and retrieval of quantum information from a single donor electron spin to its host phosphorus nucleus in isotopically-enriched ²⁸Si. We show a high fidelity memory process characterised via both state and process tomography. We use dynamical decoupling sequences during the nuclear storage to extend the memory time, and demonstrate storage and retrieval of a single qubit of information multiple times before decay. These results underline the inherent versatility and high fidelity of our two qubit system.

¹Funded by the Australian Research Council (CE11E000127) and the U.S. Army Research Office (W911NF-13-1-0024)

8:48AM A37.00003 Quantum memory in a single nucleus in silicon ², SOLOMON FREER, STEPHANIE SIMMONS, ARNE LAUCHT, JUHA MUHONEN, JUAN PABLO DEHOLLAIN, RACHPON KALRA, FAY HUDDSON, ANDREW DZURAK, UNSW Australia, KOHEI ITOH, Keio University, JEFFREY MCCALLUM, DAVID JAMIESON, University of Melbourne, ANDREA MORELLO, UNSW Australia — Long coherence times and fast manipulation are two desirable qualities of a qubit that for many systems are mutually incompatible. Storing quantum information in an ancillary qubit, i.e. a ‘quantum memory’, is a strategy to address this issue. It is a advantageous property of donor impurities in silicon to have qubits of both qualities in a single lattice site. Here we demonstrate storage and retrieval of quantum information from a single donor electron spin to its host phosphorus nucleus in isotopically-enriched ²⁸Si. We show a high fidelity memory process characterised via both state and process tomography. We use dynamical decoupling sequences during the nuclear storage to extend the memory time, and demonstrate storage and retrieval of a single qubit of information multiple times before decay. These results underline the inherent versatility and high fidelity of our two qubit system.

²Funded by the Australian Research Council (CE11E000127) and the U.S. Army Research Office (W911NF-13-1-0024)

9:00AM A37.00004 Optical quantum memory made from single nuclear spin in nitrogen vacancy in diamond. SEN YANG, YA WANG, THAI HIEN TRAN, S. ALI MOMENZADEH, RAINEER STOEHR, PHILIPP NEUMANN, 3rd Physics Institute, Universität Stuttgart, HIDEO KOSAKA, Department of Physics, Yokohama National University, JOERG WRACHTRUP, 3rd Physics Institute, Universität Stuttgart — Quantum repeater is one of the key elements to realize long distance quantum communication. In the heart of a quantum repeater is quantum memory. There are a few requirements for this memory: it needs to couple to flying qubits: photon; it needs to have long coherence time, so quantum error correction algorithm can be performed in the quantum repeater nodes; it needs to be stable under optical illuminations. Nitrogen nuclear spin is available for every nitrogen vacancy center(NV) in diamond. Besides it can be a robust quantum memory for spin qubit operations, nitrogen nuclear spin can couple to photon by taking advantage of optically resonant excitation of spin-selective transitions in low temperature. Here we demonstrate the coherent storage of quantum information from photon into nuclear spin. We show this quantum memory fulfills requirements as quantum memory for quantum repeater. Coherent time beyond 5 seconds is measured in ¹³C natural abundant sample. Under resonant laser excitations, the excited state quadruple and hyperfine interaction could lead to decoherence of nuclear spin. We show those interactions are low and nuclear spin can keep its coherence over 1000 times resonant laser excitation of electron spin.

9:12AM A37.00005 Electron Spin Resonance Experiments on a Single Electron in Silicon Implanted with Phosphorous, DWIGHT R. LUHMAN, K. NGUYEN, L.A. TRACY, S. CARR, J. BORCHARDT, N. BISHOP, G. TEN EYCK, T. PLUYM, J. WENDT, M.P. LILLY, M.S. CARROLL, Sandia Natl Labs — In this talk we will discuss the results of our ongoing experiments involving electron spin resonance (ESR) on single-electrons traps in a natural silicon sample. The sample consists of an SET, defined by lithographic polysilicon gates, coupled to nearby phosphorous donors. The SET is used to detect charge transitions and readout of the spin of the electron being investigated with ESR. The measurements were done with the sample at dilution refrigerator temperatures in the presence of a 1.3 T magnetic field. We will present data demonstrating Rabi oscillations of a single electron in this system as well as measurements of the coherence time, T₂. We will also discuss our results using these and various other pulsing schemes in the context of a donor-SET system. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a Lockheed-Martin Company, for the U. S. Department of Energy under Contract No. DE-AC04-94AL85000.

9:24AM A37.00006 Evaluation of strained silicon on insulator for SET based single donor spin read-out, PETER SHARMA, GREG TEN EYCK, DANIEL WARD, JASON DOMINGUEZ, KENTON CHILDS, JOEL WENDT, MICHAEL LILLY, MALCOLM CARROLL, Sandia National Laboratories — Recent successes in realizing single donor control and achieving very high fidelity gate operations has driven interest in silicon-based donor qubits. A number of proposals for donor to donor coupling rely on vertical field for Stark shift and ionization to a nearby interface. Back gaging silicon on insulator is one approach to achieving sufficient field strengths. We present low temperature measurements of back gatted SET structures and donor implanted SETs fabricated from strained silicon on insulator substrates with a low doped handle. This strained silicon system is useful for studying the effects of strain on both single donor physics and may provide insight into the behavior of strained silicon channels for quantum dots. We use SET thresholds to characterize the oxide/Si defect density. Back gaging influences the transient time response, mobility, and FET threshold. These parameters are also modified by above band gap light illumination. Two transport channels are observed, which also strongly depend on back gate voltage and illumination. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy Office of Science. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U. S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:36AM A37.00007 Electric field control of donor pair diatomic molecules in silicon, ALEJANDRA BAENA, Instituto de Física-Universidad Federal do Rio de Janeiro, ANDRE SARAIVA, University of Wisconsin-Madison and Instituto de Física-Universidade Federal do Rio de Janeiro, MARIA J. CALDERON, Instituto de Ciencias de Materiales de Madrid ICM-M-CSIC, BÉLITA KOILLER, Instituto de Física-Universidade Federal do Rio de Janeiro — Single donors are well-established building blocks for engineering electronic properties of semiconductors, acting effectively as giant hydrogen atoms [1]. Donor pairs, analogous to effective hydrogen molecules, were recently investigated [2,3] in the strongly interacting regime in silicon. In this regime, electric field control renders titmic results. Pairs that are more distant are more susceptible to external fields, and may harbour single electron charge control. Theoretically, the molecular quantum mechanics analogy between a donor pair and the H₂ molecule in vacuum is not as straightforward as it may seem. A detailed understanding of the electronic structure of these molecular systems is a current challenge. We analyze the lowest energy states within effective mass theory, including central cell corrected donor potential effects and the conduction band multiplicity in Si. The spectrum of ionized donor pairs and its response to an external electric field will be presented. We contemplate possible advantages of heteropolar diatomic molecules, e.g. Sb—As pairs, as more efficient elements for such devices and applications.

spin-state energetics and we discuss the effect of strain fields on the defect stability. We also discuss possible initialization schemes utilizing spin-dependent

parameters were derived from first-principles. We consider five native defects: \(V_{ab-initio}\) of defect spins with similar properties. We present a systematic study aimed at searching for localized triplet spin states in \(n\) for possible applications in quantum computing and metrology. In addition, these results stimulated an active search for other materials, which may exhibit

splitting, spin-orbit coupling, spin-spin coupling, strain and Jahn-Teller interactions. We have also carried out DFT calculations that support and complement

seen in recent experiments for the 4H-SiC defect. We have included several different mechanisms involved in the mixing of its spin states, such as crystal field

of separation, showing the transition from a Heitler-London like regime to a molecular regime. Excited valley states are found to affect the exchange energy for

to donors in silicon are important for both two qubit gates and spin readout. We present a full configuration interaction technique in the atomistic tight-binding

exploited to enable a logic operation based on selective resonant excitation. This operation has the enormous advantage that the inter-qubit interaction does not require any modification. Our calculations show that high-fidelity operations can be performed while tolerating a rather wide range of distances between atoms. This drastically reduces the demands posed on device fabrication, paving the way forward for large-scale quantum-information processing in silicon.

AS was funded by the Brazilian INCT on Quantum Information, FAPERJ, CNPq, CAPES, the William F. Vilas Trust and NSF (FRG-1206915).

10:00AM A37.00009 Robust Two-Qubit Gates for Donors in Silicon Controlled by Hyperfine Interactions

— RACHPON KALRA, ARNE LAUCHT, CHARLES D. HILL, ANDREA MORELLO, Centre for Quantum Computation and Communication Technology, Australia.

— CENTRE FOR QUANTUM COMPUTATION AND COMMUNICATION TECHNOLOGY, AUSTRALIA TEAM — The electron spin of a single atom in silicon is an excellent candidate for the building-block of a quantum computer. Recent breakthrough experiments have shown an individual phosphorus impurity atom can be used to store and elaborate one bit of quantum information. To continue along this exciting path, it is necessary to couple multiple phosphorus atoms in a controllable way and demonstrate quantum logic operations between pairs of qubits. This was thought to require exquisite control of their mutual interaction, and atomically-precise placement of the spins. Our work shows that the nuclei, to which the electrons are bound, can be exploited to realize a logic operation based on selective resonant excitation. This observation is of tremendous advantage as the inter-qubit interaction does not require any modification. Our calculations show that high-fidelity operations can be performed while tolerating a rather wide range of distances between atoms. This drastically reduces the demands posed on device fabrication, paving the way forward for large-scale quantum-information processing in silicon.

— Funded by the Australian Research Council (CE11E000127) and the U.S. Army Research Office (W911NF-13-1-0024)

10:12AM A37.00010 Triangulating the Position of Antimony Donors Implanted in Silicon

— CHLOE BUREAU-OXTON, Université de Sherbrooke, Sandia National Laboratories, ERIK NIelsen, DWIGHT LUHMAN, GREGORY TEN EYCK, TAMMY PLUYOM, JOEL WENDT, Sandia National Laboratories, MICHEL PIORO-LADRIERE, Université de Sherbrooke, MICHAEL LILLY, MALCOLM CARROLL, Sandia National Laboratories — A potential candidate for a quantum bit is a single Sb atom implanted in silicon. A single-electron-transistor (SET) situated close to an Sb donor can be used to measure the occupancy and spin of the electron on the donor while the lithographically patterned poly-silicon gates defining the SET can be used to control donor occupancy. In our samples two clusters of Sb donors have been implanted adjacent to opposite sides of the SET through a self-aligned process. In this talk, we will present experimental results that allow us to determine the approximate position of different donors by determining their relative capacitance to pairs of the SET’s poly-silicon gates. We will present the results of capacitive-based modeling calculations that allow us to further locate the position of the donors. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a Lockheed-Martin Company, for the U. S. Department of Energy under Contract No. DE-AC04-94AL85000.

10:24AM A37.00011 Atomic configuration interaction interaction simulations of two-electron states of donors in silicon

— ARCHANA TANKASALA, YU WANG, GERHARD KLIMECK, RAJIB RAHMAN, Purdue University — Two-electron states bound to donors in silicon are important for both two qubit gates and spin readout. We present a full configuration interaction technique in the atomistic tight-binding basis to capture multi-electron exchange and correlation effects taking into account the full bandstructure of silicon and the atomic scale inhomogeneity of a nanoscale device. The negatively charged two-electron \(D^-\) state of a single donor is solved as a function of a vertical field and depth from the silicon surface. Excited \(s\)-like states are found to strongly influence the charging energy. The same technique is used to solve the two-electron states of two donors as a function of separation, showing the transition from a Heitler-London like regime to a molecular regime. Excited valley states are found to affect the exchange energy for small donor separations.

10:36AM A37.0012 Electronic structure of Si vacancy centers in SiC

— ONEY SOYKAL, PRATIBHA DEV, SOPHIA ECONOMOU, Naval Research Laboratory (NRL) — The spin state of silicon vacancies in SiC is a promising candidate for applications in solid state quantum information technologies due to its long coherence time at room temperature, its technological availability and wide range of polytypism. Until recently, the electronic structure of this vacancy was not well understood. We have developed a group theoretical model that correctly predicts the spin \(3/2\) structure seen in recent experiments for the 4H-SiC defect. We have included several different mechanisms involved in the mixing of its spin states, such as crystal field splitting, spin-orbit coupling, spin-spin coupling, strain and Jahn-Teller interactions. We have also carried out DFT calculations that support and complement our analytical results.

10:48AM A37.0013 First-principles theory of defect spins in w-AlN for quantum information and sensing technologies

1 — HOSUNG SEO, MARCO GOVONI, GIULIA GALLI, The Institute for Molecular Engineering, The University of Chicago — The detection and coherent manipulations of the single nitrogen-vacancy defect spin in diamond \[1\] attracted a tremendous amount of attention for possible applications in quantum computing and metrology. In addition, these results stimulated an active search for other materials, which may exhibit defect spins with similar properties. We present a systematic study aimed at searching for localized triplet spin states in \(n\)-type \(w\)-AlN. We use a combination of \textit{ab-initio} calculations based on density functional and many-body perturbation theory and model calculations with an extended Hubbard Hamiltonian whose parameters were derived from first-principles. We consider five native defects: \(V_N\), \(V_A\), \(O_N\), \(V_AO_N\), and \(V_A/V_N\). We investigated the defect charge and spin-state energetics and we discuss the effect of strain fields on the defect stability. We will discuss how useful information can be extracted from large datasets obtained with full configuration interaction, multivalue, central-cell corrected effective mass calculations \[3\]. As examples, we will study the successful cases of theory/experiment comparison in Refs. \[1\] and \[2\], as well as provide early predictions for other systems, such as singlet-triplet donor-based qubits. \[1\] M. F. Gonzalez-Zalba, A. Saraiva, D. Heiss, M. J. Calderón, B. Koiller, and A. J. Ferguson, arXiv:1312.4589 (2013) \[2\] J. P. Dehollain, J. T. Muhonen, K. Y. Tan, A. Saraiva, D. N. Jamieson, A. S. Dzurak, and A. Morello, Phys. Rev. Lett. 112, 236801 (2014). \[3\] A. L. Saraiva, A. Baena, M. J. Calderón, and B. Koiller, arXiv:1407.8224 (2014)


Monday, March 2, 2015 8:00AM - 11:00AM

Session A38 GQI: Focus Session: Topological Quantum Information

— Mohammad Hafezi, University of Maryland
8:00AM A38.00001 Protected gates for topological quantum field theories, ROBERT KOENIG, Technical University Munich — We give restrictions on the locality-preserving unitary automorphisms U, which are protected gates, for topologically ordered systems. For arbitrary anyon models, we show that such unitaries only generate a finite group, and hence do not provide universality. For abelian anyon models, we find that the logical action of U is contained in a proper subgroup of the generalized Clifford group. In the case D(2), which describes Kitaev’s toric code, this represents a tightening of statement previously obtained within the stabilizer framework (PRL 110:170503). For non-abelian models, we find that such automorphisms are very limited: for example, there is no trivial gate for Fibonacci anyons. For Ising anyons, protected gates are elements of the Pauli group. These results are derived by relating such automorphisms to symmetries of the underlying anyon model: protected gates realize automorphisms of the Verlinde algebra. We additionally use the compatibility with basis changes to characterize the logical action. This is joint work with M. Beverland, F. Pastawski, J. Preskill and S. Sijher.

8:36AM A38.00002 Majorana Zero Modes Without Superconductivity at the Edge of Chiral Gapless Abelian Quantum Hall States, JENNIFER CANO, University of California, Santa Barbara, MENG CHENG, MAIISAM BARKESHLI, Microsoft Research, Station Q, CHETAN NAYAK, Microsoft Research, Station Q and University of California, Santa Barbara — We show that the $\nu = 8$ integer quantum Hall state can support Majorana fermion zero modes at domain walls between its two different stable chiral edge phases, even without superconductivity. This is due to the existence of an edge phase that does not support gapless fermionic excitations — all gapless excitations are bosonic in this edge phase. Majorana fermion zero modes occur at a domain wall between this edge phase and the more conventional one that does support gapless fermions. The zero modes survive the presence of gapless fermions in the conventional edge phase. Remarkably, the topological degeneracy of these zero modes has exponential protection, as a function of the relevant length scales, in spite of the presence of gapless excitations. These results are compatible with charge conservation, but do not require it. We discuss generalizations to other integer and fractional quantum Hall states.

8:48AM A38.00003 Fidelity of Majorana-based quantum operations, MOSTAFA TANHAYI AHARI, GERARDO ORTIZ, BABAK SERADJHE, Indiana Univ - Bloomington — It is well known that one-dimensional p-wave superconductor, the so-called Kitaev model, has topologically distinct phases that are distinguished by the presence of Majorana fermions. Owing to their topological protection, these Majorana fermions have emerged as candidates for fault-tolerant quantum computation. They furnish the operation of such a computation via processes that produce, braid, and annihilate them in pairs. In this work we study some of these processes from the dynamical perspective. In particular, we determine the fidelity of the Majorana fermions when they are produced or annihilated by tuning the system through the corresponding topological phase transition. For a simple linear protocol, we derive analytical expressions for fidelity and test various perturbative schemes. For more general protocols, we present exact numerics. Our results are relevant for the operation of Majorana-based quantum gates and quantum memories.

9:00AM A38.00004 Strongly interacting Majorana fermions, MARCEL FRANZ, CHING-KAI CHIU, DMITRY PIKULIN, University of British Columbia — Interesting phases of quantum matter often arise when the constituent particles — electrons in solids — interact strongly. Such strongly interacting systems are however quite rare and occur only in extreme environments of low spatial dimension, low temperatures or intense magnetic fields. Here we introduce a new system in which the fundamental electrons interact only weakly but the low energy effective theory is described by strongly interacting Majorana fermions. The system consists of an Abrikosov vortex lattice in the surface of a strong topological insulator and is accessible experimentally using presently available technology. The simplest interactions between the Majorana degrees of freedom exhibit an unusual nonlocal structure that involves four distinct Majorana sites. We formulate simple lattice models with this type of interaction and find exact solutions in certain physically relevant one- and two-dimensional geometries. In other cases we show how our construction allows for the experimental realization of interesting spin models previously only theoretically contemplated.

9:12AM A38.00005 An experimental proposal to observe non-abelian statistics of Majorana-Shockley fermions in an optical lattice, DONG-LING DENG, SHENG-TAO WANG, KAI SUN, LU-MING DUAN, Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA — Besides the conventional bosons and fermions, in synthetic two-dimensional (2D) materials there could exist more exotic quasi-particles with non-abelian statistics, meaning that the quantum states in the system will be transformed by non-commuting unitary operators when we adiabatically braid the particles one around another. The search for such non-abelian particles is of critical significance in the current investigation on quantum physics. Despite the recent great progress, it remains technically elusive to braid the quasi-particles in materials to verify their conjectured non-abelian statistics. Here, we propose an experimental scheme to observe non-abelian statistics with cold atoms in a 2D optical lattice. We show that the Majorana-Shockley modes associated with line defects can be braided with non-abelian statistics through adiabatic shift of the local potentials. Observation of the non-abelian statistics will serve both fundamental interest and practical importance, in particular for topological quantum computation.

9:24AM A38.00006 Decoherence Patterns of Topological Qubits from Majorana Modes, SUNG PO CHAO, Academia Sinica, SHIH HA-HO, National Center for Theoretical Science, CHUNG HSIEN CHOU, National Cheng Kung University, FENG LI LIN, National Taiwan Normal University — We investigate the decoherence patterns of topological qubits in contact with the environment. Each topological qubit is made of two Majorana modes of a 1D Kitaev’s chain. These two Majorana modes weakly interact with the fermionic/bosonic environments. We find the topological qubits decohere completely in the Ohmic and sub-Ohmic environments but not in the super-Ohmic ones. Though the fermion parities of the topological qubits cannot prevent the qubit states from decoherence in the sub-Ohmic environments, it can prevent the qubits turning into Gibbs state. We also study the cases in which each Majorana mode couples to different Ohmic-like environments and the time dependence of concurrence for two topological qubits.

9:48AM A38.00007 A simple quasi-1D model of Fibonacci anyons, DAVID AASEN, ROGER MONG, DAVID CLARKE, JASON ALICEA, California Institute of Technology, PAUL FENDELEY, University of Oxford — There exist various ways of understanding the topological properties of Ising anyons—from simple free-fermion toy models to formal topological quantum field theory. For other types of anyons simple toy models rarely exist; their properties have to be obtained using formal self-consistency relations. We explore a family of gapped 1D local bosonic models that in a certain limit become trivial to solve and provide an intuitive picture for Fibonacci anyons. One can interpret this model as a quasi-1D wire that forms the building block of a 2D topological phase with Fibonacci anyons. With this interpretation all topological properties of the Fibonacci anyons become manifest including ground state degeneracy and braid relations. We conjecture that the structure of the model is protected by an emergent symmetry analogous to fermion parity.

1 We thank J. Alicea, C. V. Kraus, and Y.-H Chan for discussions. D.L.D., S.T.W., and L.M.D. are supported by the NBRPC (973 Program) 2011CB900302, the IARPA MUSIQC program, the ARO and the AFSOR MURI program. K.S. is supported in part by NSF PHY-1402971.

3 FLH is supported by Taiwan’s NSC grants (grant NO. 100-2811-M-003-011 and 100-2918-I-003-008). All authors acknowledge the support by NCTS.

1) NSF grant DMR-1341822 2) Institute for Quantum Information and Matter, an NSF physics frontier center with support from the Moore Foundation. 3) NSERC-PGSD
10:00AM A38.00009 Robust quantum control using smooth pulses and topological winding
d. EDWIN BARNES, Condensed Matter Theory Center and Joint Quantum Institute, Dept. of Physics, University of Maryland, XIN WANG, Condensed Matter Theory Center, Dept. of Physics, University of Maryland — Perhaps the greatest challenge in achieving control of microscopic quantum systems is the decoherence induced by the environment, a problem which pervades experimental quantum physics and is particularly severe in the context of solid state quantum computing and nanoscale quantum devices because of the inherently strong coupling to the surrounding material. We present an analytical approach to constructing intrinsically robust driving fields which automatically cancel the leading-order noise-induced errors in a qubit’s evolution exactly. We address two of the most common types of non-Markovian noise that arise in qubits: slow fluctuations of the qubit energy splitting and fluctuations in the driving field itself. We demonstrate our method by constructing robust quantum gates for several types of spin qubits, including phosphorous donors in silicon and nitrogen-vacancy centers in diamond. Our results constitute an important step toward achieving robust generic control of quantum systems, bringing their novel applications closer to realization.

1Work supported by LPS-CMTC.

10:12AM A38.00010 Measuring second Chern number from dynamics, MICHAEL KOLODRUBETZ, Boston Univ, TIAGO SOUZA, ANATOLI POLKOVNIKOV, Boston University — By using the fact that Berry curvature acts as an effective electromagnetic field, recent work has demonstrated the direct experimental measurement of the first Chern number in systems of one and two superconducting qubits. This basic idea should extend to a number of interesting cases, including the presence of finite temperature or degenerate ground states. In this talk, I will show how in such a system one can measure the next non-trivial number in a line of topological invariants — the second Chern number. I will comment on experimental realizations of this measurement and its connection to fractionalization phenomena.

10:24AM A38.00011 Topological Phases of Sound and Light, VITTORIO PEANO CAVASOLA, CHRISTIAN BREDEL, MICHAEL SCHMIDT, FLORIAN MARQUARDT, University of Erlangen-Nuernberg — Topological states of matter are particularly robust, since they exploit global features insensitive to local perturbations. In this talk, we describe how to create a Chern insulator of phonons in the solid state. The proposed implementation is based on a simple setting, a dielectric slab with a suitable pattern of holes. Its topological properties can be wholly tuned in situ by adjusting the amplitude and frequency of a driving laser that controls the optomechanical interaction between light and sound. The resulting chiral, topologically protected phonon transport along the edges can be probed completely optically. Moreover, we identify a regime of strong mixing between photon and phonon excitations, which gives rise to a large set of different topological phases. This would be an example of a Chern insulator produced from the interaction between two physically very different particle species, photons and phonons.

10:36AM A38.00012 Topological Flux Phases of Levin-Wen String-Net Models, KAUSHAL PATEL, Univ of California - Santa Barbara, PARSA BONDERSON, Microsoft Station Q, KIRILL SHTENGEL, Univ of California - Riverside, STEVEN SIMON, Oxford — Levin-Wen string-net models provide exactly-solvable lattice models for gapped topological phases. We examine flux phases of these models, in which the lattice plaquettes contain a nontrivial flux instead of containing zero flux. In particular, we study $Z_N$ and Ising flux phases. We find that the Ising $\sigma$ flux phase is gapless, but nonetheless contains quasiparticles with topologically protected non-Abelian braiding statistics, thus providing an exactly-solvable model of a quasi-topological phase.

10:48AM A38.00013 Critical entanglement spectrum of one-dimensional symmetry protected topological phases, GUANG-MING ZHANG, Tsinghua Univ., BEIJING CHINA, XIN WAN, Zhejiang University, Hangzhou, China — Under an appropriate symmetric extensive bipartition in a one-dimensional symmetry protected topological (SPT) phase, a bulk critical entanglement spectrum can be obtained, resembling the excitation spectrum of the critical point separating the SPT phase from the trivial (vacuum) state. Such a critical point is beyond the standard Landau-Ginzburg-Wilson paradigm for symmetry breaking phase transitions. For the $S=1$ SPT (Haldane) phase with the Affleck-Kennedy-Lieb-Tasaki exact wave function, the resulting critical entanglement spectrum shows a delocalized version of the edge excitations in the SPT phase. From the wave function corresponding to the lowest entanglement energy level, the central charge of the critical point can be extracted and the critical theory can be identified as the same effective field theory as the spin-1/2 antiferromagnetic Heisenberg chain or the spin-1/2 Haldane-Shastry model with inverse square long-range interaction. (Reference: W. J. Rao, X. Wan, G. M. Zhang, Phys. Rev. B 90, 075151 (2014))

3Supported by National Science Foundation of China

Monday, March 2, 2015 8:00AM - 11:00AM — Session A39 GQI: Superconducting Qubits: Entanglement and Feedback 213AB - Leo DiCarlo, Delft University of Technology

8:00AM A39.00001 Superconducting qubits: entanglement by synchronous and asynchronous feedback, YEHAN LIU, S. SHANKAR, N. OFEK, M. HÄTRIDGE, A. NARLA, K.M. SLIWA, R.J. ŠCIOELKOPF, M.H. DEVORÉT, Department of Applied Physics, Yale University — Quantum feedback for error correction is now an important component of superconducting quantum information processing. We have implemented two feedback schemes, autonomous (AT) and measurement-based (MB), to stabilize entanglement between two transmon qubits coupled to a cavity. The two qubits are coupled with nearly equal dispersive shifts to the cavity, such that a cavity drive maps the qubits’ parity onto the cavity state. Entanglement is autonomously stabilized by applying continuous photon-number-selective Rabi drives on qubit transitions with phases conditioned on the measured signal. A synchronous protocol stabilizes entanglement for a fixed duration using either scheme resulting in a target Bell state with an unconditioned fidelity in excess of 55 % for MB and 77 % for AT. Furthermore, we have enhanced the fidelity of the entanglement by implementing an asynchronous “wait until success” protocol conditioning the tomography on a parity measurement in real time.

3Work supported by: IARPA, ARO, and ONR.
8:12AM A39.00002 Steady-state entanglement of distant transmons, stabilised against high transmission loss
FELIX MOTZOI, ELI HALPERIN, University of California, Berkeley, XIAOTING WANG, Massachusetts Institute of Technology, BIRGitta WHALEY, University of California, Berkeley, SOPHIE SCHIRMER, Swansea University — Being able to stabilise entanglement over long distances and long times provides numerous advantages over pulsed experiments (avoiding variability, synchronisation, and calibration issues) while providing an important resource on-demand, which can then be potentially distilled and used to construct a quantum network. We show how existing superconducting technologies can be entangled over distances of tens of meters providing resilient stabilisation even in the presence of high inefficiency of the transmission channel. This can be achieved both in the dispersive and non-resonant cavity regimes using simple protocols that employ correlated environmental interactions and symmetrity breaking. These require only a single-frequency drive that interacts sequentially with each cavity-qubit system. The dispersive regime protocol uses feedback while the near-resonant regime protocol is autonomous.

8:24AM A39.00003 Stochastic master equation approach for analysis of remote entanglement with Josephson parametric converter amplifier
M. SILVERI, Department of Physics, Yale University, E. ZALYS-GELLER, M. HATRIDGE, Z. LEGHTAS, M.H. DEVORET, Department of Applied Physics, Yale University, S.M. GIRVIN, Department of Physics, Yale University — In the remote entanglement process, two distant stationary qubits are entangled with separate flying qubits and the which-path information is erased from the flying qubits by interference effects. As a result, an observer cannot tell from which of the two sources a signal came and the probabilistic measurement process generates perfect heralded entanglement between the two signal sources. Notably, the two stationary qubits are spatially separated and there is no direct interaction between them. We study two transmon qubits in superconducting cavities connected to a Josephson Parametric Converter (JPC). The qubit information is encoded in the traveling wave leaking out from each cavity. Remarkably, the quantum-limited phase-preserving amplification of two traveling waves provided by the JPC can work as a which-path information eraser. By using a stochastic master approach we demonstrate the probabilistic production of heralded entangled states and that unequal qubit-cavity pairs can be made indistinguishable by simple engineering of driving fields. Additionally, we will derive measurement rates, measurement optimization strategies and discuss the effects of finite amplification gain, cavity losses, and qubit relaxations and dephasing.

8:36AM A39.00004 Optimizing JPC-based remote entanglement of transmon qubits via stochastic master equation simulations
E. ZALYS-GELLER, M. HATRIDGE, Department of Applied Physics, Yale University, M. SILVERI, Department of Physics, Yale University, A. NARLA, K.M. SLIWA, S. SHANKAR, Department of Applied Physics, Yale University, M.H. DEVORET, Department of Applied Physics, Yale University — Remote entanglement of two superconducting qubits may be accomplished by first entangling them with flying coherent microwave pulses, and then erasing the which-path information of these pulses by using a non-degenerate parametric amplifier such as the Josephson Parametric Converter (JPC). Crucially, this process requires no direct interaction between the two qubits. The JPC, however, will fail to completely erase the which-path information if the flying microwave pulses encode any difference in dynamics of the two qubit-cavity systems. This which-path information can easily arise from mismatches in the cavity linewidths and the cavity dispersive shifts from their respective qubits. Through analysis of the Stochastic Master Equation for this system, we have found a strategy for shaping the measurement pulses to eliminate the effect of these mismatches on the entangling measurement. We have then confirmed the effectiveness of this strategy by numerical simulation.

8:48AM A39.00005 Entanglement of remote transmon qubits by concurrent measurement using Fock states
A. NARLA, M. HATRIDGE, S. SHANKAR, Z. LEGHTAS, K.M. SLIWA, B. VLASTAKIS, E. ZALYS-GELLER, Department of Applied Physics, Yale University, M. MIRRAHIMI, Department of Applied Physics, Yale University and INRIA Paris Rocquencourt, M.H. DEVORET, Department of Applied Physics, Yale University — A requirement of any modular quantum computer is the ability to maintain individual qubits in isolated environments while also being able to entangle arbitrary distant qubits on demand. For superconducting qubits, such a protocol can be realized by first entangling the qubits with flying microwave coherent states which are then concurrently detected by a parametric amplifier. This protocol has a 50% success probability but is vulnerable to losses between the qubits and the amplifier which reduce the entanglement fidelity. An alternative is to use itinerant Fock states, since losses now tend to reduce the success probability of creating an entangled state but not its fidelity. Such single-photon protocols have been implemented in trapped-ion and NV-center experiments. We present such a protocol tailored for entangling two transmon qubits in the circuit QED architecture. Each qubit is entangled with a Fock state of its cavity using sideband pulses. The Fock states leak out of the cavity, interfere on a beam-splitter which erases their which-path information, and are subsequently detected using a novel photo-detector realized by another qubit-cavity system. Simulations suggest that we can realize a high-fidelity entangled state with a success probability as large as 1%.

9:00AM A39.00006 Generation of multi-qubit entanglement in a superconducting quantum circuit by parallelized parity measurements
STEFANO POLETTI, DIEGO RISTE, MENG-ZI HUANG, ALESSANDRO BRUNO, VISA VESTERINEN, OLLI-PENTTI SAIRA, LEONARDO DICARLO, QuTech and Kavli Institute of Nanoscience — We present the generation of multi-qubit entanglement using parallelized ancilla-based parity measurements in a five qubit superconducting processor. Two-qubit Bell states and three-qubit GHZ-type states are generated by single and double two-qubit parity measurements on superposition states, respectively, and characterized by both witnessing and state tomography. The protocol for generation of GHZ-type states can be used as the encoding step in the three-qubit bit-flip quantum error correction code, and made deterministic by digital feedback control. We assess its performance by state tomography of the six encoded cardinal states, and compare to the traditional method of encoding by gates.

9:12AM A39.00007 Geometry of two-qubit evolution and entanglement protection via local operations
CHARLES TAHAN, RUSKO RUSKOV, Laboratory for Physical Sciences, College Park, MD — The two-qubit pure state evolution under unitary (Hamiltonian) and measurement transformations is conveniently described via a Hopf fibration map, where an S4 sphere is the two-qubit analog of the single-qubit Bloch sphere and entanglement is encoded in an S4 subspace. We show that there exist two-qubit entanglement protection protocols based only on local operations that are as efficient as in the case of a single qubit state protection. We consider several examples related to current or near future experiments in superconducting circuits. We discuss the relevance of such ideas for quantum computing.
9:24AM A39.00008 Toward Resource-Efficient Deterministic Entanglement in 3D Superconducting Qubits, M. E. SCHWARTZ, L. MARTIN, QNL, University of California, Berkeley, C. ARON, Department of Electrical Engineering, Princeton University, M. KULKARNI, New York City College of Technology, City University of New York, H.E. TURECI, Department of Electrical Engineering, Princeton University, I. SIDDIQI, QNL, University of California, Berkeley — We present progress towards deterministic entanglement in a three-dimensional, superconducting qubit architecture, using only one continuous drive to engineer steady-state entanglement [1]. Our protocol uses two (nominally) identical copper waveguide cavities that each contain a transmon qubit. The cavities are directly coupled to one another and hybridized into symmetric and antisymmetric modes. The coupling of the cavities introduces a cavity-mediated qubit coupling that splits the degeneracy between the singlet and triplet states in the odd-parity subspace. By driving the cavities symmetrically and carefully tuning the single drive amplitude and frequency to take advantage of the hybridized cavity density of states, we aim to achieve bipartite entanglement that is stable against both dephasing and finite qubit lifetime. In this talk, we present experimental progress towards this cavity-assisted, bath engineered generation of entanglement.


This work was supported by the ARO and by the Hertz Foundation.

9:36AM A39.00009 Optimal feedback for remote entanglement, LEIGH MARTIN, Whaley Research Group and QNL, University of California, Berkeley, FELIX MOTZOI, HANHAN LI, MOHAN SAROVAR, Whaley Research Group, University of California, Berkeley, IRFAN SIDDIQI, QNL, University of California, Berkeley, BIRGITTA WHALEY, Whaley Research Group, University of California, Berkeley — Recent experiments in superconducting qubits have demonstrated measurement as a resource for entanglement, even when qubits are spatially separated to a significant degree. We consider the problem of using measurement combined with feedback to deterministically entangle remote qubits. This constraint forces us to consider only local feedback, which leads us to an interesting control-theory problem. Within this constraint, we derive a series of protocols for this system which generate entanglement as quickly as possible. We find that even in the presence of expected experimental imperfections, it should be possible to achieve high-fidelity entanglement with currently accessible experimental parameters.

This work is supported by the National Science Foundation.

9:48AM A39.00010 Robust quantum state transfer using flying microwave qubits, ERIC MLINAR, EYOB A. SETE, ALEXANDER N. KOROTKOV, University of California, Riverside — We analyze the transfer of a quantum state between two superconducting microwave resonators connected by a transmission line. Nearly perfect state-transfer efficiency can be achieved by using adjustable couplers to cancel the back-reflection from the receiving coupler with destructive interference. We show that the transfer protocol is robust to parameter variations affecting the transmission amplitudes of the couplers. We also show that the effects of Gaussian filtering, pulse-shape noise, and multiple reflections on the transfer efficiency are not significant for experimentally realistic parameters. However, the transfer protocol is very sensitive to a frequency mismatch between the two resonators. Moreover, the type of coupler we consider produces a time-dependent detuning, which requires active compensation with sufficient accuracy to yield high-efficiency state transfer.

10:00AM A39.00011 Scaleable two and four qubit parity measurement with a photon counter, LUKE C.G. GOVIA, Univ des Saarlandes, EMILY J. PRITCHETT, HRL Laboratories, R. MCDERMOTT, University of Wisconsin-Madison, FRANK K. WILHELMI, Univ des Saarlandes — Multi-qubit parity readout is a central ingredient to quantum information processing, with applications ranging from quantum error correction to entanglement generation. As the physical implementation of QIP technologies grows in size, so too does the need for scalable readout protocols. Here we present a scalable, high-fidelity, quantum non-demolition readout protocol for the parity of two or four qubits using a single dispersively coupled cavity and a photon counter. By selectively populating the cavity dependent on the qubit parity, it is possible to non-destructively read out the qubit parity using a phase insensitive photon counter, without gaining any further qubit-state resolving information. We describe our protocol in the context of superconducting integrated circuits, where the cavity is a microwave resonator, and as an example photon counter we choose the Josephson photomultiplier (PRL 107, 217401 (2011)).

10:12AM A39.00012 Analytical approach to switchoff non-leaky entangling gates in superconducting qubits, SOPHIA ECONOMOU, Naval Research Laboratory, EDWIN BARNES, Condensed Matter Theory Center and Joint Quantum Institute, Dept. of Physics, University of Maryland — We develop schemes for designing pulses that implement fast and precise entangling quantum gates in superconducting qubit systems despite the presence of nearby harmful transitions. Our approach is based on purposely involving the nearest harmful transition in the quantum evolution instead of trying to avoid it. Using analytical tools, we design simple microwave control fields that implement maximally entangling gates with fidelities exceeding 99 percent in times as low as 40 ns. We demonstrate our approach in a two-qubit circuit QED system by designing the two most important quantum entangling gates: a conditional-NOT gate and a conditional-Z gate. Our results constitute an important step toward overcoming the problem of spectral crowding, one of the primary challenges in controlling multi-qubit systems.

This work was supported by LPS-CMTC (EB) and in part by ONR (SEE).

10:24AM A39.00013 3D Multimode Cavity QED, RAVI NAIK, DAVID C. MCKAY, DAVID I. SCHUSTER, Physics Department and James Franck Institute, University of Chicago — Scalable quantum computing architectures require many long-lived and highly coherent, yet easily addressable quantum states. Photonic qubits in 3D superconducting microwave cavities are a promising approach because they are highly insensitive to decoherence and single photon lifetimes exceeding 10 ms have been demonstrated[1]. However, the plurality of current 3D cavity devices are engineered to address single photon modes. In this talk, we introduce our implementation of a multimode 3D cavity that can store greater than 20 distinct, long-lived photon modes. To perform single- and two-qubit gates between photons, each of the modes are coupled to a single flux-tunable superconducting transmon qubit. We will discuss our preliminary results towards a controlled phase gate between any pair of photons modes. This multimode circuit QED architecture may also be used as a many-body bosonic system for quantum simulation, to study multimode quantum optics, and for quantum memories as part of a larger quantum network.


10:36AM A39.00014 ABSTRACT WITHDRAWN —
10:48AM A39.00015 Design and processing considerations for superconducting qubits coupled to multiple 3D cavities

8:00AM A41.00001 n-type doping through tethered functionality: a new paradigm for molecular design of solution-processed organic thermoelectrics. BORIS RUSS, UC Berkeley, Dept of ChemE; MAXWELL J. ROBB, UCSB, Chem and Materials Deps; BHOOSHAN C. POPERE, UCSB, Dept of ChemE; ERIN PERRY, UCSB, Chem and Materials Deps; JEFFREY J. URBAN, LBNL, Molecular Foundry; MICHAEL L. CHABINYC, CRAIG J. HAWKER, UCSB, Chem and Materials Deps; RACHEL A. SEGALMAN, UCSB, Dept of ChemE — A scarcity of stable n-type doping mechanisms compatible with facile processing has been a major impediment to the advancement of n-type (electron transporting) organic thermoelectric materials. We recently demonstrated that trimethylammonium functionalization with hydroxide counterions, tethered to a perylene diimide core by alkyl spacers, facilitated solution-processing and resulted in extremely high carrier concentrations (10\textsuperscript{20} carriers/cm\textsuperscript{3}) and best-in-class thermoelectric performance in thin films. In this presentation, we report our recent findings on the underlying mechanism enabling charge carrier generation in these self-doping materials and its influence on material thermoelectric behavior. To draw these conclusions, we complement thermoelectric characterization with insights into chemical, electronic, and structural properties from XPS, optical spectroscopy, EPR, and GIWAXS experiments. Furthermore, we show that doping through tethered functionality can be extended to other n-type small molecule systems of interest, including naphthalene diimides and diketopyrrolopyrroles. Our findings help shape promising molecular design strategies for future enhancements in n-type thermoelectric performance.

Monday, March 2, 2015 8:00AM - 11:00AM
Session A41 DPOLY DMP: Focus Session: Organic Electronics and Photonics - Thermoelectric, Ferroelectric, and Piezoelectric Materials 214A - Jennifer Schaefer, National Institute of Standards and Technology

8:00AM A41.00001 n-type doping through tethered functionality: a new paradigm for molecular design of solution-processed organic thermoelectrics

8:12AM A41.00002 Silver Nafion for Thermogalvanic Applications. WILLIAM CHANG, BHOOSHAN POPERE, University of California, Berkeley, CHRIS EVANS, University of California, Santa Barbara, BORIS RUSS, University of California, Berkeley, RACHEL SEGALMAN, University of California, Santa Barbara — Thermogalvanic devices typically operate on the difference between waste heat, into electrical power using a reversible electrochemical reaction. The conversion efficiency in thermogalvanics, like with thermoelectrics, are governed by the Seebeck coefficient, the carrier conductivity and the thermal conductivity of the material. We demonstrate that the material systems silver Nafion and silver poly-styrenesulfonate are air-stable, water processable materials that demonstrate extremely high Seebeck coefficients and moderate carrier conductivities. These power factors, when coupled with the low thermal conductivities inherent in polymers, results in materials with excellent thermogalvanic figure of merits. We show the dependence of these three material properties to material composition and processing. In this talk, we show how the Seebeck coefficient in silver Nafion and silver poly-styrenesulfonate are opposite in sign, allowing construction of a thermogalvanic device. With these ion conductors, we hope to open up a flexible pathway to waste heat recovery using materials typically studied for electrochemical applications.

8:24AM A41.00003 Thermoelectric properties of hole- and electron-doped ambipolar polymers. ANNE GLAULDELL, ERIN PERRY, RUTH SCHLITZ, MICHAEL CHABINYC, Univ of California - Santa Barbara — The library of possible materials, both p- and n-type, for organic thermoelectric devices has been steadily growing with the continuous improvement in electrical properties and stability. Maximizing the thermoelectric power factor in these materials requires the simultaneous optimization of both electrical conductivity and thermopower. The challenge remains that charge transport is not well understood in organic materials due to energetic disorder from crystalline and non-crystalline domains. We have performed temperature-dependent measurements of both thermopower and electrical conductivity to uncover the relationship between microstructure and thermoelectric performance. These measurements were complemented by techniques such as electronic paramagnetic resonance (EPR) that help provide the carrier concentration to give a more complete picture of the competing charge transport mechanisms and structure-property relationships. We will present results on p- and n-type doping of ambipolar polymers that reveal the difference in thermopower for electrons and holes in the same material. An ideal thermoelectric device has n- and p-type legs with similar mechanical and thermoelectric properties, a balance more easily realized using the same polymer for each leg.

8:36AM A41.00004 Conductance and Thermopower in Thiophene and Oxidized Thiophene Single-Molecule Junctions. LATHA VENKATARAMAN, Columbia Univ — Organic electronic materials have impacted the development of semiconducting, photovoltaic and thermoelectric devices. The precise control afforded over molecular design by organic synthesis allows for device properties to be readily tailored facilitating varied functionality. Measuring charge transfer characteristics and thermoelectric properties in organic devices and across metal-organic interfaces is of critical importance for understanding structure-function relations and single molecule measurements offer an ideal test bed for such measurements. Organic materials such as thiophene and its oxidation products are prime examples of self-assembled small-molecule devices focusing on molecular systems that have strong potential for application in organic and photovoltaic devices. Specifically, I will discuss measurements of thiophene and oxidized thiophene oligomers that illustrate how structure and conformations impact both the electronic characteristics and the dominant charge carrier in these systems. I will end this talk discussing results with a new class of thiophene derivatives where the charge carriers are changed from holes to electrons as the length of the oligomer is increased. With these measurements, we illustrate a new means to tune p- and n-type transport in organic materials.

9:12AM A41.00005 Thermoelectricity in Disordered Organic Semiconductors under the Premise of the Gaussian Disorder Model and its Variants. DAN MENDELS, NIR TESSLER, TECHNION, ORGANIC MATERIALS AND DEVICES TEAM — Charge transport in disordered organic systems has been in recent decades mainly discerned from the perspective of a variety of phenomenological models prominent of which those stemming from the Gaussian Disorder Model. But while the use of these models has been prevalent, uncertainty regarding the extent of their validity remains due to the large number of free parameters they consist and their frequent deficiency to consistently account for large sets of experiments while keeping model input parameters and distributions unchanged. In the presented study, we have investigated using Monte Carlo simulations the thermoelectric properties of disordered organic semiconductors under the premise of the Gaussian Disorder Model and its variants. Doing so enabled the provision of additional directional comparison between the aforementioned theoretical frameworks and real systems, beyond those based on extensively studied charge transport properties, and the provision of a frame-of-reference for rising interest in these systems for thermoelectric applications. To illustrate the potential existing in the implementation of combined transport and thermoelectric investigation, strategies will be discussed to experimentally deduce the DOS shape, infer whether a system’s activation energy originates from its energetic disorder or a polaron activation energy (while deducing the given polaron activation energy), and discerning whether a system’s energetic disorder is spatially correlated or accompanied by off-diagonal disorder.
Nanotube Based Organic Thermoelectric Matrices, THUSITHA ETAMPAWALA, Department of Chemistry, The University of Tennessee, Knoxville, TN.

understanding illustrates that FE in even n-nylons originates from the defective crystalline phase rather than the amorphous region. The conformation is smectic-like, twisted, and the hydrogen bonds are randomized. Therefore, this mesophase is abundant in defects and poorly bonded amide dipoles, which result from the defective crystalline mesophase, play an important role in the FE behavior of nylon 12. In this mesophase, the chain

nylon 6 was due to the amorphous phase, the conclusion is debatable and the understanding of the FE mechanism is still lacking. We find that poorly bonded mesomorphic crystalline structure formed via quenching and/or stretching. Although there was an earlier claim maintaining that FE behavior in melt-quenched nanocomposites were probed by small and ultra-small angle neutron scattering (SANS and USANS respectively) as a function of CNT loading (10wt%, 30wt%, and 50wt%), sonication duration to control the CNT dispersion, and presence and absence of ethylene glycol (EG) in the deposition solution of PEDOT:PSS. The morphology of these composites is currently being correlated to their thermo-electric performance. The SANS and USANS profiles were analyzed with the hierarchical Beaucage model. Further, the USANS data were fit to a two ellipsoidal form factor, which is consistent with the analysis of the USANS data by the Beaucage model and SEM results. These results reveal that the sonication duration and presence of EG effectively de-bundle the CNTs and disperse them in the PEDOT:PSS matrix.

9:36AM A41.00007 Exploiting the Different Polarity in Piezoresistive Characteristics of Conducting Polymers for Strain Gauge Applications, MELDA SEZEN, JEFFREY T. REGISTER, Dept. of Chemical and Biological Engineering, Princeton University, YAO YAO, BRANKO GLISIC, Dept. of Civil and Environmental Engineering, Princeton University, YUEH-LIN LOO, Dept. of Chemical and Biological Engineering, Princeton University — Piezoresistivity defines the change in resistance of a material in response to mechanical stress. We exploit the effects of structural modifications on the piezoresistive properties of conducting polymers, poly(2-acrylamido-2-methyl-1-propanesulfonylic acid) doped polyaniline, PANI-PAAMPSA, and poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate), PEDOT:PSS, for strain gauge applications. Under tensile deformation, the resistances of as-cast PANI-PAAMPSA and PEDOT:PSS increase due to increased separation between the electrostatically stabilized conducting polymer particles. Upon solvent annealing in dichloroacetic acid, DCA, PANI-PAAMPSA’s resistance decreases whereas PEDOT:PSS’s resistance still increases with tension. While DCA treatment reduces the electrostatic interactions between PANI and PAAMPSA, it only removes the PSS overlay in PEDOT:PSS. The change in the polarity of PANI-PAAMPSA’s piezoresistivity is attributed to the unlocking of the globular structure of the as-synthesized conducting polymer complex with DCA-treatment, which then enables strain-induced crystallization on deformation. By tuning the piezoresistive characteristics of the polymers through structural modification, we can design strain gauge circuits for monitoring the conditions of civil structures.

9:48AM A41.00008 Temperature-dependent electrical transport in ferroelectric organic field-effect transistors, AMRIT LAUDARI, SUCHISMITA GUHA, Univ of Missouri - Columbia — Ferroelectric dielectrics, permitting access to nearly an order of magnitude range of polarization with temperature as the tuning parameter, offer a great test-bed to monitor the changes in interfacial transport in organic field-effect transistors (OFETs) as the polarization strength is tuned. Temperature-dependent transport studies have been carried out from pentacene and other organic semiconductor-based OFETs using the ferroelectric copolymer poly(vinylidene fluoride-co-trifluoroethylene) (PVDF-TrFe) as a gate insulating layer. By fits to an Arrhenius-type dependence of the charge carrier mobility as a function of temperature, the activation energy in the ferroelectric phase is found to increase as the thickness of the PVDF-TrFe layer increases. For thicknesses of the dielectric layer above 100 nm, the activation energy is found to be greater than 150 meV, which greatly reduces in the paraelectric phase of the dielectric. The weak temperature-dependence of the charge carrier mobility in the ferroelectric phase of PVDF-TrFe may be attributed to a polarization fluctuation driven transport. The threshold voltage decreases upon increasing temperatures with a large change above the ferroelectric to paraelectric phase transition temperature.

This work was supported by National Science Foundation under Grant No. ECCS-1305642

10:00AM A41.00009 Ferroelectrically-driven photocurrent in P3HT-based diodes, ELENI PAVLOPOULOU, CARINE LACROIX, ANTIGONI PASPALI, GUILLAUME FLEURY, CYRIL BROCHON, ERIC CLOUTET, LCPC, CNRS/University of Bordeaux, Bordeaux/Bordeaux INP, Pessac France, FABRICE DOMINGUES DOS SANTOS, Piezotech, France, MARIO MAGLIONE, ICMCB?CNRS, University of Bordeaux, Pessac France, GEORGES HADZIOANNOU, LCPC, CNRS/University of Bordeaux/Bordeaux INP, Pessac France — Blends of ferroelectric and semiconducting polymers are known to phase separate in thin film configuration, forming semiconducting columnar structures embedded in a ferroelectric matrix. These blends have been used in the past to fabricate non-volatile bistable diodes. In this work we demonstrate that the phase separated network of poly(3-hexylthiophene), P3HT, and poly(vinylidenefluoride-co-trifluoroethylene), P(VDF-co-TrFE), can be also used for the extraction of photocurrent under illumination. Furthermore, we provide experimental proofs on the ferroelectric origin of this photocurrent and we show that its magnitude depends on the polarization characteristics of the pre-polarized P(VDF-co-TrFe) matrix. The devices we propose herein can provide an alternative to the existing organic photovoltaic devices.

10:12AM A41.00010 Ferroelectricity and Double Hysteresis Loop Behavior in Even-Numbered n-Nylons, ZHONGBO ZHANG, LEI ZHU, MORTON LITT, Case Western Reserve Univ — Ferroelectric (FE) property in odd-numbered n-nylons has been known for a long time. In comparison, even-numbered n-nylons are claimed to be non-ferroelectric due to their non-polar crystalline structure, where the direction of hydrogen bonded dipoles alternates. Nevertheless, in this presentation, FE property is discovered in even n-nylons, and it is related to the mesomorphic crystalline structure formed via quenching and/or stretching. Although there was an earlier claim maintaining that FE behavior in melt-quenched nylon 6 was due to the amorphous phase, the conclusion is debatable and the understanding of the FE mechanism is still lacking. We find that poorly bonded amide dipoles, which result from the defective crystalline mesophase, play an important role in the FE behavior of nylon 12. In this mesophase, the chain conformation is smectic-like, twisted, and the hydrogen bonds are randomized. Therefore, this mesophase is abundant in defects and poorly bonded dipoles, which can easily flip under electric field. In addition, the hydrogen-bonded amides can serve as pinning points and induce double hysteresis loop behavior. This understanding indicates that FE in even n-nylons originates from the defective crystalline phase rather than the amorphous region.

1 NSF (DMR0907580)
10:24AM A41.00011 Relaxor Ferroelectric Behavior from Strong Physical Pinning in a Poly(vinylidene fluoride-co-trifluoroethylene-co-chlorotrifluoroethylen) Random Terpolymer 1
LEI ZHU, LIANYUN YANG, Dept. of Macromolecular Sci. & Eng., Case Western Reserve University, Cleveland, OH 44106, BRADY TYBURSKI, Dept. of Chemistry, Central Michigan University, Mount Pleasant, Michigan 48859, FABRICE DOMINGUES DOS SANTOS, Pliezotech S.A.S, Arkema-CRAA, Rue Henri Moissan 69493 Pierre-Benite Cedex, France — Although narrow single hysteresis loop (SHL) is observed for electron beam (e-beam) irradiated poly(vinylidene fluoride-co-trifluoroethylene) [P(VDF-TrFE)] random copolymers owing to strong chemical pinning in isomorphic (or defect-modified) crystals, it has not been achieved for P(VDF-TrFE)-based random terpolymers, such as P(VDF-TrFE-CFE) (CFE is 1,1-chlorofluoroethylene), which only exhibits double hysteresis loops (DHLs). This is attributed to the weak physical pinning of CFE units in isomorphic crystals. In this work, the comonomer CFE in the terpolymer was replaced by the larger chlorotrifluoroethylene (CTFE). Intriguingly, narrow SHLs were exclusively observed for the P(VDF-TrFE-CTFE) terpolymer above room temperature. This was attributed to the stronger physical pinning force of the larger CTFE, which has a smaller dipole moment (only 0.64 Debye). This result provides further insight into the structure and behavior of relaxor ferroelectric polymers, which can help to design and develop new ferroelectric polymers with more desirable properties and enhanced performance.

1This work is supported by National Science Foundation (DMR-0907580 and DMR-1402733).

10:36AM A41.00012 ABSTRACT MOVED TO M6.00013 —

10:48AM A41.00013 Enhanced Electrical Conductivity due to Morphological Changes in Polyanailine-Titania Core-Shell Nanocomposites
NELSON COATES, California Maritime Academy, JIANFENG LIU, University of California, Berkeley, RACHEL SEGALMAN, University of California, Santa Barbara, JEFFREY URBAN, Lawrence Berkeley National Laboratory — Conducting polymer-inorganic nanoparticle composites are a valuable class of advanced materials with a wide range of applications due to extensive physical and chemical tunability. Although effective medium theories are often used to predict the behavior of these materials, the actual physical properties can be distinctly different from the predictions of the effective medium interactions that they manifest. Here, we present electrical conductivity data for TiO2 nanoparticles coated with polyaniline, along with structural characterization of the conducting polymer as a function of component volume fraction. For these composites, we find that the electrical conductivity cannot be explained by a 2-component effective medium theory, but rather is correlated to a structural change in the polymer. We hypothesize that the organic-inorganic interface induces a structural change in a region of polymer surrounding the nanoparticle which improves the electrical conductivity of the composite. These results emphasize the importance of controlling interfacial interactions in organic-inorganic composites, and demonstrate the potential for using such interactions as a way to tune electrical transport.

Monday, March 2, 2015 8:00AM - 11:00AM — Session A42 DPOLY: Polymeric Elastomers and Gels 214B - Edwin Chan, National Institute of Standards and Technology

8:00AM A42.00001 Tailoring Phase Behavior and Mechanical Properties in Thermoplastic Elastomers through Block Sequence and Macromolecular Architecture
ADAM BURNS, RICHARD REGISTER, Princeton University — Block copolymers exhibit unique properties which depend not only on the identities of the constituent blocks but also the block sequence and macromolecular architecture. Thermoplastic elastomers (TPEs) are a prime example. In TPEs the arrangement of glassy end blocks flanking a long rubbery midblock gives rise to a physically cross-linked, elastic solid. Exchanging the glassy blocks for crystalline blocks can improve the processability and solvent resistance, but adversely affects the mechanical performance. The block sequence crystalline-glassy-rubber-crystalline has been developed to combine the advantages of both crystalline and glassy blocks. Careful selection of block lengths produces materials in which the order-disorder transition temperature lies below the melting point of the crystalline block, ensuring that the melt will be homogeneous above the melting point. Access to single-phase melts provides a large reduction in viscosity and elasticity over conventional TPEs, which remain microphase-separated in the melt. Inserting the glassy blocks between the crystalline and rubbery blocks produces a vitreous layer surrounding the crystalline domains, which improves the room-temperature mechanical performance. Incorporating the crystalline-glassy-rubber motif into the arms of star block copolymers adds another level of control. The star architecture introduces a permanent cross-link at the center of the star without appreciatively affecting the phase behavior.

8:12AM A42.00002 Shear Induced Morphology Evolution and Dynamic Viscoelastic Behavior of Binary and Ternary Elastomer Blends 1
XIA DONG, XIAOJIANG LIU, WEI LIU, CHARLES C. HAN, DUJIN WANG, Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Engineering Plastics, Institute of Chemistry Chinese Academy of Sciences — The morphology evolution and rheological response of a near-critical composition polybutadiene/polyisoprene blend and solution-polymerized styrene-butadiene rubber/polyisoprene/silica ternary composites after various shear flow were in situ studied with the rheological and rheo-optical techniques. The relationship between the morphology of the blend during the relaxation after the cessation of steady shear with different shear rates and their corresponding rheological properties was successfully established. It was found that the different shear-induced morphologies under steady shear would relax to the equilibrium states via varied mechanisms after the shear cessation. The storage modulus G' increased significantly in the breakup process of the string-like phase. In long time scale, silica slowed down the succeeding breakup of the string-phase domains and simultaneous coalescence of broken droplets, and then effectively reduced the droplets size and stabilized the morphology.

1The authors thank the financial support from National Natural Science Foundation of China (No.51173195).

8:24AM A42.00003 Structure and mechanical properties of isotactic polypropylene (iPP) gels formed at different cooling temperatures
RYUSUKE OKOSHI, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University — The effects of the cooling temperature on the crystalline network formation and the mechanical properties of isotactic polypropylene (iPP) gels were evaluated. iPP-decallydroonaphthalene gels were prepared at different cooling temperatures varying from 25 degrees C to -196 degrees C. Tensile test was carried out to measure the mechanical properties of the gels. Scanning electron microscopy (SEM) and differential scanning calorimetry (DSC) analyses were conducted to observe the density and the homogeneity of the network structures. It was found that the iPP gel quenched at -196 degrees C was highly elastic, exhibiting the highest fracture strain and stress of 2500% and 230 kPa. The SEM analysis revealed that nano-crystals were formed, which acted as crosslinkers that were distributed throughout the gels by quenching below -40 degrees C. By contrast, spherulites were observed to have grown inhomogeneously by cooling above -20 degrees C. It was found by DSC that the amount of decreasing the cooling temperatures, indicating an increase in the density of the network structures. From these results, it was therefore concluded that iPP gel quenched at -196 degrees C possessed the highest mechanical property due to its dense and homogeneous network structures.
Copolymers parameters obtained from PRI with results from neutrons scattering studies of the same series of hydrogels. Applying various thermodynamic network swelling models to describe the mechanical response of these gels as measured from PRI, we are able to extract *glycol* chains. We use PRI to quantify the mechanical and transport properties of a series of "click" hydrogels with different crosslink densities. By

9:00 AM A42.00006 Wide bicontinuous compositional windows from co-networks made with telechelic macromonomers, Gregory TeW, Polymer Science and Engineering, University of Massachusetts, Amherst — Phase-separated and self-assembled co-network materials offer a simple route to bicontinuous-like morphologies, which are expected to be highly beneficial for applications such as ion, charge, and oxygen transport. Despite these potential advantages, the systematic definition of co-network structures has not been achieved, largely due to the lack of well-controlled chemistries for their preparation. Here, a thiol-ene end-linking platform enables the systematic investigation of phase-separated poly(ethylene glycol) (PEG) and polystyrene (PS) networks in terms of the molecular weight and relative volume fractions of precursor polymers. The ion conductivity and storage modulus of these materials serve as probes to demonstrate that both phases percolate over a wide range of compositions, spanning PEG volume fractions from ∼0.3 - 0.65. These findings demonstrate that this approach to thiol-ene co-networks is a versatile platform to create bicontinuous morphologies.

9:12 AM A42.00007 Squeezing a gel to establish network structure-transport property relationships, Edwin Chan, Nichole Nadermann, Material Science and Engineering Division, National Institute of Standards and Technology, Gaithersburg, MD, 20899, USA — Gels are used in many applications, ranging from drug delivery to water purification, where regulating transport of a particular permeant is crucial. The structure of the gel determines its transport properties but developing the gel structure-transport property relationships often require multiple measurement techniques. In this work, we demonstrate poroelastic relaxation indentation (PRI) as a single measurement tool to establish the relationships between the polymer network structure and the transport properties of well-defined hydrogel networks synthesized via a thiol-norbornene click reaction of poly(ethylene glycol) (PEG) chains. We use PRI to quantify the mechanical and transport properties of a series of “click” hydrogels with different crosslink densities. By applying various thermodynamic network swelling models to describe the mechanical response of these gels as measured from PRI, we are able to extract thermodynamic parameters of these hydrogels including the Flory chi parameter and the mesh size. We validate our approach by comparing the thermodynamic parameters obtained from PRI with results from neutrons scattering studies of the same series of hydrogels.

9:24 AM A42.00008 Tensile Deformation and Morphological Evolution of Precise Acid Copolymers, Luri Robert Middleton, Steve Szewczyk, Eric Schwartz, University of Pennsylvania, Jason Azoulay, Dustin Murtagh, Joseph Cordon, Sandia National Laboratory, Kenneth Wagen, University of Florida, Karen Winney, University of Pennsylvania — Acid- and ion-containing polymers have specific interactions that produce complex and hierarchical morphologies that provide tunable mechanical properties. We report tensile testing and in situ x-ray scattering measurements of a homologous series of precise poly(ethylene-co-acrylic acid) copolymers (pXAA). Upon variation of the number of backbone carbons (x = 9, 15, 21) between pendant acrylic acid groups along the linear polyethylene chain, these materials exhibit pronounced changes in both their tensile properties as well as their morphological evolution during deformation. The hierarchical layered acid aggregate structure coincides with the onset of a strain hardening mechanism and was observed in both a semi-crystalline sample (p21AA) as well as an amorphous sample (p15AA). The polymer with the shortest spacing between acid groups (p9AA) maintains a liquid-like distribution of acid aggregates during deformation, exhibiting low tensile strength which we attribute to facile acid exchange between acid aggregates during deformation. Our results indicate that the formation of the hierarchical layered structure, which coincides with polymer strain-hardening regime, originates from the associating acid groups cooperatively preventing disentanglement.

9:36 AM A42.00009 Nonlinear behavior of ionically and covalently cross-linked alginate hydrogels, Seyedmeymans Hasmemnejad, Mahla Zabet, Santanu Kundu, Dave C. Swalm School of Chemical Engineering, Mississippi State University, MS State, MS — Gels deform differently under applied load and the deformation behavior is related to their network structures and environmental conditions, such as pH and ionic strength. Conventional linear theories are not suitable to describe the mechanical behavior of both ionically and covalently cross-linked alginate hydrogel using large amplitude oscillatory shear (LAOS) and cavitation experiments. Ionically-bound alginate gels were obtained by using divalent calcium. Alginate volume fraction and alginate to calcium ratio were varied to obtain gels with different mechanical properties. Chemical gels were synthesized using adipic acid dihydrazide (AAD) as a cross-linker. The non-linear rheological parameters are estimated from the stress responses to elucidate the strain softening behavior of these gels. Fracture initiation and propagation mechanism during shear rheology and cavitation experiments will be presented. Our results provide a better understanding on the deformation mechanism of alginate gel under large-deformation.

9:48 AM A42.00010 Nonlinear Elasticity and Cavitation of a Triblock Copolymer Gel, Santanu Kundu, Seyedmeymans Hasmemnejad, Mahla Zabet, Satish Mishra, Dave C. Swalm School of chemical engineering, Mississippi State University, MS State, MS — Polymer gels are subjected to large-strain deformation during their applications. The gel deformation at large-strain is non-linear and can often lead to failure of the material. Here, we report the large-strain deformation behavior of a physically cross-linked, swollen polymer gel, which displays unique strain-stiffening response at large-strain. Investigations were performed using large amplitude oscillatory shear (LAOS) and custom designed cavitation rheology techniques. Gent constitutive model, which considers finite extensibility of midblock, was fitted with the LAOS data, therefore, linking the estimated parameters from LAOS analysis to the structure of the gel. Cavitation experiments were conducted as a function of temperature. Both analytical method and finite-element based modeling have been implemented to capture the pressure response in cavitation experiments. Our results provide a critical understanding of gel failure mechanism at large-strain.
and compared with literature data of other known glass formers. Contrary, we observed formation of highly stable glasses of ethylcyclohexane and 1-pentene. The results on ethylcyclohexane and 1-pentene will be presented.

0.2 Hz to 4 kHz. Ethylcyclohexane and 1-pentene are both strong glass formers, for which possibility of stable glass formation has been questioned. On the contrary, we observed formation of highly stable glasses of ethylcyclohexane and 1-pentene. The results on ethylcyclohexane and 1-pentene will be presented and compared with literature data of other known glass formers.

1 NSF DMR-1409710, DMR-1407645, DMR-1122483

10:12AM A42.00012 On the role of geometric non-linearities in the mechanics of nematically ordered semi-flexible networks, LOUIS FOUCARD, Department of Chemistry and Biochemistry, UCLA, JORDAN KAZUO PRICE, WILLIAM KLUG, Department of Mechanical and Aerospace Engineering, UCLA, ALEX LEVINE, Department of Chemistry and Biochemistry, UCLA — Extending previous studies on the affine-nonaffine transition of nematically ordered semiflexible networks, we investigate numerically the effect of geometric non-linearities on the mechanical response of anisotropic networks of elastic filaments. We find that the strong dependence of buckling susceptibility on segment length has a pronounced effect on the nonlinear elastic behavior of anisotropic networks; contrary to isotropic networks, highly ordered ones show an important softening of the shear modulus at nonlinear (finite) strains. We compute the spatial correlation of the Conti/McKintosh buckling order parameter and show that the particularity of the nonlinear response of nematic networks resides in the cooperativity of the buckling events. We also show that dependence of the shear modulus on the nematic order parameter can be predicted using the assumption of affine deformation at small shear, and in terms of a generalized floppy mode analysis of the nonaffine mechanics at larger deformation.

10:24AM A42.00013 Using stability analyses to predict dynamic behaviour of self-oscillating polymer gels, VAIBHAV PALKAR, GAURAV SRIVASTAVA, Indian Institute of Technology Gandhinagar, OLAGA KUKSENOK, ANNA C. BALAZS, University of Pittsburgh, PRATYUSH DAYAL, Indian Institute of Technology Gandhinagar — Use of chemo-mechanical transduction to produce locomotion is one of the significant characteristics of biological systems. Polymer gels, intrinsically powered by oscillatory Belousov-Zhabotinsky (BZ) reaction, are biomimetic materials that exhibit rhythmic self-sustained mechanical oscillations by chemo-mechanical transduction. Via simulations, based on the 3D gel lattice spring model, we have successfully captured the dynamic behaviour of BZ gels. We have demonstrated that it is possible to direct the movement of BZ gels along complex paths, guiding them to bend, reorient and turn. From a mathematical perspective, the oscillations in the BZ gels occur when the gel's steady states lose stability by virtue of Hopf bifurcations (HB). Through the use of stability analyses, we predict the conditions under which gel switches from stationary to oscillatory mode and vice versa. In addition, we characterize the nature of HB and also identify other types of bifurcations that play a critical role in governing the dynamic behaviour of BZ gels. Also, we successfully predict the frequency of chemo-mechanical oscillations and characterize its dependency on the model parameters. Our approach not only allows us to establish optimal conditions for the motion of BZ gels, but also can be used to design other dynamical systems.

1 IIT Gandhinagar and DST-SERB for funding.

10:36AM A42.00014 Shape Actuation of Competitive Networks, YUAN MENG, JISU JIANG, MITCHELL ANTHAMATTEN, University of Rochester, Department of Chemical Engineering — We demonstrate a single phase, two-way shape actuator that, in the absence of an external load, elongates upon cooling and reversibly contracts upon heating. In a simple and straightforward process, a partially crosslinked, semi-crystalline PCL network is melted, stretched to several hundred percent strain, and further crosslinked. Upon removal of the applied load, the elastic ‘double network’ adopts a ‘state-of-ease’ that retains part of its former strain. When cooled, internal stress-induced crystallization causes further elongation of the configurational biased chains; and when heated, crystallites melt, and the sample returns to its equilibrium state-of-ease. Under optimized conditions, reversible actuation of over 15 percent strain can be reproducibly achieved, and samples can be cycled multiple times with highly uniform actuation with no observable creep. The mechanism behind such actuation was further confirmed via calorimetry and X-ray scattering.

1 Pump Primer Grant, Univ. of Rochester

10:48AM A43.00015 Shape Memory Polymers from Blends of Elastomers and Crystalline Small Molecules, KEVIN CAVICCHI, NICOLE BROSTOWITZ, Dept of Polymer Engineering, University of Akron, BRENT HUKILL, Dept of Chemical Engineering, Rose Hulman Institute of Technology, HEATHER FAIRBAIRN, Dept of Chemical Engineering, University of Akron — This talk will present work on the fabrication of shape memory polymers (SMPs) by swelling natural with molten fatty acids. By this method a SMP with excellent shape recovery can be obtained during free recovery after uniaxial deformation to 100% strain. Experiments to measure the shape memory properties under both stress and strain controlled conditions will be reported and compared. This fabrication method offers a number of advantages for preparing SMPs. First, it utilizes natural rubber as the base material for the SMP, which capitalizes on a high performance, commodity elastomer. Second, by blending a commercial polymer with a small molecule additive no additional chemistry is needed for the preparation of the SMP. Third, this route inverts the typically processing steps by crosslinking the permanent network prior to formation of the physically crosslinked reversible network. This offers a means to potentially generate a SMP from any preformed elastomer article.

Monday, March 2, 2015 8:00AM - 11:00AM –
Session A43 DPOLY: Focus Session: Stable Glasses and Their Properties

8:00AM A43.00001 Stable glasses from strong liquids, YEONG ZEN CHUA, MATHIAS AHRENBERG, University of Rostock, MICHAEL TYLINSKI, MARK D. EDIGER, University of Wisconsin-Madison, CHRISTOPH SCHICK, University of Rostock — To date, only several materials have been observed to form ultra-stable glasses by vapor deposition. Some authors have suggested that fragility might be a controlling factor in the ability to form stable glasses by vapor deposition, with highly stable glasses only being possible for highly fragile liquids. Glasses of ethylcyclohexane, fragility index 56.5, and 1-pentene, a very small molecule, produced by physical vapor deposition have been characterized by in situ AC chip nanocalorimetry. Since the fragility index of 1-pentene was not available, it was determined as 52 from the calorimetric glass transition temperatures measured in the frequency range from 0.2 Hz to 4 kHz. Ethylcyclohexane and 1-pentene are both strong glass formers, for which possibility of stable glass formation has been questioned. On the contrary, we observed formation of highly stable glasses of ethylcyclohexane and 1-pentene. The results on ethylcyclohexane and 1-pentene will be presented and compared with literature data of other known glass formers.
8:12AM A43.00002 Stable Glasses of a Low Fragility Organic Liquid. M. TYLINSKI, A. SEPULVEDA, Univ of Wisconsin, Madison, A. GUISEPPI-ELIE, Clemson University, R. RICHERT, Arizona State University, Y.Z. CHUA, C. SCHICK, University of Rostock, M.D. EDIGER, Univ of Wisconsin, Madison — We have created stable glasses of the low fragility liquid methyl-m-toluate (MMT, m = 60). The MMT stable glass films are prepared by physical vapor deposition and characterized in situ with AC nanocalorimetry and dielectric spectroscopy. Stable glasses of MMT have lower heat capacities and increased kinetic stability compared to the liquid-cooled glass. The films transform into the supercooled liquid via two mechanisms. A propagating front controls the transformation of thin films while a bulk mechanism dominates the transformation of thick films. This behavior is similar to other stable glass systems and shows that stable glasses can be prepared from liquids with a very wide range of fragilities (60 < m < 147). In one respect MMT stands out from previously studied systems. When a stable glass of MMT is annealed above $T_g$ the surface-initiated front propagates 5 $\mu$m into the sample before the bulk mechanism dominates the transformation. This 5 $\mu$m length scale is significantly larger than what has been observed in other stable glass systems.

8:24AM A43.00003 Synthesis and Characterization of Exceptionally Stable Glasses of 1,3-Bis(1-naphthyl),5-(2-aryl)benzene. TIANYI LIU, KEVIN CHENG, ELMIRA SALAMI, FENG GAO, CHEN LI, Department of Chemistry, University of Pennsylvania, XIAO TONG, Brookhaven National Lab, YUE ZHANG, YI-CHIH LIN, WILLIAM ZHANG, ETHAN GLOR, PATRICK WALSH, ZAHRA FAKHRAAI, Department of Chemistry, University of Pennsylvania — Stable glasses can be prepared by physical vapor deposition (PVD). Compared to ordinary glasses, stable glasses have exceptional properties such as higher density and thermal stability. Deposition temperature is one of the most important parameters that controls the properties of PVD glasses. When scaled to the glass transition temperature ($T_g$), most stable glasses are usually obtained at deposition temperatures around 0.85 $T_g$. Chemical structure, entropy of super-cooled liquid, fragility and enhanced mobility may all affect the most stable structure obtained via PVD. To examine the effect of chemical structure, specifically the molecular weight effect on the stability of PVD glasses, we synthesized and characterized stable glasses of small organic molecule 1,3-bis(1-naphthyl),5-(2-aryl)benzene ($\alpha_{10\beta\gamma}$) and its molecular analogues. With systematically changing its chemical structure, thermal expansion coefficients, fictive temperature and density of stable glasses all vary systematically. These results indicate the robust nature of stable glass formation and can elucidate the processes by which these glasses are formed.

8:36AM A43.00004 Using deposition rate as a means to alter the properties of small molecule organic glasses for OLED applications. KENNETH KEARNES, The Dow Chemical Company, PAIGE KRZYSKOWSKI, ZACHARY DEVEREAX, Department of Chemistry, Saginaw Valley State University — Organic light emitting diode (OLED) devices rely on vapor-deposited, small molecule organic glasses. Recent work has shown that deposition condition plays a critical role in altering OLED device performance. Here it will be shown that the deposition rate alters the onset and fictive temperatures measured by differential scanning calorimetry (DSC) of the deposited glass. Glasses of the common hole transport materials NPD and TPD were prepared with onset temperatures 17 and 16 K higher, respectively, than the ordinary glass prepared by cooling the supercooled liquid. The thermal stability of glasses in functioning devices can be underestimated due to increases in onset temperature relative to $T_g$. The fictive temperatures for NPD and TPD were 32 and 27 K lower, respectively, than the $T_g$ of the ordinary glass. These results are consistent with literature reports on other non-OLED glasses where enhanced mobility allows for glasses with similar properties to be made. Ellipsometry studies on NPD showed that the fictive and onset temperatures were consistent with the DSC results. Additionally, the modeled birefringence of the as-deposited NPD glass was non-zero and quickly decreased upon heating above the onset temperature, which has implications for device performance.

8:48AM A43.00005 Structural equivalence of equal-energy vapor deposited and liquid cooled films in two dimensions. DANIEL REID, IVAN LYUBIMOV, JUAN DE PABLO, Univ of Chicago — Vapor deposition has been shown to provide a means of producing supercooled liquids with exceptional structural and kinetic stability compared to samples prepared by gradual cooling of a liquid. In this work, we study two-dimensional binary glassy films formed by vapor deposition and liquid cooling. We show that distinctive local structural regimes correspond directly to the structural energy of these films. We find the path towards equilibrium to be characterized by a transition in these structural regimes from medium sized square-ordered clusters to states with significant pentagonal local order. Tracking the degree of local order over a range of structural energies using both formation strategies, we find that the structure of vapor deposited and liquid cooled films are equivalent in films with equal inherent structural energies. Previous work has found that the substrate temperature that yields minimum energy for a vapor deposited film lies near 85% of the material’s glass transition temperature. Our simulations indicate that in two dimensions, the optimal substrate temperature for stable glass formation decreases with deposition rate.

9:00AM A43.00006 Do Two-Level-Systems and Boson Peak persist or disappear in highly stable glasses? MIGUEL A. RAMOS, TOMAS PEREZ-CASTANEDA, Univ Autonoma de Madrid, RAFAEL JIMENEZ-RIOBOO, Inst Ciencia de Materiales de Madrid, CRISTIAN RODRIGUEZ-TINOCO, JAVIER RODRIGUEZ-VIEJO, Univ Autonoma de Barcelona — We have investigated how deep kinetic and thermodynamic stabilization in glasses can affect their universal properties at low temperatures. In particular, we have studied two different kinds of material which allow us to access highly-stable glassy states, as well as their corresponding conventional glasses: (i) ancient amber, which is a glass which has experienced an extremely long hyperaging process; and (ii) ultrastable thin-film glasses of indomethacin, prepared by physical vapor deposition at temperatures around 85% of its glass-transition temperature. Specifically, we have studied 110-million-year-old amber samples from El Soplao (Spain). Specific heat Cp measurements of pristine and rejuvenated samples were conducted in the temperature range 0.07K < T < 30K, as well as around its glass-transition temperature $T_g = 150^\circ C$. A modest increase of the boson-peak height (in Cp/T$^3$) with increasing rejuvenation was observed. The amount of two-level systems (TLS) was however found to decrease as the surface-initiated-front propagates 5 $\mu$m into the surface-initiated-front propagates 5 $\mu$m into the

9:12AM A43.00007 Dielectric Relaxation of Materials that Form Ultra-Stable Glasses RANKO RICHERT, Arizona State University — Physical vapor deposition of glass forming materials onto substrates at temperatures around 0.8 $T_g$ produces glasses of high density and low enthalpy. Using interdigitated electrode cells as substrates, such stable glasses can be studied by dielectric spectroscopy in situ. This technique is applied to monitor the dynamics of stable films upon their conversion to the ordinary supercooled liquid state. The dielectric loss during transformation indicates that the softening occurs by a growth front mechanism generating the ordinary liquid state without forming intermediates. The same technique is also used to assess the residual dynamics of the stable glassy state. We observe that processes such as the Johari-Goldstein beta relaxation are strongly suppressed in this stable state, consistent with the relatively low fictive temperature of these glassy glasses.

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[3] coauthors: Hai-Bin Yu, Department of Chemistry and Biochemistry, Arizona State University, Tempe, Arizona 85278; Michael Tylini, and Mark D. Ediger, Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53706.
N,N-deposition temperature to generate films with moduli nearly twice that obtained for analogous films fabricated under normal vapor deposition conditions. For decreased in ultrathin films for materials deposited at low temperatures. Moreover, the thin film behavior of these small molecule glasses are altered by the and this can be used to tune the modulus of bulk-like glasses. Here, examination of ultrathin (<30 nm) films provides a route to further test hypotheses about mobile surface layers near Tg. We find that the proximity of the mechanical testing temperature to bulk Tg controls if the modulus is increased or decreased in ultrathin films for materials at low temperatures. Moreover, the thin film behavior of these small molecule glasses are altered by the deposition temperature to generate films with moduli nearly twice that obtained for analogous films fabricated under normal vapor deposition conditions. For N,N′-Di-(1-Naphthyl)-(N,N-diamine (NPD) with a bulk Tg of \sim 90\textdegree C, the modulus of the material is optimized if deposited at 70 C (0.9Tg). The stable glass deposition temperature of 0.85Tg reported originally by Ediger and coworkers results in more than 20% decrease in the elastic modulus. This suggests that the optimum deposition temperature depends on property of interest.
to the electronic behavior of 2D materials. Finally, using graphene as an example, we demonstrate that the kirigami structure may open up interesting opportunities in coupling molecular dynamics simulations that have been used almost exclusively for macroscale structures to dramatically enhance their stretchability. Specifically, we show using classical mechanics and numerical simulations that the yield and fracture strains of graphene and MoS$_2$ that have been used to improve the stretchability of elastic materials can be enhanced by about a factor of three using kirigami as compared to standard monolayers. We explore the emergence of elastic properties in smocked fabrics as functions of both fabric elasticity and smocking pattern.

8:12AM A44.00002 Miura Tubes and Assemblages: Theory and Applications, EVGENI FILIPOV, GLAUCIO PAULINO, University of Illinois at Urbana Champaign. TOMOHIRO TACHI, University of Tokyo — Origami systems inspired from the Miura-ori pattern are rigid and flat foldable meaning that they can fold completely by deforming only about prescribed fold lines. We investigate origami tubes and assemblages constructed from Miura-ori inspired sheets and use eigenvalue analyses to study their stiffness characteristics. A simplified bar model is used to model the stretching and shear of the flat panel segments and rotational hinges are used to simulate the bending stiffness of the panels and prescribed fold lines. We discuss the small to large deformation bending of thin sheets and show an improved method to estimate stiffness when modeling origami structures. The tube assemblages show interesting behaviors that make them suitable for applications in science and engineering.

8:24AM A44.00003 Multishape Origami Metasheets, SCOTT WAITUKAITIS, MARTIN VAN HECKE, Leiden University — We show how origami-based folding structures are a platform for multistable metamaterials. Our focus is the simplest building block, rigid 4-vertices, which we demonstrate can have up to six stable states. We extend our results to non-Euclidean vertices, which enables us fine-control over the number of minima. Our results lay the foundation for building designer, origami-based shape-shifting structures.

8:36AM A44.00004 Multi-stability in folded shells: non-Euclidean origami, ARTHUR EVANS, University of Massachusetts, Amherst — Both natural and man-made structures benefit from having multiple mechanically stable states, from the quick snapping motion of hummingbird beaks to micro-textured surfaces with tunable roughness. Rather than discuss special fabrication techniques for creating bi-stability through material anisotropy, in this talk I will present several examples of how folding a structure can modify the energy landscape and thus lead to multiple stable states. Using ideas from origami and differential geometry, I will discuss how deforming a non-Euclidean surface can be done either continuously or discontinuously, and explore the effects that global constraints have on the ultimate stability of the assemblings.

9:12AM A44.00005 Prediction of the force required to unwrap a thin-film origami structure, LEE WILSON, SERGIO PELLEGRINO, Caltech — We consider thin film membranes wrapped around a polygonal hub according to the origami crease pattern developed by Guest and Pellegrino [1]. The problem of unwrapping such membranes is important for applications such as space solar sails. Their deployment can be controlled by displacing four edge points radially outwards. During deployment the film buckles multiple times, creating a complex deployment force profile. We have used finite element simulations to investigate how different models of the creases affect the predicted force profile and we have compared the results of our simulations with experimental results for Kapton thin film thicknesses of 50um, 25um, 12.5um and 7.5um. The deployment force profile is also highly dependent on the initial packaged configuration of the film, which in our model is obtained by simulating the folding process from a flat state. [1] S.D.Guest and S. Pellegrino, Proc. First Int. Seminar on Struct. Morphology, R. Motro and T. Wester, eds. (1992) pp 203-215

9:24AM A44.00006 Making the Cut: Lattice Kirigami Rules, TOEN CASTLE, YIGIL CHO, XINGTING GONG, EUIYEON JUNG, DANIEL SUSSMAN, SHU YANG, RANDALL KAMEN, University of Pennsylvania — Complex 3D structures can be built by bending and folding a flat sheet, as is done in origami. This paradigm can be extended by cutting and gluing the sheet as well as folding. The principles manifest in manipulating a piece of paper can translate across many length scales, limited only by fabrication methods. We explore and develop a simple set of rules that apply to cutting, pasting, and folding honeycomb lattices. We consider origami-like structures that are extrinsically flat away from zero-dimensional sources of Gaussian curvature and one-dimensional sources of mean curvature, and our cutting and pasting rules maintain the intrinsic bond lengths on both the lattice and its dual lattice. We find that a small set of rules is allowed, providing a framework for exploring and building kirigami - folding, cutting, and pasting the edges of paper.

9:36AM A44.00007 Kirigami for Two-Dimensional Electronic Membranes, ZENAN QI, Boston University, DARIO BAHAMON, Mackenzie Presbyterian University, DAVID CAMPBELL, HAROLD PARK, Boston University — Two-dimensional materials have recently drawn tremendous attention because of their unique properties. In this work, we introduce the notion of two-dimensional kirigami, where concepts that have been used almost exclusively for macroscale structures are applied to dramatically enhance their stretchability. Specifically, we show using classical molecular dynamics simulations that the yield and fracture strains of graphene and MoS$_2$ can be enhanced by about a factor of three using kirigami as compared to standard monolayers. Finally, using graphene as an example, we demonstrate that the kirigami structure may open up interesting opportunities in coupling to the electronic behavior of 2D materials.

Authors acknowledge Mechanical Engineering and Physics departments at Boston University, and Mackgrafe at Mackenzie Presbyterian University.

Department of Mechanical Engineering

Graphene and Nano-Materials Research Center

Department of Physics

Department of Mechanical Engineering
10:00AM A44.00009 Optimization of Actuating Origami Networks1, PHILLIP BUSKOHL, Air Force Research Laboratory, KAZUKO FUCHI, Wright State Research Institute, GIORGIO BAZZÁN, JAMES JOO, REICH GREGORY, RICHARD VAIA, Air Force Research Laboratory – Origami structures morph between 2D and 3D conformations at predetermined fold lines that efficiently program the form, function and mobility of the structure. By leveraging design concepts from action origami, a subset of origami art focused on kinematic mechanisms, reversible folding patterns for applications such as solar array packaging, tunable antennae, and deployable sensing platforms may be designed. However, the enormity of the design space and the need to identify the requisite actuation forces within the structure places a severe limitation on design strategies based on intuition and geometry alone. The present work proposes a topology optimization method, using truss and frame element analysis, to distribute foldline mechanical properties within a reference crease pattern. Known actuating patterns are placed within a reference grid and the optimizer adjusts the fold stiffness of the network to optimally connect them. Design objectives may include a target motion, stress level, or mechanical energy distribution. Results include the validation of known action origami structures and their optimal connectivity within a larger network. This design suite offers an important step toward systematic incorporation of origami design concepts into new, novel and reconfigurable engineering devices.

1This research is supported under the Air Force Office of Scientific Research (AFOSR) funding, LRIR 13RQ02COR.

10:12AM A44.00010 Origami folding of polymer sheets by inkjet printing, YING LIU, BRANDI SHAW, MICHAEL D. DICKEY, JAN GENZER, North Carolina State University — In analogy to the ancient Japanese art of paper folding (Origami), self-folding is an attractive strategy to induce the formation of three-dimensional (3D) objects with well-defined shapes and dimensions using conventional two-dimensional (2D) patterning techniques, such as lithography and inkjet printing. Self-folding can be applied in the areas of reconfigurable devices, actuators, and sensors. Here we demonstrate a simple method for self-folding of polymer sheets utilizing localized light absorption on selected areas of the pre-strained polymer sheet. The ink is patterned via a desktop printer and it defines the location of the ‘hinge’ on the sheet. The inked areas on the 2D sheet absorb light preferentially, thus causing the polymer sheet to fold locally in the inked areas. The temperature gradients through the depth of the sheet induce localized shrinkage and the sheet folds within seconds. This patterned polymer sheets act as shape memory materials which can be programmed to fold into various 3D structures based on the nature of the light source, the shape and size of the ink patterns, and ink property. By controlling the aforementioned parameters we achieve a complete control of the time and degree of folding, which ultimately govern the final 3D shape of the folded object.

10:24AM A44.00011 Actuated 3D origami-like structures with tunable volume and stiffness, JOHANNES OVERVELDE, TWAN DE JONG, JAMES WEAVER, CHUCK HOBERMAN, KATIA BERTOLDI, Harvard University — Recent years have seen an upsurge of new materials with interesting and unusual properties that result from their regular periodic microstructure. Origami-based metamaterials based on the Miura fold pattern have recently gained a lot of attention for their ability to drastically change their shape and therewith creating a programmable metamaterial. In this work, we propose a completely new class of actuated 3D foldable materials with three degrees of freedom that can drastically change their shape and volume by folding. These materials do not only change their shape, but also have a tunable stiffness that can vary two orders of magnitude by making use of contact interaction between different parts of the material. We experimentally show their effectiveness by building a metamaterial consisting of 64 unit cells and by incorporating local inflatant actuators in the material to enable large on demand changes in shape and stiffness.

10:36AM A44.00012 Stress Focusing in Creased Shells, SARAH SELDEN, ARTHUR EVANS, NAKUL BENDE, RYAN HAYWARD, CHRISTIAN SANTANGELO, Univ of Mass - Amherst — Upon indentation, thin shells react by localizing strain energy in polygonal structures as opposed to a uniform axisymmetric distribution. While the formation of these localized structures are well-characterized for perfect shells, the introduction of a crease fundamentally changes the nature of the shell deformation. We perform finite element simulations, in tandem with experiments to explore the effect of a creased shell on the energy landscape. We find that the crease induces a new symmetry-breaking localization that does not appear in perfect shells, and we explore the deformation characteristics of the creased shell over a wide range of crease sizes, shell thickness, and crease orientations.

10:48AM A44.00013 Folding and bending of self-assembled nanoparticle membranes, YIFAN WANG, The University of Chicago, JIANHUI LIAO, Peking University, SEAN MCBRIDE, EFI EFRATI, The University of Chicago, XIAO-MIN LIN, Argonne National Laboratory, HEINRICH JAEGER, The University of Chicago — We demonstrate that self-assembled nanoparticle monolayers can be folded into 3 dimensional hollow structures. Using a force-volume Atomic Force Microscope (AFM), indentation measurements were made on these nanoparticle scrolls, and the bending modulus of the nanoparticle membrane is obtained for the first time. The resulting bending modulus is two orders of magnitude larger than that predicted by classical continuum elastic theory, we show this can be explained by a micropolar theory as the material makes on these nanoparticle scrolls, and the bending modulus of the nanoparticle membrane is obtained for the first time. The resulting bending modulus is two orders of magnitude larger than that predicted by classical continuum elastic theory, we show this can be explained by a micropolar theory as the material makes on these nanoparticle scrolls, and the bending modulus of the nanoparticle membrane is obtained for the first time. The resulting bending modulus is two orders of magnitude larger than that predicted by classical continuum elastic theory, we show this can be explained by a micropolar theory as the material makes on these nanoparticle scrolls, and the bending modulus of the nanoparticle membrane is obtained for the first time. The resulting bending modulus is two orders of magnitude larger than that predicted by classical continuum elastic theory, we show this can be explained by a micropolar theory as the material makes on these nanoparticle scrolls, and the bending modulus of the nanoparticle membrane is obtained for the first time. 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The resulting bending modulus is two orders of magnitude larger than that predicted by classical continuum elastic theory, we show this can be explained by a micropolar theory as the material makes on these nanoparticle scrolls, and the bending modulus of the nanoparticle membrane is obtained for the first time. The resulting bending modulus is two orders of magnitude larger than that predicted by classical continuum elastic theory, we show this can be explained by a micropolar theory as the material makes on these nanoparticle scrolls, and the bending modulus of the nanoparticle membrane is obtained for the first time. The resulting bending modulus is two orders of magnitude larger than that predicted by classical continuum elastic theory, we show this can be explained by a micropolar theory as the material makes on these nanoparticle scrolls, and the bending modulus of the nanoparticle membrane is obtained for the first time. 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Monday, March 2, 2015 8:00AM - 11:00AM Session A45 DPOLY: Crystalline Polymers 216AB - Christopher Li, Drexel University 8:00AM A45.00001 Interplay Between a Strong Memory Effect of Crystallization and Liquid-Liquid Phase Separation in Melts of Broadly Distributed Ethylene 1-Alkene Copolymers, RUFINA G. ALAMO, AL MAMUN, XUEJIAN CHEN, FAMU-FSU College of Engineering, Department of Chemical and Biomedical Engineering, Tallahassee, FL 32310 — Ethylene-1-alkene copolymers with a broad, bimodal comonomer distribution display acceleration and retardation of the crystallization rate when cooling from a range of melt temperatures where narrow copolymers show a continuous acceleration of the rate. The acceleration of the rate is observed in a range of melt temperatures between 165 and 150 °C, and is due to a strong memory effect of crystallization above their equilibrium melting point. The retardation or inversion of the rate, observed in a range of 150 to 123 °C, demarcates the onset of a self-seeded assisted liquid-liquid phase separation (LLPS) between comonomer-rich and comonomer poor molecules. The interplay between number of self-seeds at the initial melt temperature and chain diffusion during LLPS causes a decrease in the crystallization rate with decreasing melt temperature. When crystallites remain in the melt at temperatures <123 °C, the crystallization rate again accelerates quickly. The crystallization rates were studied by DSC, and the effect in nucleation density and in overall crystalline morphology of crystallizations from one phase or two liquid phases was followed by polarized optical microscopy and transmission electron microscopy.
8:12AM A45.00002 Butyl Branch Partitioning to the Crystal Surface in Polyethylenes Detected by NMR. KLAUS SCHMIDT-ROHR, Brandeis University, Department of Chemistry, Waltham, MA 02453, USA, ALLISON WHITE, Iowa State University, Department of Chemistry, Ames, IA 50011, USA, KANMI MAO, DIANA SMIRNOVA, ExxonMobil Research and Engineering, 1545 Route 22 East, Annandale, NJ 08801, USA — Short-chain branches have pronounced effects on the structure and properties of semicrystalline polyethylenes. Distinct partitioning of butyl branches in high- and linear low-density polyethylenes (HDPEs and LDLDPEs) synthesized with hexene comonomers has been detected by solid-state $^{13}$C NMR. In mobility-selective $^{13}$C NMR spectra, distinct signals of mobile amorphous and of trans-rich immobilized branches are observed, the latter with longer $^{13}$C spin lattice relaxation times and limited mobility. This analysis takes advantage of double inverse filtering, which provides the signals of limited-mobility noncrystalline segments selectively. The location of the dynamically constrained branches near the crystal surface has been confirmed by $^1$H spin diffusion measurements. The fraction of immobilized butyl branches is approximately constant at about 0.5 mol% for a series of copolymers with 0.35 – 3.3 mol% hexene. It is close to the percentage expected if one surface site is freely available for each crystalline chain stem. Lower molecular weight appears to enable better ordering of branches at the crystal surface. Further, it more strongly limits a fast-relaxing component in $^{13}$C spin-lattice relaxation of the crystalline signal that can be attributed to chain diffusion. In a HDPE with 0.35 mol % hexene content, nearly all branches are at the crystal surface.

8:24AM A45.00003 Chain Trajectory of Polymer Chains in Bulk and Single Crystals: Molecular Weight Effect. TOSHIKAZU MIYOSHI, YOULEE HONG, The University of Akron, THE UNIVERSITY OF AKRON TEAM — Semicrystalline polymers are crystallized as folded chains in thin lamellae of ca. 5-20 nm from random coils in the melt and solution states. Recently, we developed a novel strategy to access chain trajectory of semi-crystalline polymers using $^{13}$C/$^{13}$C double Quantum (DQ) NMR combined with selectively isotopic labeling. This approach does not suffer from morphology (bulk vs single crystals), molecular weight distribution, and crystallization temperatures. Thereby, DQ NMR has been successfully applied to determination of chain trajectory of semi-crystalline polymer with a relatively low molecular weight in bulk as well as single crystals in wide crystallization temperatures. In this work, we will report chain-folding structure of a semicrystalline polymer with a high molecular weight in bulk as well as single crystals. Molecular weight effects on chain trajectory in different morphology will be demonstrated.

8:36AM A45.00004 SAXS/WAXS measurements of HDPE crystallization during uniaxial extensional flow.ERICA MCCREADY, WESLEY BURGHARDT, Northwestern University — We report studies of flow-induced crystallization of high density polyethylene during uniaxial extensional flow. Flow was applied using an SER extensional fixture housed in a custom built oven designed to facilitate in situ synchrotron x-ray experiments. Samples were loaded onto the fixture, heated to well above the melting temperature, and then cooled to the desired crystallization temperature. Extent of crystallization, orientation of crystallites, and extensional viscosity were determined throughout the entire uniaxial extensional flow, using simultaneous small- and wide-angle x-ray scattering (SAXS and WAXS) and torque measurements. Both temperature and extension rate were varied. SAXS patterns show distinct shapes characteristic of shish kebab morphology formation. WAXS peaks indicate high alignment of unit cell structure along the flow direction. Evolution of both SAXS and WAXS patterns can be correlated to each other and to extensional viscosity features during the crystallization process.

8:48AM A45.00005 Selective crystallization of conjugated polymer nanowires from graphene-coated surfaces. DANIEL ACEVEDO CARTAGENA, YUE ZHANG, University of Massachusetts, ELVIRA TRABANINO, None, EMILY PENTZER, Case Western Reserve University, TODD EMRICK, ALEJANDRO BRISEN0, RYAN HAYWARD, University of Massachusetts — Solution-based crystallization of conjugated polymers is a promising route to develop hierarchical structures for organic electronic devices, especially solar cells. Well-defined nucleation sites in supersaturated solutions can regulate the crystallization behavior to control the morphology of the material. We have developed an approach to tune the hysteresis between melting and crystallization of poly(3-hexylthiophene) in a marginal solvent, using temperature controlled fractionation. This process produces supersaturated solutions in a metastable state at room temperature, suppressing homogeneous nucleation of crystals but allowing for heterogeneous crystallization on nucleation sites. We show that in these metastable solutions, crystalline nanowires are selectively grown on graphene-coated surfaces and highly oriented pyrolytic graphite.

9:00AM A45.00006 Mesomorphic State in Early Stage Crystallization of Polyethylene. KALMAN MIGLER, ANGELA HIGHT WALKER, ANTHONY KOTULA, NIST — The kinetic pathway by which a molten polymer transforms into a multi-length scale, semi-crystalline structure upon cooling is an unsolved problem in polymer physics, yet it is critical to the processing, properties and ultimate performance of these materials. Here we utilize Raman spectroscopy to probe the early stage crystallization kinetics of a high-density polyethylene during low undercooling. The importance of Raman as a tool stems from its ability to measure the mass fraction of conformations that are in consecutive trans sequences (locally straight) but are not in an orthorhombic configuration, which we term non-orthorhombic continuous-trans (NOCT). We find that the Raman peaks indicative of NOCT precede the appearance of the peak which indicates orthorhombic crystallinity. We analyze the spectra within the context of a three-state conformational model to extract the mass fractions of the NOCT and the orthorhombic conformational states as crystallization proceeds. Concomitant birefringence and turbidity measurements indicate that this NOCT state can be understood as a separate mesomorphic phase which emerges from the melt state and precedes crystallization.

9:12AM A45.00007 Morphology and Crystallization Behavior of Poly(3-(2'-ethyl)hexthiophene) (P3EHT) Containing Diblock Copolymers. EMILY DAVIDSON, BRYAN BECKINGHAM, VICTOR HO, UC Berkeley, RACHEL SEGALMAN, UC Santa Barbara — Poly(3-alkylthiophene) crystallites are confined within classical diblock copolymer microphase separated domains by substituting the alkyl side chain to reduce the crystalline driving force. Previously, we determined that the P3AT chain axis is oriented perpendicular to the domain interface within crystallites. Here, we find that following block copolymer self-assembly in the melt, crystallite growth drives expansion of microdomains, indicating that chains adopt an extended conformation within confined crystallites. In addition, we demonstrate that the degree of perfection of crystallites confined within lamellae may be tuned via the degree of undercooling.
9:24AM A45.00008 Exploring Molecular Dimension and Trajectory of Polymer Chains Embedded in Single Crystals1, YOULEE HONG, TOSHIKAZU MIYOSHI. University of Akron — Semicrystalline polymers are crystallized as folded chains in thin lamellae of ca. 5-20 nm from random coils in the melt and solution states. Even though there are continuous efforts on understanding of crystallization mechanisms at molecular levels for understanding of crystallization mechanism of polymers at molecular levels, the fundamental questions - when, where, and how do semicrystalline polymers fold during crystallization? - have not been clarified due to experimental limitations. Recently, we developed a novel strategy to access chain trajectory of semi-crystalline polymers using 13C-13C double Quantum (DQ) NMR. In this work, we recently investigated determined molecular dimension as well as chain-trajectory of 13C CH3-labeled isotactic poly(1-butene) (iPB1) in form III chiral single crystals blended with nonlabeled iPB1 crystallized under low supercooling, using solid-state NMR. Comparisons of 13C-13C double quantum (DQ) NMR results at multiple sites with spin dynamics simulation revealed individual chains form the three dimensional nanoclusters via folding. This result supports proves two step process of i) cluster formation by chain-folding the prestige of crystallization, and ii) depositions of the cluster on the growth front of single crystal.

1National Science Foundation

9:36AM A45.00009 On the strain-induced structural evolution upon uniaxial stretching of Poly(Vinylidene Fluoride): influence of secondary crystals and crystalline relaxation, JULIETTE DEFEBVIN, SOPHIE BARRAU, GRÉGORY STOCLET, JEAN-MARC LEFEBVRE. Umet-Université Lille1, POLYMER ENGINEERING SCIENCE TEAM — Development of more efficient piezoelectric devices tends to innovate and create materials able to combine flexibility and electro-mechanical conversion. Poly(vinylidene fluoride) (PVDF) is a semi-crystalline polymer that exhibits interesting piezoelectric properties. Besides PVDF is able to convert an electric energy and vice versa. However these physical properties are highly dependent on the polymer crystal structure. PVDF presents at least two main crystalline forms. The most common phase is the α-phase that is non-polar. On the other hand, the β phase is the most polar one and it can be obtained by a stretching of the α-phase. Knowing the influence of the drawing conditions on the strain-induced structural evolution is thus of prime interest. To assess this point the strain-induced structural evolution of PVDF, stretched under different conditions, has been followed in-situ by means of WAXS/SAXS experiments. As a main result, this study shows that drawing conditions strongly affect both the α to β phase conversion degree and the crystalline morphology. Moreover the key role played by the crystalline relaxation of PVDF on the strain-induced structural evolution is also highlighted for the first time.

9:48AM A45.00010 Quantifying tie-chain content in semicrystalline polyolefins with vapor-flow small-angle neutron scattering, AMANDA MCDERMOTT, CHAD SNYDER. National Institute of Standards and Technology (NIST), PAUL DESLAURIERS, Chevron Phillips Chemical Company, RONALD JONES. National Institute of Standards and Technology (NIST) — Tie molecules bridging adjacent crystalline lamellae in semicrystalline polymers strongly impact mechanical properties, but they remain difficult to characterize. In this work we apply equilibrium swelling theory, balancing the entropic cost of tie-chain extension against the free energy of mixing, to small-angle neutron scattering patterns from semicrystalline polyethylene films whose interlamellar amorphous regions are swollen with deuterated organic solvent. Results show that for a linear polyethylene and several ethylene-hexene copolymers, these vapor-flow SANS measurements of tie-chain content compare favorably with a primary structural parameter (PSP2) that is calculated from molecular architecture and correlates with slow crack growth behavior.

10:00AM A45.00011 Isothermal Programming Triple Shape Memory1, SERGEI SHEIKO, JING ZHOU, QIAOXI LI, SARA TURNER, VALERIE ASHBY, University of North Carolina at Chapel Hill, ANDREY DOBRYNIN, University of Connecticut — While a variety of shape memory materials have been developed for triple shape memory (TSM), different fixation temperatures are required for memorizing different shapes, with imposed limitations on materials design. We present a new strategy for TSM, where different shapes are programmed at a constant fixation temperature and can be applied to a variety of semi-crystalline elastomers. This universal strategy is based on controlling the interplay between shape-memory thermodynamics and kinetics of polymer crystallization. We have developed a composite model to study correlations between the control parameters (chemical composition, crosslinking density, crystallization rate) and TSM performance (shape fixation and recovery). Furthermore, the isothermal TSM allows one-way reversible shape memory.

1Acknowledge financial support from the NSF DMR-1122483, DMR-1004576, and DMR-1206957.

10:12AM A45.00012 Flow-induced crystallinity in polyethylene as probed by time-resolved Raman spectroscopy and optical microscopy, ANTHONY KOTULA, ANGELA HIGHT WALKER, KALMAN MIGLER, National Institute of Standards and Technology — The crystallization of polymer melts under flow is critically relevant to the polymer processing industry. Optical, thermal, and mechanical properties of semi-crystalline polymer products depend on the final crystallinity of the material, which depends on the structure and orientation of the initial molecular-scale crystal nuclei formed in flow. Here, we present a combination of optical microscopy and Raman scattering techniques to analyze structure formation in high density polyethylene during steady shear at low degrees of undercooling. When low shear rates (~ 1 s-1) are imposed after a temperature quench to less than 10 °C undercooling, fibrous structures aligned parallel to the flow direction appear over a period of minutes. Raman spectra indicate that chain straightening (consecutive trans chain conformation) precedes the growth of the crystalline phase, and increased shear increases the rate of growth of the consecutive trans and crystalline fractions. Complimentary Raman scattering experiments are performed on n-alkanes to compare conformational similarities in the molecular structure during the crystallization process.

10:24AM A45.00013 Short-Range Order of Mesomorphic Phase of a Semi-crystalline Polymer by Solid-State NMR: Isotactic Polypropylene1, SHICHEN YUAN, TOSHIKAZU MIYOSHI, Univ of Akron — Mesophase is intermediate phase between crystalline and melt state. Characterization of short-range structures of disordered mesomorphic phase without long-range order is challenging issue in polymer characterization. The short range order was considered same as α or β . However, in this work, a new strategy using 13C-13C through space interactions as well as molecular dynamics based on chemical shift anisotropy (CSA) re-orientation is proposed for evaluating short-range order of mesophase of isotactic-polypropylene (iPP). 13C-13C double quantum (DQ) build up curves of 13C 15 percent CH3 selectively labeled iPP and spin dynamics simulations elucidate that local packing structures in mesophase is very close to that in β phase. Moreover, exchange NMR proves that the crystalline chains perform large amplitude motions in all α, β, and mesophase. The correlation time of overall dynamics of stems in mesophase follows the same Arrhenius line with that of β phase but is largely deviated from the Arrhenius line of the α phase. Through the obtained results, it is concluded that short-range order in mesophase is exceedingly close or same to those in β phase.

1This work was financially supported by the National Science Foundation (Grant no. DMR-1105829) and by UA startup funds.
10:36AM A45.00014 Stress induced reversible crystal transition in poly(butylene succinate)\(^1\). GUOMING LIU, LIUCHUN ZHENG, XIQIN ZHANG, CHUNCHENG LI, DUJIN WANG, CAS Key Laboratory of Engineering Plastics, Institute of Chemistry, the Chinese Academy of Sciences, Beijing, 100190, China — The plastic deformation mechanism of semi-crystalline polymers is a long-studied topic, which is crucial for establishing structure/property relationships. For polymers with stress induced crystal transition, some open questions still need to be answered, such as on which stage of plastic deformation does the crystal transition take place, and more importantly, what happens on the lamellar structure during crystal transition. In this talk, stress-induced reversible crystal transition in poly(butylene succinate) was systematically investigated by in-situ WAXS and SAXS. A "lamellar thickening" phenomenon was observed during stretching, which was shown to mainly originated from the reversible crystal transition. This mechanism was shown to be valid in poly(ethylene succinate). The critical stress for the transition was measured in a series of PBS-based crystalline-amorphous multi-block copolymers. Interestingly, these PBS copolymers exhibited identical critical stress independent of amorphous blocks. The universal critical stress for crystal transition was interpreted through a single-microfibril-stretching mechanism.

\(^1\)The work is financially supported by the National Natural Science Foundation of China (Grant No. 51203170).

10:48AM A45.00015 Crystallization of low molecular weight atactic polystyrene, YU CHAI, JAMES GILBERT, CHAD DALEY, JAMES FORREST, Univ of Waterloo — It is well known that atactic polystyrene does not crystallize. However, it is also true that even in pure atactic polystyrene, there is a small fraction of isotactic and syndiotactic moieties due to random statistics, which are crystallizable. Using small molecular weight atactic polystyrene, we are able to observe crystallization in an acceptable time window. We characterize the crystals in terms of both the morphology and dynamics by using atomic force microscopy and differential scanning calorimetry and the results are consistent with that from the bulk isotactic and syndiotactic polystyrene. As the molecular weight increases, the fraction of pure isotactic and syndiotactic components becomes smaller, and crystallization is not observed.

Monday, March 2, 2015 8:00AM - 11:00AM —
Session A46 DBIO: Invited Session: DNA Physics and Chromatin Organization 217A - Alexandre Morozov, Rutgers University

8:00AM A46.00001 Dynamics of the Competition Between Nucleosome Unwrapping and DNA Binding Proteins\(^1\), RALF BUNDSCHUH, Ohio State Univ - Columbus — In eukaryotic organisms DNA is tightly wrapped into nucleosomes. This bears the question how this DNA can be accessed in order to be copied, transcribed, or repaired. A process that allows access to the DNA is transient unwrapping of the DNA from the histone proteins. We have developed a quantitative model of this unwrapping process which we calibrate by comparison to nucleosome unzipping experiments by the Wang group. We then apply this model to quantitatively explain the dynamics of transcription factor binding within nucleosomal DNA. In this context, it has been well known that nucleosomes reduce the affinity for transcription factors to binding sites covered by the nucleosome. It has been assumed that this is due to a reduction in on-rate since a transcription factor can only bind when a rare thermal fluctuation of the nucleosome makes the DNA accessible. However, recent experimental data surprisingly shows that the off-rate of transcription factors is also strongly affected in the presence of a nucleosome. The application of our nucleosome unwrapping free energy landscape demonstrates that this increase in off-rate by several orders of magnitude is a consequence of a competition between partial binding events of dimeric transcription factors and the nucleosome.

\(^1\)This material is based upon work supported by the National Science Foundation under Grant Nos. 1105458 and 1410172.

8:36AM A46.00002 Hydrodynamics, ROBijn Bruinsma, Department of Physics and Astronomy, University of California, Los Angeles — The talk will present a hydrodynamic description of large-scale cooperative movement of chromatin that have been observed by particle tracking methods. The results of the hydrodynamic description will be compared with the tracking data. Passive thermal fluctuations and active "scalar" events - associated with local chromatin condensation - are found to dominate cooperative motion at shorter length scales while active "vector" events - associated with chromatin remodeling - driving transverse hydrodynamic modes dominate at large length scales.

9:12AM A46.00003 A physical analysis of nucleosome positioning, ULRICH GERLAND, Physik Department, Technische Universität München, Munich, Germany — The first level of genome packaging in eukaryotic cells involves the formation of dense nucleosome arrays, with DNA coverage near 90% in yeasts. A high nucleosome coverage is essential for cells, e.g. to prevent cryptic transcription, and the local positions of specific nucleosomes can play an important role in gene regulation. It is known that in vivo nucleosome positions are affected by a complex mix of passive and active mechanisms, including sequence-specific histone-DNA binding, nucleosome-nucleosome interactions, AT-dependent remodeling enzymes, transcription, and DNA replication. Yet, the statistical distribution of nucleosome positions is extremely well described by simple physical models that treat the chromatin fiber as an interacting one-dimensional gas. I will discuss how can we interpret this surprising observation from a mechanistic perspective. I will also discuss the kinetics of the interacting gas model, which is pertinent to the question of how cells achieve the high nucleosome coverage within a short time, e.g. after DNA replication.

9:48AM A46.00004 DNA-protein recognition and sequence-dependent variations of DNA conformational properties, ALEXANDER VOLOGODSKII, New York University — Parameters of B-DNA, the major form of the double helix, depend on its sequence. This dependence can contribute to the recognition of specific DNA sequences by proteins. Here we try to analyze this contribution quantitatively. In the first approach to this goal we used experimental data on the sequence dependence of DNA bending rigidity and its helical repeat. The solution data on these parameters of B-DNA were derived from the experiments on cyclization of short DNA fragments with specially designed sequences. The data allowed calculating the sequence variations of DNA bending energy, as well as the variations of the energy of torsional deformation of the double helix associated with a protein binding. The results show that DNA conformational parameters can have very limited influence on the sequence specificity of protein binding. In the second approach we analyzed the experimental data on the binding affinity of the nucleosome core with DNA fragments of different sequences. The conclusions derived in these two approaches are in a good agreement with one another.

10:24AM A46.00005 Polymer Models of Looping in Genome, ANIRVAN SENGUPTA, Rutgers University — Regions of the chromosome that are many thousands of bases away often have to come in contact for turning some genes on or off. To discover the specific and highly regulated contacts, we need to have a good statistical description of the strength of non-specific ones. We model the chromatin fiber as a potentially heterogeneous polymer and discuss how to use such a model in the analysis of chromatin conformation capture data.

Monday, March 2, 2015 8:00AM - 11:00AM —
Session A47 DBIO: Focus Session: Physics of Behavior I 217B - Greg Stephens, Vrije Universiteit Amsterdam & Okinawa Institute of Science and Technology
8:00AM A47.00001 ABSTRACT WITHDRAWN

8:12AM A47.00002 How to catch a falling fruit , ANDREW MARANTAN, LAKSHMINARAYANAN MAHADEVAN, Harvard Univ — A variety of fish engage in complex hunting behaviors involving catching airborne prey falling to the surface of the water. In principle this requires that the fish develop internal models describing both the falling prey and its own motion relative to that prey. However learning such models is complicated by the fact that the fish must also account for noise in optical measurements and the refraction occurring at the air/water interface. Inspired by experimental observations, we describe how one such species (Brycon guatemalensis) might feasibly overcome these obstacles and learn a model accurate enough to catch falling fruit. Instead of learning a model for how the fruit falls and a model for how it moves in the water and a model accounting for refraction, we argue that the fish could instead learn one approximate linear model relating a set of measured inputs to a set of measured outputs valid in a limited domain of initial conditions. The fish could then make its control decisions based on the outcome predicted by this combined linear model. We also discuss how the fish can leverage neural transformations of raw data to learn a model with a larger domain of validity and yet more sensitive to noise due to nontrivial Jacobians arising from the neural transformations.

8:24AM A47.00003 Growth behaviors of bacteria reveal the evolutionary significance of energy-efficiency1. ARJIT MAITRA, KEN DILL, Stony Brook University — Microorganisms have evolved a mosaic of gene expression changes to adapt their growth behaviors to changing environmental conditions. The subset of genes coding for the protein translation machineries, the ribosomes, however display robust linear activities with growth rates. Such patterns are considered to be the source of growth itself. There is another robust growth law, observed by Monod in the 1940s, in which bacteria are able to scale their growth with food concentration before plateauing off to a constant value. To interlink these observed growth laws we derive an analytical network model that leverages metabolic data to capture how the cell manages its exchange of energy to support costly gene expression. The model explores the limits of energy allocation for function and reveals evolutionary principles. Among others, we find, in glucose medium the fastest growing *E. coli* operate close to their maximum energy-efficiency. Optimization of energy efficiency provides a quantitative limit to how much energy is allocated for protein synthesis and it is determined by evolutionarily selected structural and biophysical constants. We conclude that energy efficiency has played a key role in bacterial evolution.

1Supported by the Laufer Center for Physical and Quantitative Biology, SBU

8:36AM A47.00004 Migration of amoeba cells in an electric field1. ISABELLA GUIDO, EBERHARD BODENSCHATZ, Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — Exogenous and endogenous electric fields play a role in cell physiology as a guiding mechanism for the orientation and migration of cells. Electrotaxis of living cells has been observed for several cell types, e.g. neurons, fibroblasts, leukocytes, neural crest cells, cancer cells. Dictyostelium discoideum (Dd), an intensively investigated chemotactic model organism, also exhibits a strong electrotactic behavior moving toward the cathode under the influence of electric fields. Here we report experiments on the effects of DC electric fields on the directional migration of Dd cells. We apply the electric field to cells seeded into microfluidic devices equipped with agar bridges to avoid any harmful effects of the electric field on the cells (ions formation, pH changes, etc.) and a constant flow to prevent the build-up of chemical gradient that elicits chemotaxis. Our results show that the cells linearly increase their speed over time when a constant electric field is applied for a prolonged duration (2 hours). This novel phenomenon cannot be attributed to mechanotaxis as the drag force of the electroosmotic flow is too small to produce shear forces that can reorient cells. It is independent of the cellular developmental stage and to our knowledge, it was not observed in chemotaxis.

1This work is supported by MaxSynBio project of the Max Planck Society

8:48AM A47.00005 Rhythmicity, recurrence, and recovery of flagellar beating4. KIRSTY WAN, RAY-MOND GOLDSTEIN, DAMTP, Univ. of Cambridge — The eukaryotic flagellum beats with apparently unfailing periodicity, yet responds rapidly to stimuli. Further, we quantify the recovery of periodic breaststroke beating from transient hydrodynamic forcing. These results will help constrain microscopic theories on the origins and regulation of flagellar beating.

4Financial support is acknowledged from the EPSRC, ERC Advanced Investigator Grant No. 247333, and a Senior Investigator Award from the Wellcome Trust.

9:00AM A47.00006 Crosslink dynamics in a model of two filaments of actin under shear, ARJAN BOERMA, ERIK VAN DER GIJSEN, STEFANOS PAPANIKOLAOU, University of Groningen — We seek to elucidate the dynamic mechanisms underlying the stress dependent effects of the cellular cytoskeleton, as they are observed in the storage and loss modulus as a function of frequency and cross-linker concentration. We report on the statistical behavior of the effects originating from cross-linker dynamics in the basic constituent of a cytoskeleton network: two mutually cross-linked filaments. We model each of the filaments and the cross-linkers in terms of elastic finite elements. Unbinding of individual cross-linkers takes place through a realistic constitutive model and re-binding may occur to maintain the average cross-linker density. Our approach provides a direct analysis of the athermal interplay of the elastic filament interactions with the dynamics of the cross-linking molecules.

9:12AM A47.00007 Neuromechanics of crawling in *D. melanogaster* larvae, CENGIZ PEHLEVAN, HHMI Janelia Research Campus. PAOLO PAOLETTI, University of Liverpool, L. MAHADEVAN, Harvard University — Nervous system, body and environment interact in non-trivial ways to generate locomotion and thence behavior in an organism. Here we present a minimal integrative mathematical model to describe the simple behavior of forward crawling in *Drosophila* larvae. Our model couples the excitation-inhibition circuits in the nervous system to force production in the muscles and body movement in a frictional environment, which in turn leads to a proprioceptive signal that feeds back to the nervous system. Our results explain the basic observed phenomenology of crawling with or without proprioception, and elucidate the stabilizing role of proprioception in crawling with respect to external and internal perturbations. Our integrated approach allows us to make testable predictions on the effect of changing body-environment interactions on crawling, and serves as a substrate for the development of hierarchical models linking cellular processes to behavior.
Entropy measures of collective cell migration. ARIADNE WHITBY, Imperial College London & MRC Clinical Sciences Centre, SIMONA PARRINELLO, MRC Clinical Sciences Centre, ALDO FAISAL, Imperial College London — Collective cell migration is a critical process during tissue formation and repair. To this end there is a need to develop tools to quantitatively measure the dynamics of collective cell migration obtained from microscopy data. Drawing on statistical physics we use entropy of velocity fields derived from dense optic flow to quantitatively measure collective migration. Using peripheral nerve repair after injury as experimental system, we study how Schwann cells, guided by fibroblasts, migrate in cord-like structures across the cut, paving a highway for neurons. This process of emergence of organised behaviour is key for successful repair, yet the emergence of leader cells and transition from a random to ordered state is not understood. We find fibroblasts induce correlated directionality in migrating Schwann cells as measured by a decrease in the entropy of motion vector. We show our method is robust with respect to image resolution in time and space, giving a principled assessment of how various molecular mechanisms affect macroscopic features of collective cell migration. Finally, the generality of our method allows us to process both simulated cell movement and microscopic data, enabling principled fitting and comparison of in silico to in vitro.

9:36AM A47.00009 Sensory-motor system identification of active perception in ecologically valid environments. WILLIAM ABBOTT, ANDREAS THOMIK, A. ALDO FAISAL, Imperial College London — The brain is a dynamical system mapping sensory inputs to motor actions. This relationship has been widely characterised by reductionist controlled experiments. Here we present working models out of the lab “into the wild” to capture, rather than constrain, sensory inputs and motor outputs, by recording 90% of sensory inputs using head mounted eye-tracking, scene camera and microphone as well as recording 95% of skeletal motor outputs by motion tracking 51 degrees of freedom in the body and a total of 40 degrees of freedom from the hands. We can thus begin to systematically characterise the perception-action loop through system identification. This enables us to evaluate classical relationships in ecologically valid settings and behaviours including 3 daily scenarios: breakfast in the kitchen, evening chores and activities and in-door ambulation. This level of data richness (97 DOF, 60Hz), coupled with the extensive recordings of natural perceptual and behavioural data (total > 30 hrs, 10 subjects) enables us to answer general questions of how lab tasks and protocols will produce systematically different results from those found in daily life.

9:48AM A47.00010 Animal and robot experiments to discover principles behind the evolution of a minimal locomotor apparatus for robust legged locomotion. BENJAMIN MCMINROE, HENRY ASTLEY, Georgia Tech, SANDY KAWANO, NIMBioS, RICHARD BLOB, Clemson University, DANIEL I. GOLDMAN, Georgia Tech — In the evolutionary transition from an aquatic to a terrestrial environment, early walkers adapted to the challenges of locomotion on complex, flowable substrates (e.g. sand and mud). Our previous biological and robotic studies have demonstrated that locomotion on such substrates is sensitive to both limb morphology and kinematics. Although reconstructions of early vertebrate skeletal morphologies exist, the kinematic strategies required for successful locomotion by these organisms have not yet been explored. To gain insight into how early walkers contended with complex substrates, we developed a robotic model with appendage morphology inspired by a model analog organism, the mudskimmer. We tested mudskippers and the robot on different substrates, including rigid ground and dry granular media, varying incline angle. The mudskippers moved effectively on all level substrates using a fin-driven gait. But as incline angle increased, the animals used their tails in concert with their fins to generate propulsion. Adding an actuated tail to the robot improved robustness, making possible locomotion on otherwise inaccessible inclines. With these discoveries, we are elucidating a minimal template that may have allowed the early walkers to adapt to locomotion on land.

This work was supported by NSF PoLS

10:00AM A47.00011 Evolution of foraging behavior in Drosophilid larvae. MARTA RIVERA-ALBA, MAYANK KABRA, KRISTIN BRANSON, Janelia Research Campus, HHMI, CHRISTEN MIRTH, Instituto Gulbenkian de Ciencia — Drosophilids, like other insects, go through a larval phase before metamorphosing into adults. Larvae increase their body weight by several orders of magnitude in a few days. We therefore hypothesized that foraging behavior is under strong evolutionary pressure to best fit the larval environment. To test this hypothesis we used a multidisciplinary approach to analyze foraging behavior across species and larval stages. First, we recorded several videos of larvae foraging for each of 4 Drosophilid species. Then, using a supervised machine learning approach, we automatically annotated the video collection for the foraging sub-behaviors, including crawling, turning, head casting or burrowing. We also computed over 100 features to describe the posture and dynamics of each animal in each video frame. From these data, we fit models to the behavior of each species. The models each had the same parametric form, but differed in the exact parameters. By simulating larva behavior in virtual arenas we can infer which properties of the environments are better for each species. Comparisons between these inferred environments and the actual environments where these animals live will give us a deeper understanding about the evolution of foraging behavior in Drosophilid larvae.

10:12AM A47.00012 Collective workload organization in confined excavation of granular media. DARIA MONAENKOVA, VADIM LINEVICH, MICHAEL A. GOODISMAN, DANIEL I. GOLDMAN, Georgia Institute of Technology — Many social insects collectively construct large nests in complex substrates: such structures are often composed of narrow tunnels. The benefits of collective construction, including reduced construction costs per worker come with challenges of navigation in crowded, confined spaces. Here we study the workforce organization of groups of S. invicta fire ants creating tunnels in wet granular media. We monitor the activity levels of marked (painted) workers—defined as a number of tunnel visits over 12 hours—during initiation of tunnels. The activity levels are described by a Lorenz curve with a Gini coefficient of ∼0.7 indicating that a majority of the excavation is performed by a minority of workers. We hypothesize that this workload distribution is beneficial for excavation in crowded conditions, and use a 2D cellular automata (CA) model to reproduce behaviors of the excavating ants. CA simulations reveal that tunnel construction rates decrease in groups of equally active animals compared to groups with the natural workload distribution. We use predictions of the CA model to organize collective excavation of granular material by teams of digging robots, and use the robots to test hypotheses of crowded excavation in the physical world.

1We acknowledge support of National Science Foundation, Physics of Living Systems division.

10:24AM A47.00013 Nociception and escape behavior in planarians. EVA-MARIA SCHOEZT COLLINS, University of California, San Diego — Planarians are famous and widely studied for their regenerative capabilities. When a moving planarian is cut through the middle, the resulting head and tail pieces instantaneously retract and exhibit a characteristic escape response that differs from normal locomotion. In asexaul animals, a similar reaction is observed when the planarian undergoes fission, suggesting that reproduction through self-tearing is a rather traumatic event for the animal. Using a multiscale approach, we unravel the dynamics, mechanics, and functional aspects of the planarian escape response. This musculature-driven gait was found to be a dominating response that supersedes the urge to feed or reproduce and quantitatively differs from other modes of planarian locomotion (gliding, peristalsis). We show that this escape gait constitutes the animal’s pain response mediated by TRP like receptors and the neurotransmitter histamine, and that it can be induced through adverse thermal, mechanical, electrical or chemical stimuli. Ultimately, we will examine the neuronal subpopulations involved in mediating escape reflexes in planarians and how they are functionally restored during regeneration, thereby gaining mechanistic insight into the neuronal circuits required for specific behaviors.

1Supported by BWF CASI and Sloan Foundation.
An explicitly solvated full atomicistic model of the cardiac thin filament and application on the calcium binding effects from familial hypertrophic cardiomyopathy linked mutations, MICHAEL WILLIAMS, STEVEN SCHWARTZ, Dept. of Chemistry and Biochemistry, The University of Arizona — The previous version of our cardiac thin filament (CTF) model consisted of the troponin complex (cTn), two coiled-coil dimers of tropomyosin (Tm), and 29 actin units. We now present the newest revision of the model to include explicit solvation. The model was developed to continue our study of genetic mutations in the CTF proteins which are linked to familial hypertrophic cardiomyopathies. Binding of calcium to the cTnC subunit causes subtle conformational changes to propagate through the cTnC to the cTnI subunit which then detaches from actin. Conformational changes propagate through to the cTnT subunit, which allows Tm to move into the open position along actin, leading to muscle contraction. Calcium disassociation allows for the reverse to occur, which results in muscle relaxation. The inclusion of explicit TIP3 water solvation allows for the model to get better individual local solvent to protein interactions; which are important when observing the N-lobe calcium binding pocket of the cTnC. We are able to compare in silica and in vitro experimental results to better understand the physiological effects from mutants, such as the R92L/W and F110V/I of the cTnT, on the calcium binding affinity compared to the wild type.

Proteins and Complexity, JOELLE MURRAY, DANA GIBBON, ALISSA RUNYON, ARUN BA-JRACHARYA, Linfield College — A protein’s tertiary structure determines its function in living organisms. The different functions proteins serve necessitate variety in native structures. How is variation in tertiary structure created from a common set of amino acids and molecular forces? In other words, what generates complexity in structures across all types of native proteins? To explore this question, a simple HP model of protein folding was explored for evidence of self-organized criticality, a potential generator of complexity.

Interaction and dynamics of homologous pairing protein 2 (HOP2) and DNA studied by MD simulation, HEM MOKTAN, Oklahoma State University, ROBERTO PEZZA, Oklahoma Medical Research Foundation, DONGHUA ZHOU, Oklahoma State University — The homologous pairing protein 2 (HOP2) plays an important role in meiosis and DNA repair. Together with protein Mnd1, HOP2 enhances the strand invasion activity of recombinase Dmc1 by over 30 times, facilitating proper synopsis of homologous chromosomes.

We recently determined the NMR structure of the N-terminal domain of Hop2 and proposed a model of Protein-DNA complex based on NMR chemical shift perturbations and mutagenesis studies (Moktan, J Biol Chem 2014 10.1074/jbc.M114.548180). However structure and dynamics of the complex have not been studied at the atomic level yet. Here, we used classical MD simulations to study the interactions between the N-terminal HOP2 and DNA. The simulated results indicate that helix3 (H3) interacts with DNA in major groove and wing1 (W1) interacts mostly in minor groove mainly via direct hydrogen bonds. Also it is found that binding leads to reduced fluctuations in both protein and DNA. Several water bridge interactions have been identified. The residue-wise contributions to the interaction energy were evaluated. Also the functional motion of the protein is analyzed using principal component analysis. The results confirmed the importance of H3 and W1 for the stability of the complex, which is consistent with our previous experimental studies.

Principles of allosteric mechanisms in cell signaling, RUTH NUSSINOV, National Cancer Institute — Linking cell signaling events to the fundamental physicochemical basis of the conformational behavior of single molecules and ultimately to cellular function are key challenges facing the life sciences. Specific protein function is determined by the extent to which the protein populates a distinct active state. Allostery, an inherent physical property of proteins, is a key factor governing the relative populations among accessible conformational states. Allostery can be defined as the change in the distribution of the conformational ensemble through some perturbation. Nature has co-evolved ligand-host protein interactions, optimizing them to tune the populations of the active (or inactive) states for function, either by stabilizing the active conformation and/or destabilizing the inactive conformations, or vice versa. More and more data attest to the significance of allostery in cell life under physiological conditions and in disease. We aim to delineate key challenging questions, such as can we predict a priori- and quantify changes incurred by allosteric mutations or specific binding events to increase/decrease the population of the active or inactive state to up- or down- regulate the protein? I will provide an overview of the fundamental underpinnings of allostery.

Interaction of albumin with perylene-diimides with aromatic substituents, MOHAMMED FAROOQI, MARK PENICK, JESSICA BURCH, GEORGE NEGRETE, LORENZO BRANCALON, University of Texas at San Antonio — Perylene diimide (PDI) derivatives, a class of synthetic organic dyes, serve as useful tools in biology to study fundamental aspects of protein-protein interactions, protein-ligand binding and to probe the conformational change of unliganded proteins. Using ultrafast IR spectroscopy, we have been able to track the conformational changes of a single protein-binding groove of an allosteric protein domain, a conformational change can be initiated by a laser pulse. This transition mimics the conformational change of the unmodified domain upon ligand binding. We have studied this light induced conformational change by ultrafast IR spectroscopy. So far, we have probed two IR absorption bands: First, the amide I band which arises from the carbonyl stretch vibration of all amide groups in the protein and is sensitive to overall structural changes, and second, a vibration localized on the photoswitch, which is sensitive to its local environment, namely the opening of the binding groove. We have found that the binding groove opens on a timescale of 100 ns in a non-exponential manner. Even after the binding groove has equilibrated, the protein conformation still continues to change. Currently, we are incorporating site-specific IR labels, to learn more about the response of the protein to the perturbation of the binding groove.

Probing a Conformational Change of a Photoswitchable Allosteric Protein with Ultrafast IR Spectroscopy, BRIGITTE STUCKI-BUCHLI, STEVEN A. WALDHAUER, RETO WALSER, ROLF PFISTER, PETER HAMM, Department of Chemistry, University of Zurich, Switzerland — By covalently linking an azobenzene photoswitch across the binding groove of an allosteric protein domain, a conformational transition can be initiated by a laser pulse. This transition mimics the conformational change of the unmodified domain upon ligand binding. We have studied this light induced conformational change by ultrafast IR spectroscopy. So far, we have probed two IR absorption bands: First, the amide I band which arises from the carbonyl stretch vibration of all amide groups in the protein and is sensitive to overall structural changes, and second, a vibration localized on the photoswitch, which is sensitive to its local environment, namely the opening of the binding groove. We have found that the binding groove opens on a timescale of 100 ns in a non-exponential manner. Even after the binding groove has equilibrated, the protein conformation still continues to change. Currently, we are incorporating site-specific IR labels, to learn more about the response of the protein to the perturbation of the binding groove.

Funded by RCM grant.

Kinetic response of a photoperturbed allosteric protein, BRIGITTE STUCKI-BUCHLI, STEVEN A. WALDHAUER, RETO WALSER, ROLF PFISTER, PETER HAMM, Department of Chemistry, University of Zurich, Switzerland — By covalently linking an azobenzene photoswitch across the binding groove of an allosteric protein domain, a conformational transition can be initiated by a laser pulse. This transition mimics the conformational change of the unmodified domain upon ligand binding. We have studied this light induced conformational change by ultrafast IR spectroscopy. So far, we have probed two IR absorption bands: First, the amide I band which arises from the carbonyl stretch vibration of all amide groups in the protein and is sensitive to overall structural changes, and second, a vibration localized on the photoswitch, which is sensitive to its local environment, namely the opening of the binding groove. We have found that the binding groove opens on a timescale of 100 ns in a non-exponential manner. Even after the binding groove has equilibrated, the protein conformation still continues to change. Currently, we are incorporating site-specific IR labels, to learn more about the response of the protein to the perturbation of the binding groove.

9:36 AM A48.00007 Global Low Frequency Protein Motions in Long-Range Allosteric Signaling


The proposed model allows to combine prior knowledge with additional sources of information (likelihood) from another neural population, and to implement in dynamics and recurrent inhibitory connections, enables a neural population to learn the statistical properties of the received sensory input (prior). Moreover, resource to implement close-to-optimal inference by sampling. Specifically, we derive a synaptic plasticity rule which, coupled with integrate-and-fire neural

9:48 AM A48.00008 Modulation of Allostery by protein intrinsic Disorder

ASHOK DENIZ, The Scripps Research Institute — No abstract available.


10:24 AM A48.00009 Functionally important residues from mode coupling during short-time protein dynamics

ALKAN KABAKCIIOGLU, Koc Univ, ONUR VAROL, Indiana Univ, DENIZ YURET, BURAK ERMAN, Koc Univ — Relevance of mode coupling to energy/information transfer during protein function, particularly in the context of allosteric interactions is widely accepted. However, existing evidence in favor of this hypothesis comes essentially from model systems. We here report a novel formal analysis of the near-native dynamics for proteins, which allows us to explore the impact of the interaction between possibly non-Gaussian vibrational modes on fluctutational dynamics. We show that, an information-theoretic measure based on mode coupling alone yields a ranking of residues with a statistically significant bias favoring the functionally critical locations identified by experiments on Myosin II and AncGR1.2.


1Supported by TUBITAK-MFG113F092.

10:36 AM A48.00010 Optical observation of correlated motions in dihydrofolate reductase

MENGYANG XU, KATHERINE NIESSEN, State Univ of NY - Buffalo, JAMES PACE, VIVIAN CODY, Hauptman-Woodward Medical Research Institute, ANDREA MARKELZ, State Univ of NY - Buffalo — Enzyme function relies on its structural flexibility to make conformational changes for substrate binding and product release. An example of a metabolic enzyme where such structural changes are vital is dihydrofolate reductase (DHFR). DHFR is essential in both prokaryotes and eukaryotes for the nucleotide biosynthesis by catalyzing the reduction of dihydrofolate to tetrahydrofolate. NMR dynamical measurements found large amplitude fast dynamics that could indicate rigid-body, twisting-hinge motion for ecDHFR that may mediate flux [1]. The role of such long-range correlated motions in function was suggested by the observed sharp decrease in enzyme activity for the single point mutation G121V, which is remote from active sites [2]. This decrease in activity may be caused by the mutation interfering with the long-range intramolecular vibrations necessary for rapid access to functional configurations. We use our new technique of crystal anisotropy terahertz microscopy (CATM) [3], to observe correlated motions in ecDHFR crystals with the bonding of NADPH and methotrexate. We compare the measured intramolecular vibrational spectrum with calculations using normal mode analysis. 1. Cameron C.E. and Benkovic S.J., Biochemistry, 1997. 36(50): p. 15792-15800. 2. Bhabha G., et al., Nat Struct Mol Biol, 2013. 20(11): p. 1243-9. 3. Acbas, G., Niessen K.A., Snell E. H., and Markelz A.G., Nat Commun, 2014. 5, 3076.

10:48 AM A48.00011 Non-linear dynamics in recurrently connected neural circuits implement Bayesian inference by sampling

ALESSANDRO TICCHI, ALDO A. FAISAL, Imperial College London, BRAIN AND BEHAVIOUR LAB TEAM — Experimental evidence at the behavioural-level shows that the brains are able to make Bayes-optimal inference and decisions (Kording and Wolpert 2004, Nature: Ernst and Banks, 2002, Nature), yet at the circuit level little is known about how neural circuits may implement Bayesian learning and inference (but see Ma et al. 2006, Nat Neurosci)). Molecular sources of noise are clearly established to be powerful enough to pose limits to neural function and structure in the brain (Faisal et al. 2008, Nat Rev Neurosci; Faisal et al. 2005, Curr Biol). We propose a spiking neuron model where we exploit molecular noise as a useful resource to implement close-to-optimal inference by sampling. Specifically, we derive a synaptic plasticity rule which, coupled with integrate-and-fire neural dynamics and recurrent inhibitory connections, enables a neural population to learn the statistical properties of the received sensory input (prior). Moreover, the proposed model allows to combine prior knowledge with additional sources of information (likelihood) from another neural population, and to implement in spiking neurons a Markov Chain Monte Carlo algorithm which generates samples from the inferred posterior distribution.

Monday, March 2, 2015 8:00AM - 11:00AM –
Session A49 GSOFT: Focus Session: Self-Phoretic Colloids and Active Emulsions I

8:00AM A49.00001 Swarming of active colloidal Janus particles: Polar waves and vortices

Cong Xu, Jing Yan1, University of Illinois at Urbana-Champaign, Ming Han, Erik LuuTEN, Northwestern University, Steve Granick, University of Illinois at Urbana-Champaign — The synthesis of artificial “swarming” particles with tunable interaction represents a strong interest of the soft active matter community. Here, we demonstrate a straightforward design of swarming Janus colloids that exhibit transient mutual alignment within a certain frequency range of an applied AC electric field. In a dense two-dimensional suspension of these Janus colloids, we observe that coherent polar waves emerge at first, which then collide and merge into stable discrete vortices. Based upon a careful analysis of the pair interaction, we propose a simple mechanism that explains the formation of the polar waves, with agreement between experiment and simulation. A rich spectrum of phenomena, including dimer swarming, chain formation, and particle clustering, can be further achieved by changing the frequency of the AC electric field.

1Currently working as a postdoctoral researcher in Princeton University.
8:12 AM A49.00002 Confining collective motion, DENIS BARTOLO, ANTOINE BRICARD, JEAN-BAPTISTE CAUSSIN, ENS Lyon, DEBASHIS DAS, UCSD, CHARLES SAVOIE, VIJAYAKUMAR CHIKKADI, ENS Lyon, KYOEI SHITARA, Kyushu University, OLESKAR CHEP-IZHKO, Odessa National University, FERNANDO PERUANI, 61030775, DAVID SAINTILLAN, UCSD — Confined active materials are often found to display self-organization in the form of a macroscopic steadily rotating vortex, yet a unified description of the formation and structure of this pattern based on microscopic interaction rules remains lacking. We use a combination of experiments, numerical simulations and theory to address this question in the case of a confined population of colloidal rollers. We first demonstrate experimentally that upon increasing density this system undergoes a continuous phase transition from a dilute isotropic-gas phase to a heterogeneous polar-liquid phase. In the ordered phase, the entire population self-organizes into a single vortex lying at the onset of a phase separation. Numerical simulations confirm the existence of this non-equilibrium phase transition, and make it possible to single out the very ingredient responsible for the emergent-vortex structures: the competition between alignment and repulsive interactions. Building on this observation, we also establish a continuum theory and lay out a strong foundation for the description of emergent collective behavior in a broad class of motile populations constrained by geometrical boundaries.

8:24 AM A49.00003 Flocking at a distance in granular matter, HARSH SONI, Indian Institute of Science, SRIRAM RAMASWAMY, TIFR Hyderabad — A mixture of polar granular rods and spherical beads on a vibrated plate undergoes a phase transition to an orientationally ordered state above a critical bead concentration. We study this system using large scale numerical simulations with periodic boundary conditions. We find an intermediate state with banded structures between the disordered and the globally ordered state. We observe a single band whose width increases with rod concentration. We find that at high densities the rods and the beads phase separate. We also test the various theoretical predictions of the hydrodynamic theory in the ordered state. Our results, which are in good agreement with the theory, are following: We see a highly anisotropic dispersion relation are exhibited with geometrical boundaries.

8:36 AM A49.00004 Exploring flocking via quantum many-body physics techniques, ANTON SOUSLOV, BENJAMIN LOEWE, PAUL M. GOLDBART, Georgia Institute of Technology — Flocking refers to the spontaneous breaking of spatial isotropy and time-reversal symmetries in collections of bodies such as birds, fish, locusts, bacteria, and artificial active systems. The transport of matter along biopolymers using molecular motors also involves the breaking of these symmetries, which in some cases are known to be broken explicitly. We study these classical nonequilibrium symmetry-breaking phenomena by means of models of many strongly interacting particles that hop on a periodic lattice. We employ a mapping between the classical and quantum dynamics of many-body systems, combined with tools from many-body theory. In particular, we examine the formation and properties of nematic and polar order in low-dimensional, strongly-interacting active systems using techniques familiar from fermionic systems, such as self-consistent field theory and bosonization. Thus, we find that classical active systems can exhibit analogs of quantum phenomena such as spin-orbit coupling, magnetism, and superconductivity. The models we study connect the physics of asymmetric exclusion processes to the spontaneous emergence of transport and flow, and also provide a soluble cousin of Vicsek’s model system of self-propelled particles.

8:48 AM A49.00005 Dynamics of cluster growth in a system of self-propelled particles, MICHELLE DRISCOLL, MELISSA FERRARI, JEREMIE PALACCI, PAUL CHAIKIN, New York Univ NYU — Self-propelled particles are a simple realization of an active-matter system; particles are continuously driven and thus inherently out of equilibrium. It has recently been shown that this leads to a rich variety of behaviors, including self-organization into dynamic clusters. Particles aggregate into clusters which are not static, but are constantly growing and shrinking by exchanging particles, coalescing, and breaking apart. Here we study in detail the dynamics of this process in a system of photo-activated colloidal swimmers. Soon after the self-propulsion mechanism is activated, a large fraction of the swimmers quickly incorporate into clusters. We measure the distributions of cluster size, and show that a substantial population of small clusters can persist even at late times. Additionally, we examine how geometric confinement of the system can alter cluster growth dynamics.

9:00 AM A49.00006 Transitions between homogeneous phases of polar active liquids, OLIVIER DAUCHOT, CNRS, UMR Gulliver, PSL University, KHANH DANG NGUYEN THU LAM, ESPCI-Paris Tech, PSL University, MICHAEL SCHINDLER, CNRS, UMR Gulliver, PSL University, EC2M TEAM, PCT TEAM — Polar active liquids, composed of aligning self-propelled particles, exhibit large scale collective motion. Simulations of Vicsek-like models of constant-speed point particles, aligning with their neighbors in the presence of noise, have revealed the existence of a transition towards a true long range order polar-motion phase. Generically, the homogeneous polar state is unstable; non-linear propagative structures develop; and the transition is discontinuous. The long range dynamics of these systems has been successfully captured using various scheme of kinetic theories. However the complexity of the dynamics close to the transition has somewhat hindered more basics questions. Is there a simple way to predict the existence and the order of a transition to collective motion for a given microscopic dynamics? What would be the physically meaningful and relevant quantity to answer this question? Here, we tackle these questions, restricting ourselves to the study of the homogeneous phases of polar active liquids in the low density limit and obtain a very intuitive understanding of the conditions which particle interaction must satisfy to induce a transition towards collective motion.

9:12 AM A49.00007 Active self-assembly and collective chemotaxis of catalytic colloids, RAMIN GOLESTANIAN, Rudolf Peierls Centre for Theoretical Physics, University of Oxford — The equilibrium dynamics of phoretically active colloids could lead to spontaneous formation of interesting structures and patterns due to the presence of long-range Coulomb-like interactions. We examine theoretically the consequences of this interaction, and present some results that exemplify the type of emergent properties that could result from them. In particular, we discuss the following: (1) spontaneous formation of small stable clusters or “molecules” that can exhibit functionality that depends on geometry (2) collective chemotaxis in a solution of catalytically active colloids that could lead to cluster formation, aster condensation, and spontaneous oscillations, and (3) swarming in the form of a comet - of light-induced thermally active colloids with negative Soret coefficient due to a shadowing interaction.

9:48 AM A49.00008 Hydrodynamics of Turning Flocks1, XINGBO YANG, M. CRISTINA MARCHETTI, Syracuse University — We present a hydrodynamic model of flocking that generalizes the familiar Toner-Tu equations to incorporate turning inertia of well polarized flocks. The continuum equations are derived by coarse graining the inertial spin model recently proposed by Cavagna et al. The interplay between orientational inertia and bend elasticity of the flock yields spin waves that mediate the propagation of turning information throughout the flock. When the inertia is large, we find a novel instability that signals the transition to complex spatio-temporal patterns of continuously turning and swirling flocks.

This work was supported by the NSF awards DMR-1305184 and DGE-1068780 at Syracuse University and NSF award PHY11-25915 and the Gordon and Betty Moore Foundation Grant No. 2919 at the KITP at the University of California, Santa Barbara.

10:00 AM A49.00009 Interactions and Collective Behaviour of Chemotactic Active Colloids, SUROPRIYA SAHA, Indian Institute of Science, SURBHI HABLANI, TIFR Centre for Interdisciplinary Sciences, 21 Brundavan Colony, Narsingi, Hyderabad 500075, RAMAN RAGHUPATI, ESRIIRAM, Rudolf Peierls Center for Theoretical Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, United Kingdom, SRIRAM RAMASWAMY, TIFR Centre for Interdisciplinary Sciences, 21 Brundavan Colony, Narsingi, Hyderabad 500075 — Artificial realizations of motility in the ordered state. Our results, which are in good agreement with the theory, are following: We see a highly anisotropic dispersion relation are exhibited with two sound modes in all directions except along the flock. Further the rods are super diffusive in the transverse direction and exhibit large number fluctuations.
10:12AM A49.00010 The Swim Pressure of Active Matter. JOHN BRADY, SHO TAKATORI, WEN YAN. California Institute of Technology — Through their self-motion, active matter systems generate a unique "swim pressure" that is entirely athermal in origin. This new source for the active stress exists at all scales in both living and nonliving active systems, and also applies to larger organisms where inertia is important. Here we explain the origin of the swim stress and develop a simple thermodynamic model to study the self-assembly and phase separation in active soft matter. Our new swim stress perspective may help analyze and exploit a wide class of active soft matter, from swimming bacteria and catalytic nanobots, schools of fish and birds, and molecular motors that activate the cellular cytoskeleton.

10:24AM A49.00011 Diffusive properties of Brownian agents interacting via metric-free aligning-forces1. FRANCISCO J. SEVILLA, LUIS ALBERTO GÓMEZ NAVA, JOSÉ LUIS MIRADA OLVERA, MIGUEL ALEJANDRO PÉREZ CONTRERAS. Instituto de Física, Universidad Nacional Autónoma de México — The diffusive properties of active particles moving at constant speed in two dimensions and interacting through metric-free aligning-forces are studied. Exponential and scale free networks are used as the backbone for the interactions among agents. Averages over the trajectories of hundred thousand agents are performed to compute the single particle mean-square displacement, and the Kurtosis of the spatial distribution, as a function of time. These quantities provide a mean to evaluate the effects of interaction. In contrast to what one would expect, the diffusion constant, increases with the intensity of the alignment.

1FIS, LAGN. JLMO and MAPC acknowledge support from PAPIIT-UNAM through the grant IN113114.

10:36AM A49.00012 Self-consistent nonlocal feedback theory for electrocatalytic swimmers2. AMIR NOURHANI, VINCENT H. CRESPI, PAUL E. LAMMERT. Department of Physics, The Pennsylvania State University — The phoretic propulsion mechanisms of electrocatalytic micro/nano-motors has received considerably more theoretical attention than the heterogeneous electrochemical processes underlying their operation. We present a flexible approach to such heterogeneous electrochemistry with nonlocal feedback using a surface bias potential field as a control parameter field with a locally open-circuit reference state. The framing in operational terms permits both convenient contact to experiment and potential for implementation in Frumkin-Butler-Volmer kinetics. Previous results are recovered in a simple approximation, and an approximate scaling form is deduced for motor speed as function of fuel concentration and swimmer size which is more consistent with data from the literature than the original linear fits.

2This work was supported by the National Science Foundation under Grant No. DMR-0820404 through the Penn State Center for Nanoscale Science.

10:48AM A49.00013 ABSTRACT MOVED TO Z49.00009 –

Monday, March 2, 2015 8:00AM - 10:48AM –

8:00AM A50.00001 Multiple networks in soft materials: polycontinuity. STEPHEN HYDE, Australian National University — Bicontinuous network phases contain a pair of interwoven labyrinths. Analogous patterns with 3, 4, ..., 8, ..., 54,... labyrinths are readily constructed via 2d hyperbolic geometry. Some of these have been realised in synthetic materials, from mesoporous silicates and lyotropic liquid crystals to metal-organic frameworks. We stumbled on polycontinuous forms while exploring 2d hyperbolic geometry. The only known tricontinuous phase found to date in mesoscale self-assembled materials was described via 2d non-euclidean geometry many years before its discovery. This example demonstrates the relevance of regular patterns in non-euclidean spaces to self-assembled morphologies in actual materials. One route to explicit ground-up design of mesoscale polycontinuous phases is via star-shaped molecules with immiscible arms, such as Y-shaped “polyphiles.” Some results of theoretical geometric modelling and experimental formulation of lyotropic LC mesophases with polyphile will be discussed.

3Nat Chem 1, 123127 (2009)
5Proc Natl Acad Sci. USA, 111, 12711276 (2014)
6Chem Mat, in press (2015); in preparation

8:36AM A50.00002 Hard Spheres on the Primitive Surface. TOMONARI DOTERA, YUSUKE TAKAHASHI, Dept. of Physics, Kinki Univ. — Recently hierarchical structures associated with the gyroid in several soft-matter systems have been reported [1,2]. One of fundamental questions is regular arrangement or tiling on minimal surfaces [3]. We have found certain numbers of hard spheres per unit cell on the gyroid surface are entropically self-organized [4,5]. Here, new results for the primitive surface are presented. 56/64/72 per unit cell on the primitive minimal surface are entropically self-organized. Numerical evidences for the fluid-solid transition as a function of hard sphere radius are obtained in terms of the acceptance ratio of Monte Carlo moves and order parameters. These arrangements, which are the extensions of the hexagonal arrangement on a flat surface, can be viewed as hyperbolic tiling on the Poincaré disk with a negative Gaussian curvature.

Real time SANS studies on the transformation between the hexagonal cylinder phase and the bi-continuous gyroid structure: transient structures\textsuperscript{1}.

KELL MORTENSEN, Univ of Copenhagen, MARTIN VIGILD, Technical University of Denmark, RUYA ESKIMERGEN, Leo Pharma, Denmark — Combined application of SANS and oscillatory shear is effective tools for studying structure and real-time dynamics of soft matter materials. Large-amplitude oscillatory shear can be used to effectively control the texture of soft materials in the ordered states. We will show experimental data proving that the 10-spot pattern often characterizing the gyroid phase of block copolymer melts as well as surfactant systems is a 2D powder-pattern, originating from the dominating structure of the cylinder axis when grown from single-domain hexagonal structures. We show that the gyroid state is unstable when exposed to large amplitude / large frequency shear, transforming into the a hexagonal cylinder phase: the transformation is completely reversible. With the slow kinetics, it is possible in detail to follow the complex materials transformation from one-dimension cylinders to the complex three-dimensional gyroid phase of block copolymers. The transformation kinetics is different within the various crystallographic directions, and shows the transformation through a transient structure rather similar to that found in SCFT-studies\textsuperscript{2}.

\textsuperscript{1}Supported by the Danish Research Council, Natural Sciences.
\textsuperscript{2}Eskimergen et al., \textit{Macromol} 38, 1286 (2005)
\textsuperscript{3}Mortensen et al, unpubl.

Towards complex network droplets — a computational study of bicontinuous network regions in star polymer droplets, RYAN MARSON, SHARON GLOTZER, Univ of Michigan - Ann Arbor — The complexity and functionality of network phases in soft matter systems offer a wealth of possible technological applications ranging from photonics to medicine. Through Dissipative Particle Dynamics (DPD) simulations, with explicit solvent, of over 1 million particles we demonstrate control of nano- and micro-scale ordering in star polymer droplets. By tuning the building block geometry and interactions between star polymer components we produce a droplet phase diagram. In particular we highlight regions of the structure that contain phase separated bicontinuous network domains. This system demonstrates the possibility of functional droplets composed of complex networks, with a hierarchy of scales that can be tuned for specific applications.

Free Energy-Based Monte Carlo Determination of a Model Microphase Former, YUAN ZHUANG, Duke Univ, KAI ZHANG, Yale Univ, PATRICK CHARBONNEAU, Duke Univ — Determining the equilibrium phase behavior of microphase formers from particle-based simulations is particularly challenging because the occupancy of the various microphase features (clusters, layers, cylinders, etc.) fluctuates and varies from one state point to the next. Here, we compute the phase diagram of a schematic microphase former, the square well-linear model, using a novel free energy-based Monte Carlo simulation methodology. Our approach surmounts traditional equilibration difficulties by including modulated reference fields and developing the expanded isothermal-isobaric [N]PT ensemble. Our results for the square-well-linear model goes beyond other descriptions of the equilibrium phase behavior of simple microphase formers by revealing the complex thermodynamic interplay of various microphases with micelle formation and percolation.

Structural Diversity of Self-Assembled Iridescen Arthropod Biophotonic Nanostructures, VINOD KUMAR SARANATHAN, Division of Physics and Applied Physics, Nanyang Technological University, RICHARD O. PRUM, Department of Ecology and Evolutionary Biology, Yale University — Many organisms, especially arthropods, produce vivid interference colors using diverse mesoscopic (100-350 nm) integumentary biophotonic nanostructures that are increasingly being investigated for technological applications. Despite a century of interest, we lack precise structural knowledge of many biophotonic nanostructures and mechanisms controlling their development, when such knowledge can open novel biomimetic routes to facilely self-assemble tunable, multi-functional materials. Here, we use synchrotron small angle X-ray scattering and electron microscopy to characterize the photonic nanostructure of 140 iridescent integumentary scales and setae from 127 species of terrestrial arthropods in 85 genera from 5 orders. We report a rich nanostructural diversity, including triply-periodic bicontinuous networks, close-packed spheres, inverse columnar, perforated lamellar, and disordered sponge-like morphologies, commonly observed as stable phases of amphiphilic surfactants, block copolymer, and lyotropic lipid-water systems. Diverse arthropod lineages appear to have independently evolved to utilize the self-assembly of infolding bilayer membranes to develop biophotonic nanostructures that span the phase-space of amphiphilic morphologies, but at optical length scales.

The Tricontinuous 3ths(5) Phase: A New Morphology in Copolymer Melts, MICHAEL FISCHER, Adolphe Merkle Institute, Chemin des Verdiers 4, CH-1700 Fribourg, Switzerland, LILIANA DE CAMPO, Australian National Science and Technology Organisation, Bragg Institute, New Illawarra Road, Lucas Heights NSW 2234, Australia; JACOB KIRKENSGAARD, Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, 2100 København Ø, Denmark, STEPHEN HYDE, Applied Maths, Research School of Physics & Engineering, The Australian National University, Canberra ACT 0200, Australia, GERD SCHROEDER-TURK, Institut für Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstr. 7B, 91058 Erlangen, Germany — Self-assembly remains one of the most efficient routes to the formation of ordered nanostructures, but at optical length scales. Here, we demonstrate the existence of a tricontinuous morphology, called 3ths(5), based on the intergrowth of three distorted nths nets, in an equilibrium phase of triblock star-copolymer melts when an extended molecular core is introduced. The introduction of the core enhances the role of chain stretching by enforcing larger structural length scales, thus destabilizing the hexagonal columnar phase in favor of morphologies with less packing frustration. This study further demonstrates that the introduction of molecular cores is a general concept for tuning the relative importance of entropic and enthalpic free energy contributions, hence providing a tool to stabilize an extended repertoire of self-assembled nanostructured materials.

Group Theory of Circular-Polarisation Effects in Chiral Photonic Crystals with Four-Fold Rotation Axes, Applied to the Eight-Fold Intergrowth of Gyroid Nets, MATTHIAS SABA, Theoretische Physik, FAU Erlangen-Nuremberg, MARK D. TURNER, CUDOS & Centre for Micro-Photonics, Swinburne University of Technology, KLAUS MECKE, Theoretische Physik, FAU Erlangen-Nuremberg, MIN GU, CUDOS & Centre for Micro-Photonics, Swinburne University of Technology, GERD E. SCHRODER-TURK, Theoretische Physik, FAU Erlangen-Nuremberg — The 8-srs PhC of body-centered cubic f\textit{\textalpha}3 symmetry consists of eight interwoven equal-handed dielectric Gyroid networks. The complete resolution of the scattering matrix parameters to derive analytical results for the band structure topology and the circular polarization scattering parameters of the 8-srs PhC and any other lossless f\textit{\textalpha}3 photonic crystal. All results are supported by numerical. We demonstrate in particular that all bands along the cubic [100] direction can be identified with the irreducible representations \textit{E}±, \textit{A} and \textit{B} of the \textit{C}4 point group. The \textit{E}± (\textit{E}) representation can be identified as the only transmission channel for right(left)-circularly polarized light. We derive explicit relationships for the (zero Bragg order) transmission and reflectance amplitudes which guarantee equal transmission rates for both polarizations and vanishing ellipticity below a critical frequency, yet allowing for finite rotation of the polarization plane. The combination of vanishing losses, vanishing ellipticity, near-perfect transmission and optical activity comparable to that of metallic meta-materials makes this geometry an attractive design for nanofabricated photonic materials.
non-Hermitian systems, and show new experiments exploring their properties. Time permitting, I will discuss the question of what it means to have topological interface states in an anomalous Hall effect. I will also present experimental results on the first realization of a “topological Anderson insulator” (in a similar setting), where the symmetry. This leads to bands with non-zero Chern number, and thus topologically-protected edge states (protected in the quantum Hall sense – not by any materials that are insulators in the bulk, but conduct electricity along their surfaces - and are intrinsically robust to disorder. In particular, when a surface

Measures of the detailed molecular conformations of the surfactants that stem from the length of the bridging moiety, which suggests that this molecular design strategy may generally extend to other surfactant classes.

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8:36 AM A51.00002 Proposed Realization and Signatures of Floquet Topological Superconductors and Insulators\(^1\), BABAK SERADJEH, Indiana Univ.-Bloomington — As understood recently, a topological state may be generated dynamically in an otherwise normal combination of materials by a periodic driving force. These states can only occur when the system is driven out of equilibrium. A Floquet topological insulator can be realized, for example, in a two-dimensional system of Dirac fermions, such as graphene, irradiated by a circularly polarized laser [1]. It is characterized by steady state edge modes and two separate integer-valued topological invariants. A Floquet topological superconductor, on the other hand, is characterized by two types of Floquet Majorana fermions—steady states of equal superposition of electrons and holes—with a period that is the same or twice that of the drive [2]. I introduce these concepts and present our recent theoretical work on the realization and detection of these Floquet topological states. First, I discuss how Floquet Majorana fermions can be realized in a highly tunable setup consisting of two coupled quantum dots and detected by a third probe dot [3]. More generally, Floquet Majorana fermions can be detected by measuring a quantized conductance sum rule over discrete values of lead bias differing by multiples of drive frequency [4]. This quantized sum rule is robust against weak disorder. Finally, I present an effective theory of Floquet topological insulators and use it to study their transport signature [5]. Remarkably, we find that disorder can enhance transport at certain Floquet topological transitions by several orders of magnitude.\(^1\)


\(^1\)Work supported in part by Indiana University College of Arts and Sciences, NSF, and BSF.

9:12 AM A51.00003 Interactions and dissipation in Floquet-Bloch systems\(^1\), NETANEL LINDNER, Technion - Israel Institute of Technology — Time periodic driving fields provide a versatile route for dynamically altering band structures. Particular excitement surrounds the possibility of controlling the topology of the resulting “Floquet bands,” whose topological classification is even richer than the one describing their static counterparts. While many schemes have been proposed for realizing interesting Floquet band structures, crucial questions remain regarding the many-body steady states of these systems. In this work we study the roles of interactions, heating, and dissipation in the population kinetics of many-particle Floquet systems. While a naive picture might lead one to expect rapid heating of any strongly driven interacting system, we find wide parameter regimes in which non-trivial Floquet steady states are obtained at intermediate and long times. Prospects for obtaining and probing the physics of these many-body Floquet systems will be discussed.

\(^1\)In collaboration with: Karthik Seetharam (Caltech), Charles-Edouard Bardyn (Caltech), Mark Rudner (Copenhagen), and Gil Refael (Caltech).

9:48 AM A51.00004 Topology in Floquet-Bloch systems: physics beyond the topological insulators\(^1\), MARK RUDNER, Copenhagen University — Floquet theory provides a powerful framework for understanding the dynamics of periodically-driven quantum systems. When applied to systems with spatially periodic potentials, the emergence of Floquet-Bloch quasiequation bands suggests many exciting opportunities to explore topological phenomena through analogies to those known in equilibrium. Due to the periodicity of quasienergy, however, the topological classification of the resulting Floquet states is richer than that of static systems. This opens the way for discovering truly new, non-equilibrium topological phenomena. For example, a one dimensional Floquet system may host chiral bands, while in two dimensions a system whose Floquet bands all have zero Chern numbers may support robust chiral edge states. In this talk I will address the question: when is a Floquet-Bloch system not like a static system? I will discuss both general considerations, based on the structure of the time-dependent Floquet-Bloch evolution operator, and specific examples which highlight the possibilities available in both non-interacting and interacting systems.

\(^1\)In collaboration with: Frederik Nathan (Copenhagen), Erez Berg (Weizmann), Netanel Lindner (Technion), Michael Levin (Chicago).

10:24 AM A51.00005 Observation of topological transitions in interacting quantum circuits\(^1\), PEDRAM ROUSHAN, Google Inc., Santa Barbara, CA — Topology, despite its mathematical abstractness, often manifests itself in physics and plays a pivotal role in our understanding of natural phenomena. Notable examples include the discoveries of topological phases in condensed matter systems which have changed the modern conception of phases of matter. The global nature of topological ordering, however, makes direct experimental probing an outstanding challenge. Present experimental tools are mainly indirect and inadequate for studying such properties at a fundamental level. Here, we employ the exquisite control afforded by superconducting quantum circuits to directly investigate topological properties of quantum spin systems. The essence of our approach is to infer local curvature by measuring the deflection of quantum trajectories topological properties are then revealed from a quantum analog of the Gauss-Bonnet theorem. We benchmark our technique by constructing the topological phase diagram of the celebrated Haldane model. The nature of the individual phases is revealed by visualizing their microscopic spin texture and evolution across the transition. Furthermore, we demonstrate the power of our method in studying the topology of interacting quantum systems, utilizing a novel qubit architecture which enables control over every term in a two-qubit Hamiltonian. We discovered an interaction-driven topological phase, whose emergence is understood by fully exploring the parameter-space of the Hamiltonian. Our work establishes a generalizable experimental platform to study fundamental aspects of topological phenomena in quantum systems.

\(^1\)NSF grants: DMR-0907039 and DMR-1029764

Monday, March 2, 2015 8:00AM - 11:00AM – Session A52 DCMP: Invited Session: Coherent Flow and Vortices in Polariton Condensates

8:00 AM A52.00001 Quantum features in the hydrodynamic flow of a superfluid of light, IACOPO CARUSOTTO, INO-CNR BEC Center — After a number of experiments showing the power of fluids of light in semiconductor microcavity devices for superfluid hydrodynamic studies, a growing activity is being devoted to quantum hydrodynamic features, where hydrodynamic quantities such as density, current, etc. must be described by quantum operators. As a concrete example, we shall consider the emission of phonon pairs from a sonic horizon via analog Hawking radiation processes. The robustness of entanglement against the driven-dissipative nature of the microcavity photon fluid will be discussed and perspectives to detect it will be sketched. In the last part, I will discuss the potential of a different, propagating architecture in view of studies of the conservative quantum dynamics of a photon fluid. After a brief summary of the general theoretical framework, our attention will be focused to a slab geometry able to exploit the power of quantum fluids of light to study the physics of quantum quenches.
8:36AM A52.00002 Half-quantum flow of a polariton spinor condensate in a ring geometry¹. DAVID SNOKE, University of Pittsburgh — We have created a macroscopic ring trap for exciton-polaritons with long lifetime, about 200 ps at resonance. In this trap we have observed Bose condensation of the polaritons, as seen in the strongly peaked energy spectrum and in the phase coherence across the trap, with coherence length of at least 50 microns. Studies of the phase gradient of the ring condensate show that it spontaneously goes into a quantized circulation state, sometimes circulating one way, sometimes the opposite way. Because this is a spinor condensate, states with only a half quantum of angular momentum are possible, accompanied by a 180-degree rotation of the polarization angle between the two spinor states. The circulating states with lowest energy in our experiments have this property, and in addition, the sign of the spin flips from one side of the ring to the other, unlike the case of a standard “half-quantum vortex.”

¹Supported by the National Science Foundation under Grant No. DMR-1104383.

9:12AM A52.00003 Hydrodynamics and coherence properties of polaritons in lattices, FLORENT BABOUX, Laboratoire de Photonique et Nanostructures, LPN/CNRS — At the frontier between non-linear optics and the physics of Bose-Einstein condensation, microcavity polaritons opened a new research field, both for fundamental studies of bosonic quantum fluids in a driven dissipative system, and for the development of new devices for all optical information processing. In this talk, I will review how semiconductor microcavities can be engineered into 1D and 2D lattices, allowing to implement complex hamiltonians and to study the hydrodynamics and coherence properties of polaritons in a novel and controlled environment. I will first show how we could generate polaritons in a 1D quasi-periodic Fibonacci potential and reveal features characteristic for a fractal energy spectrum, opening the way to the investigation of the anomalous propagation (neither ballistic nor diffusive) predicted in such structures. Then I will present a 2D honeycomb lattice for polaritons, which allows direct imaging of Dirac cones, paving the way for studies of the hydrodynamics of massless Dirac polaritons. Finally 1D lattices sustaining a non-dispersive band or “flat band” will be presented: here reduced spatial coherence is evidenced as a consequence of phase frustration.

9:48AM A52.00004 Pattern formation in interacting exciton-polariton condensates, PAVLOS SAVVIDIS, Nanophotonics Centre, Cavendish Lab, University of Cambridge, UK FORTH-IESL and Dept. of Materials S — Strongly coupled semiconductor microcavities support the formation of the exciton-polaritons, which can condense into macroscopically occupied quantum states or quantum liquids. The investigation of such systems revealed a number of effects commonly associated with the formation of a macroscopic phase, for instance superfluid-like behavior [1] or the appearance of quantized vortices. One of the focal points of current research regards the possibility of optically manipulating polariton condensates to realize new experiments and potential applications like all-optical polariton circuits. We develop this vision by employing a spatial light modulator to create arbitrary excitation patterns, where nonresonant excitation of polariton condensates allows us to define the potential landscape experienced by the condensates. Novel effects regarding the interaction of multiple polaritonic quantum liquids are revealed, in particular phase-locking between freely-flowing condensates [2], the formation of vortex lattices for multiple pump spots at large separations and the transition to a trapped configuration as the pump spots are moved closer together [3,4]. These results enhance our ability to explore new features in macroscopic coherent systems and bring us closer to practical applications with polariton condensates such as creating all-optical coherent circuits [5].


10:24AM A52.00005 Vortex-lattice phase order in a microcavity exciton-polariton lattice system, NA YOUNG KIM, Stanford University — Microcavity exciton-polaritons are bosonic quasi-particles in microcavity-quantum-well structures, exhibiting spontaneous coherence to form condensates. We have engineered two-dimensional polariton-lattice systems for investigating quantum phase order associated with high-ordinal symmetry. In particular, we have observed two-degenerate vortex-antivortex lattice order at the inequivalent K and K' points in the honeycomb lattice. Under the inversion symmetry, we identify the handedness of the vortex-antivortex phase order via an interferometry technique, which leads the quest for the nature of degenerate condensates at zero-momentum values. We envision that the polariton-lattice systems will provide exciting opportunities to explore new quantum order arising from the interplay of topology, spin, orbital and various symmetry properties. We embark on a journey to deepen our understandings in quantum nature and to develop its novel applications.

Monday, March 2, 2015 8:00AM - 11:00AM –
Session A53 DCMP: Invited Session: Optoelectronic Response of Low Dimensional Materials
Grand Ballroom C3 - Nathaniel Gabor, University of California, Riverside

8:00AM A53.00001 Electrical control and detection of nanoscale optical fields with 2d materials, FRANK KOPPENS, ICFO, the Institute of Photonic Sciences — No abstract available.

8:36AM A53.00002 Hot Carriers and Photoresponse in Graphene, QIONG MA, Massachusetts Institute of Technology — The photoresponse of materials, which determines the performance of optoelectronic devices, is governed by energy relaxation pathways of photo-excited electron-hole pairs. In graphene, with the electron-lattice coupling strongly quenched by the vanishing electronic density of states, a novel transport regime is reached in which the photo-generated carrier population can remain hot while the lattice stays cool. In this talk, I will review how semiconductor microcavities can be engineered into 1D and 2D lattices, allowing to implement complex hamiltonians and to study the hydrodynamics and coherence properties of polaritons in a novel and controlled environment. I will first show how we could generate polaritons in a 1D quasi-periodic Fibonacci potential and reveal features characteristic for a fractal energy spectrum, opening the way to the investigation of the anomalous propagation (neither ballistic nor diffusive) predicted in such structures. Then I will present a 2D honeycomb lattice for polaritons, which allows direct imaging of Dirac cones, paving the way for studies of the hydrodynamics of massless Dirac polaritons. Finally 1D lattices sustaining a non-dispersive band or “flat band” will be presented: here reduced spatial coherence is evidenced as a consequence of phase frustration.
survives to temperatures well above the Neel ordering $T_x$, liquid-like state with local order in the form of weakly correlated, co-aligned four-spin plaquettes. Additionally, this dynamical magnetism is extremely robust. It exhibits a small but measurable response, suggesting dynamical correlation length of only 1-2 lattice repeats. The wave-vector structure of magnetic fluctuations can be best described by a

GARLEA, DOUGLAS ABERNATHY, Oak Ridge National Lab — Neutron scattering in the chalcogenide parent material FeTe reveals diffuse dynamical magnetic

1Work supported by KAKENHI, The Canon Foundation, The Asahi Glass Foundation, and JSPS Open Partnership Joint Projects, as well as the Nanotechnology Platform and Photon Frontier Network Program of MEXT, Japan.

9:48AM A53.00004 Single carbon-nanotube photonics and optoelectronics1, YUICHIRO K. KATO, The University of Tokyo — Single-walled carbon nanotubes have unique optical properties as a result of their one-dimensional structure. Not only do they exhibit strong polarization for both absorption and emission, large exciton binding energies allow for room-temperature excitonic luminescence. Furthermore, their emission is in the telecom-wavelengths and they can be directly synthesized on silicon substrates, providing new opportunities for nanoscale photonics and optoelectronics. Here we discuss the use of individual single-walled carbon nanotubes for generation, manipulation, and detection of light on a chip. Their emission properties can be controlled by coupling to silicon photonic structures such as photonic crystal microcavities [1] and microdisk resonators [2]. Simultaneous photoluminescence and photocurrent measurements show that excitons can dissociate spontaneously [3], enabling photodetection at low bias voltages despite the large binding energies. More recently, we have found that alternating gate-voltages can generate optical pulse trains from individual nanotubes [4]. Ultimately, these results may be combined to achieve further control over photons at the nanoscale.


10:24AM A53.00005 Many-body interactions in atomically thin 2D materials, ALEXEY CHERNIKOV, Columbia University — Since the discovery of graphene, a single sheet of carbon atoms, research focused on two-dimensional (2D) materials evolved rapidly due to the availability of atomically thin, thermally stable crystals with intriguing physical properties. The 2D materials naturally inherit major traits associated with systems of reduced dimensionality: strongly enhanced Coulomb interactions, efficient light-matter coupling, and sensitivity to the environment. In particular, the considerable strength of the Coulomb coupling between the charge carriers introduces a rich variety of many-body phenomena. In the class of 2D semiconductors, e.g., this leads to the emergence of strongly bound electron-hole quasi-particles, such as excitons, tripons, and biexcitons, with unusually high binding energies and efficient light absorption. In this talk, I will present a study of the excitonic properties of 2D semiconductors, as exemplified in recent works on atomically thin transition metal dichalcogenides [1-4]. The observation of exciton binding energies on the order of 0.5 eV and the marked deviation of the exciton Rydberg series from the hydrogenic model will be discussed. The results reflect both strong carrier confinement and the distinctive nature of dielectric screening in atomically thin materials. I will further describe how carrier doping and strong photo-excitation can profoundly alter the many-body interactions in these 2D systems.


11:15AM B0.00001 Nematic spin correlations in the tetragonal state of uniaxial-strained BaFe$_{2-x}$Ni$_x$As$_2$1, PENGCHENG DAI, Rice Univ — Understanding the microscopic origins of electronic phases in high-transition temperature (high-$T_c$) superconductors is important for elucidating the mechanism of superconductivity. In the paramagnetic tetragonal phase of BaFe$_{2-x}$Ni$_x$As$_2$ (where $T_c$ is $\sim$ 60 K, and even exhibits unusual temperature-induced enhancement. More surprisingly, no coherent excitation was seen to emerge when system is cooled into magnetically ordered state. Nevertheless, spin-wave theory has been applied to interpret the measured spectra, but the agreement of its predictions with the experiment was found to be marginal at best. Here we report the discovery of a coherent magnetic excitation in the magnetically ordered state at low temperature, which coexists with the diffuse, liquid-like magnetic response. This resolves puzzle of surprising absence of coherent excitations associated with magnetic order in FeTe, where emergence of sharp electronic resonance near the Fermi energy has been observed by ARPES. This work was supported by the US DOE under Contract DE-AC02-98CH10886.

1This work is supported by MOST of China, US NSF, and Welch foundation grants.

11:51AM B0.00002 Coexistence of diffuse liquid-like scattering and emergent coherent mode in Fe$_{1+y}$Te, IGOR ZALIZNYAK, DAVID FOBES, ZHIJUN XU, GENDA GU, JOHN TRANQUADA, Brookhaven Natl Lab, ANDREI SAVICI, OVIDIU GARLEAN, DOUGLAS ABERNATHY, Oak Ridge National Lab — Neutron scattering in the chalcogenide parent material FeTe reveals diffuse dynamical magnetic response, suggesting dynamical correlation of the form of only 1-2 lattice repeats. The wave-vector structure of magnetic fluctuations can be best described by a liquid-like state with local order in the form of weakly correlated, co-aligned four-spin plaquettes. Additionally, this dynamical magnetism is extremely robust. It survives to temperatures well above the Neel ordering $T_N$ ~ 60 K, and even exhibits unusual temperature-induced enhancement. More surprisingly, no coherent excitation was seen to emerge when system is cooled into magnetically ordered state. Nevertheless, spin-wave theory has been applied to interpret the measured spectra, but the agreement of its predictions with the experiment was found to be marginal at best. Here we report the discovery of a coherent magnetic excitation in the magnetically ordered state at low temperature, which coexists with the diffuse, liquid-like magnetic response. This resolves puzzle of surprising absence of coherent excitations associated with magnetic order in FeTe, where emergence of sharp electronic resonance near the Fermi energy has been observed by ARPES. This work was supported by the US DOE under Contract DE-AC02-98CH10886.
12:03PM B0.00003 Decoupling neutron resonances from superconducting transition temperatures in NaFe$_{1-x}$Co$_x$As. CHENGLIN ZHANG, Rice University, EGAMI TAKEISHI, University of Tennessee, PENGCHENG DAI, Rice University, RICE UNIVERSITY TEAM, UNIVERSITY OF TENNESSEE TEAM — We report a comprehensive study of the evolution of neutron resonance modes in wide doping range of NaFe$_{1-x}$Co$_x$As. Double resonances, a sharp followed by a broad one, are observed in certain underdoped region. Surprisingly, the sharp resonance energy is nearly unchanged with variation of doping concentrations and therefore $T_c$. In overdoped region without competing phases, single resonance present and is gradually broadening with further increasing doping. Nevertheless, the resonances peak at the same energy while $T_c$ falls half from slightly overdoped one ($T_c=18$ K) to heavily overdoped one ($T_c=9$ K). The decoupling between $E_r$ and $T_c$ indicates unappreciated cooperation which had not been predicted by any theoretical model. Our results manifest the distinct multibarital character in FeSeC, guiding a new direction in the pursuit of a generic connection in diversified unconventional superconductors.

12:15PM B0.00004 Elastic and Inelastic neutron scattering results in heavily Cu doped NaFe$_{1-x}$Cu$_x$As with $x$ approaching 0.5. YU SONG, Rice University, DAVID TAM, Rice Univ, MENG WANG, UC Berkeley, RICE UNIVERSITY TEAM — We performed inelastic neutron scattering on Co-doped LiFeAs material. In 12% Co doped LiFeAs, where $T_c$ is dramatically suppressed, the low energy spin excitation is commensurate at $(p,0)$ point which is different from pure LiFeAs case. Based on the fact that in the material the perfect nesting exists between outer hole pocket and electron pocket and is dominated by $d_{xy}$ orbital, we argue that the superconductivity is actually associated with electron scattering from $d_{xz}/d_{yz}$ orbital and $d_{xy}$ orbital bare contributes to the superconducting pairing.

12:27PM B0.00005 Inelastic neutron scattering study on Co-doped LiFeAs, YU LI, Rice University, DAVID TAM, Rice Univ, Ming WANG, UC Berkeley, Rice University — We performed inelastic neutron scattering on Co-doped LiFeAs. In 12% Co doped LiFeAs, where $T_c$ is dramatically suppressed, the low energy spin excitation is commensurate at $(p,0)$ point which is different from pure LiFeAs case. Based on the fact that in the material the perfect nesting exists between outer hole pocket and electron pocket and is dominated by $d_{xy}$ orbital, a wave that the superconductivity is actually associated with electron scattering from $d_{xz}/d_{yz}$ orbital and $d_{xy}$ orbital bare contributes to the superconducting pairing.

12:39PM B0.00006 Phase diagram of BaFe$_2$(As$_{1-x}$P$_x$)$_2$. DING HU, SHILIANG LI, HUIQIAN LUO, Chinese Academy of Sci (CAS), PENGCHENG DAI, Chinese Academy of Sci (CAS):Rice University — As a unique system of high temperature Iron-based superconductors, recent experimental results indicate that there is a quantum critical point (QCP) around the optimal level in BaFe$_2$(As$_{1-x}$P$_x$)$_2$. We use neutron diffraction, high resolution X-ray scattering and NMR techniques to map out the detailed phase diagram. It is found that the long-range antiferromagnetic (AF) order survives up to the optimal doping level within the instrument resolution. Our results suggest that the evolution of the AF order upon doping in BaFe$_2$(As$_{1-x}$P$_x$)$_2$ is different from that in the electron-doped Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ or Ba(Fe$_{1-x}$Ni$_x$)$_2$As$_2$.

12:51PM B0.00007 Magneto-elastic coupling in detwinned Sr(Fe$_{1-x}$Co$_x$)$_2$As$_2$ by inelastic x-ray scattering. NAOKI MURAI, RIKEN SPing-8 Center and Osaka University, TATSUO FUKUDA, RIKEN SPing-8 Center and JAEA, MASAMICHI NAKAJIMA, TATSUYA KOBAYASHI, Osaka University, HIROSHI UCHIYAMA, RIKEN SPing-8 Center and JASRI, SATOSHI TSUTSUI, JASRI, DAISUKU ISHIKAWA, RIKEN SPing-8 Center and JASRI, HIROKI NAKAMURA, MASAKI MACHIDA, JASRI, SHIGEKI MIYASAKA, SETSUKO TAJIMA, Oska University, ALFRED BARON, RIKEN SPing-8 Center and JASRI — We measured magneto-elastic coupling in Sr(Fe$_{1-x}$Co$_x$)$_2$As$_2$ with different doping levels ($x=0$ and 0.08) using inelastic x-ray scattering with 1.5 meV resolution at SPing-8. The crystals were detwinned by application of in-plane uniaxial stress. This allowed us to measure single domain phonon structure in the magnetically ordered state. We clearly identified the change in the phonon dispersion induced by the onset of magnetic order, with phonon energies depending on orientation of the phonon wave vector relative to the Fe moment. We compare our results to ab-initio pseudo potential calculations: Magnetic calculations give better agreement than non-magnetic calculations, in but in most parts of the Brillouin zone investigated, they overestimate the magnitude of the mode splitting and in fact often fail to predict even the correct sign of the splitting. 1

1 This work was partly supported JST, EU-Japan program “IRON-SEA”.

1:03PM B0.00008 Magnetic phase diagram of Ca(1-x)Co$_x$Fe$_2$As$_2$ ($x \leq 0.1$) single crystals. W.T. JAYASEKARA, B.G. UELAND, ABHISHEK PANDEY, V.K. ANAND, N.S. SANGEETHA, Ames Laboratory U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA, W. TIAN, Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, D.C. JOHNSTON, A. KREYSSIG, A.I. GOLDMAN, Ames Laboratory U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA. Both CaCo$_2$As$_2$ and CaFe$_2$As$_2$ possess the tetragonal ThCr$_2$Si$_2$ crystal structure and are paramagnetic at room temperature and ambient pressure. Upon cooling, CaCo$_2$As$_2$ shows A-type antiferromagnetic (AFM) order below a Neel temperature of $T_N = 50-70$ K, while CaFe$_2$As$_2$ transitions to an orthorhombic lattice with stripe-type AFM order below $T_N \approx 170$ K. Here, we present results from neutron diffraction experiments on a series of Ca(1-x)Co$_x$Fe$_2$As$_2$ single crystals ($x = 0$ to 0.1) studying the evolution of CaCo$_2$As$_2$'s low-temperature state upon substituting Fe for Co. We find that A-type magnetic order persists for all of the values of $x$ studied with suppressed $T_N$ and ordered moment for increasing Co concentration and present the magnetic phase diagram for the Co rich region.

Work at Ames Laboratory was supported by US DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Contract No. DE-AC02-07CH11358. Research conducted at ORNL’s High Flux Isotope Reactor was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, US DOE.

1:15PM B0.00009 Study of lattice distortion in Sr(Fe$_{1-x}$Co$_x$)$_2$As$_2$ single crystals employing high-energy x-ray diffraction. A. SAPKOTA, W.T. JAYASEKARA, ABHISHEK PANDEY, SHREE R. BANJARA, P. DAS, N.S. SANGEETHA, D.C. JOHNSTON, A. KREYSSIG, A.I. GOLDMAN, Ames Laboratory U.S. DOE, Department of Physics and Astronomy, Iowa State University — For the iron arsenide family of superconductors, the interplay between structure, magnetism, and superconductivity is a major theme of research. Among $A$Fe$_2$As$_2$ ($A =$ Ca, Sr, Ba), a difference lies in the strength of magnetoelectric coupling: it is strongest in CaFe$_2$As$_2$ as indicated by strongly coupled first order phase transitions (structural and magnetic) and modest in BaFe$_2$As$_2$ in which the two phase transitions split with Co-substitution. Moreover, similar to the structural transition, the magnetic transition becomes second order with higher Co-concentration. SrFe$_2$As$_2$ shows intermediate behavior. Here we present a temperature-dependent study of the lattice distortion from tetragonal to orthorhombic in Sr(Fe$_{1-x}$Co$_x$)$_2$As$_2$ single crystals through diffraction measurements using x-ray radiation of two energies: 8.047 keV and 100 keV. The lower energy probes a few micrometers down from the surface of the sample whereas the higher energy characterizes the bulk. Details of the lattice distortion obtained with these two probes will be discussed.

The work at Ames Laboratory was supported by US DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Contract DE-AC02-07CH11358. This research used resources of Advanced Photon Source, a US DOE, Office of Science User Facility.
Tetragonal-to-orthorhombic lattice distortion and domains in Ca\(\text{Fe}_{1-x}\text{Co}_x\)\_2As\_2 single crystals, A. KREYSSIG, E.C. BLOMBERG, G.S. TUCKER, A. SAPKOTA, S. RAN, S.L. BUD’KO, P.C. CANFIELD, M.A. TANATAR, R. PROZOROV, A.I. GOLDMAN, Ames Laboratory US DOE, Department of Physics and Astronomy, Iowa State University — Similarly to other Fe-based pnictide superconductors, Ca\(\text{Fe}_{1-x}\text{Co}_x\)\_2As\_2 single crystals show a tetragonal-to-orthorhombic lattice distortion that is suppressed with increasing Co concentration. However, in contrast to other Fe-based pnictide superconductors, an unprecedented 45° rotation of the domain patterns in polarized-light microscopic studies has been observed for Co concentrations \(x \approx 0.2\) at temperatures around the onset of antiferromagnetic order and lattice distortion. We present a high-resolution high-energy x-ray diffraction study demonstrating that the observed change in domain arrangement is related to the coexistence of the tetragonal and orthorhombic phases in a well-defined geometric configuration allowed by a special relationship between the lattice parameters of both phases in these compounds.

The work at the Ames Laboratory was supported by US DOE, Office of Basic Energy Sciences, Department of Materials Sciences and Engineering under contract DE-AC02-07CH11358. This research used resources of the Advanced Photon Source, a US DOE, Office of Science User Facility.

Competing magnetic and superconducting order and the role of vortices in iron-based superconductors, B. MENCIA URANGA, Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark, J. LARSEN, Department of Physics, Technical University of Denmark. 2800 Kgs. Lyngby, Denmark, G. STIEBER, S.L. HOLM, K. LEFFMANN, Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark, C. NIEDERMAYER, Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, CH-5232 Villigen, Switzerland, T. WOLF, Karlsruher Institut fuer Technologie, Institut fuer Festkoerperfysik, D-76021 Karlsruhe, Germany, B.M. ANDERSEN, Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark — We discuss recent neutron and muSR measurements of the magnetic and superconducting (SC) properties of Co-doped Ba-122 as a function of temperature and external magnetic field \([1]\). Below the \(T_c\), the magnetic and SC order parameters coexist and compete. A magnetic field can significantly enhance the magnetic scattering in the SC state \([1]\). We perform a microscopic modeling of the data by use of a five-band Hamiltonian relevant to iron pnictides. In the SC state, vortices can slow down and freeze spin fluctuations locally. When such regions couple they result in a long-range ordered antiferromagnetic phase producing the enhanced magnetic elastic scattering in agreement with experiments \([1]\). Lastly, we also study the low energy bound states in the vortex core of LiFeAs, where the quasiparticle states in the vortex core can provide useful information about the gap structure \([2]\).


Itinerant ferromagnetism in the As \(4p\) conduction band of Ba\(0_x\)K\(0.4\)Mn\(2As_2\) identified by x-ray magnetic circular dichroism, B. G. UELAND, ABHISHEK PANDEY, A. SAPKOTA, Y. LEE, Ames Laboratory, Dept. of Physics and Astronomy, Iowa State University, Y. CHOI, D. HASKEL, R. A. ROSENBERG, J. C. LANG, Advanced Photon Source, Argonne National Laboratory, B. N. HARMON, D. C. JOHNSTON, A. KREYSSIG, A. I. GOLDMAN, Ames Laboratory, Dept. of Physics and Astronomy, Iowa State University — X-ray magnetic circular dichroism (XMCD) measurements on single-crystal and powder samples of Ba\(0_x\)K\(0.4\)Mn\(2As_2\) show that the ferromagnetism (FM) below \(T_c\) \(\approx 100\) K arises in the As \(4p\) conduction band. No XMCD signal is observed at the Mn \(x\)-ray absorption edges, however, a clear XMCD signal is found below \(T_c\) at the As \(K\) edge which increases with decreasing temperature. The XMCD signal is absent with the beam directed parallel to the crystalline c-axis, indicating that the ordered orbital moment lies in the basal plane of the tetragonal lattice. These results show that the previously reported itinerant FM is associated with the As \(4p\) conduction band and that distinct local-moment antiferromagnetism and itinerant FM coexist at low temperature.

Work at the Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences, Division of Materials Sciences & Engineering, under Contract No. DE-AC02-07CH11358. This research used resources of the Advanced Photon Source, a U.S. Department of Energy Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

Collapsed tetragonal phase in SrCo\(_2\)As\(_2\) under high pressure, W.T. JAYASEKARA, B.G. UELAND, A. KREYSSIG, ABHISHEK PANDEY, N.S. SANGEETHA, Ames Laboratory U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA, G. FABBRI, YEJUN FENG, D. HASKEL, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA, D.C. JOHNSTON, A.I. GOLDMAN, Ames Laboratory U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — SrCo\(_2\)As\(_2\) possesses the same tetragonal ThCr\(_2\)Si\(_2\) structure as the \(\text{AFe}_2\text{As}_2\) (\(A = \text{Ca, Sr, Ba}\)) family of high-temperature superconductors but does not manifest magnetic order or superconductivity down to a temperature of 1.8 K. Nevertheless, inelastic neutron scattering data show the presence of magnetic fluctuations peaked at a wavevector of \((1/2 1/2 1)\), which corresponds to the stripe antiferromagnetic propagation vector found for \(\text{AFe}_2\text{As}_2\). Here, we present evidence from high-energy x-ray diffraction experiments which show that SrCo\(_2\)As\(_2\) undergoes a transition to a collapsed-tetragonal phase characterized by a 10% reduction of the \(c\)-lattice parameter for an applied pressure of 5 GPa at 7 K. This fascinating result opens another path for studying the role of magnetic ordering, spin fluctuations, and magnetoelastic coupling in the development of superconductivity in the Fe-pnictides and related materials.

— Work at Ames Laboratory was supported by US DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Contract No. DE-AC02-07CH11358. This research used resources of the Advanced Photon Source, a US DOE, Office of Science User Facility.

Monday, March 2, 2015 11:15AM - 2:15PM —
Session B1 DMP: Focus Session: Graphene - Point Defects and Structural Defects 001A - Benjamin Butz, Friedrich Alexander Universitaet Erlangen

Spontaneous Boron-doping of Graphene at Room Temperature, LIDA PAN, Vanderbilt Univ, YANDE QUE, SHIXUAN DU, HONGJUN GAO, Institute of Physics, Chinese Academy of Sciences, SOKRATES T. PANTELIDES, Vanderbilt Univ — Doping graphene with boron or nitrogen is an effective way to modify its electronic properties. However, the reaction barrier for introducing these impurities is quite high, making the doping process difficult. In this work, we propose a low-energy reaction route derived from first-principles calculations and subsequently validated by experiments. The calculations show that, when graphene is placed on a ruthenium substrate and exposed to atomic boron, boron atoms can incorporate substitutionally into the graphene sheet with an energy barrier about 0.1 eV, displacing carbon atoms below the graphene sheet where they migrates away. This result suggests that spontaneous doping by boron can take place at room temperature. Following the prediction, we grew high-quality graphene on the Ru(001) surface and then expose it to B\(_2\)H\(_6\) which decomposes into atomic boron. XPS and STM results indicate that boron dopes graphene substantially without disturbing the graphene lattice, confirming the theoretical predictions. Doping by nitrogen and co-doping by B and N will also be discussed.
11:27AM B1.00002 Boron Substitution in Disordered Graphene-like Carbon. JOE SCHAEPPERKOETTER, ANDREW GILLESPIE, CARLOS WEXLER, PETER PFEIFER, University of Missouri, MATERIALS RESEARCH INSTITUTE—MISSOURI S&T COLLABORATION—X-ray photoelectron spectroscopy was used to determine both the elemental composition of boron doped carbons as well as gain insight into the arrangement of atoms in the material. The hypothesized arrangement of atoms is a direct substitution of boron for carbon into a graphene like sheet, maintaining the hexagonal honeycomb lattice of sp² sigma bonds. Such a boron atom would have an electronic configuration of 1s²(sp³)². With a graphitic carbon atom, the p_st orbitals are maintained and participate in mobile pi bonds with neighboring carbon atoms, as understood in the aromatic model. Boron, however, would require a charge donation to fill its p_z orbital. Thus, three possible models are proposed for the out of plane electron density: (1) the orbital remains unoccupied and the boron is a free radical, (2) charge is donated from a neighboring atom and the boron atom is ionic, (3) the delocalization of charge in the aromatic system results in a partial charge transfer with an effective charge somewhere between neutral and anionic. Our results suggest that boron is not in an anionic state, and, by doing a quantitative and simultaneous analysis from multiple elemental spectra, we conclude that no more than 2 wt% of boron is being substitutionally doped into the system.

11:39AM B1.00003 Stabilities and electronic structures of B and N defects in bilayer graphene. YOSHITAKA FUJIMOTO, SUSUMU SAITO, Department of Physics, Tokyo Institute of Technology — Since its discovery, atomically thin monolayer of graphene has attracted great attention both scientifically and technologically since they exhibit different electronic structures from monolayer graphene. One of the effective ways to tune the electronic properties of carbon-based nanomaterials is to dope them with B and N atoms. Here, we study energetics and electronic properties of B and N defects in bilayer graphene, based on the first-principles density-functional theory. All kinds of dopant sites and stacking patterns (AA and AB) of bilayer sheets are studied and the site-dependent and independent behaviors of the dopants are found. We also report the electronic structures and study the STM images of doped bilayer graphene. While B-doped and N-doped defects show different STM images, the STM images are shown to be similar for AA and AB stacking patterns in both B- and N-doped defect cases.

1 Supported by the JSPS 26390062 and MEXT 25107005, and TIES (MEXT Elements Strategy Initiative).

11:51AM B1.00004 Imaging the Individual Nitrogen Dopant Atoms in Graphene with Thermoelectric Measurements. HO-KI LYEO, SANGHEE CHO, Korea Research Institute of Standards and Science, EUI-SUB LEE, YONG-HYUN KIM, Korea Advanced Institute of Science and Technology, JUNSTIN BULT, JEFFREY BLACKBURN, National Renewable Energy Laboratory — Chemical doping of nitrogen has been known as a means of modifying the electronic structure of graphene grown on a Cu substrate. We used scanning thermoelectric microscope to investigate the influence of individual nitrogen dopant atoms in monolayer graphene. Nitrogen-doped graphene was grown on a single crystal Cu substrate by using the chemical vapor deposition of pyridine molecules that contain a nitrogen atom substituting a carbon atom in the carbon hexagon. Thermoelectric voltage measurements, which have been shown to be differentially sensitive to the Fermi energy state, can produce two-dimensional images of electronic signature near the individual nitrogen dopants on the atomic scale. The measurements yielded a more complicated and extended modification of electronic structure than previously measured by using tunneling spectroscopy, which can be accounted for by the theoretical simulation and experimental evidences of nitrogen inclusion obtained from Raman and XPS measurements.

12:03PM B1.00005 Manipulate the Doping of Graphene at Nanoscale with Intercalated Oxygen. XIN ZHANG, HONG LUO, Department of Physics, University at Buffalo, the State University of New York, LEI LIU, GONG GU, Department of Electrical Engineering and Computer Science, the University of Tennessee, DANIELE STRADI, MADS BRANDBYGE, Department of Micro- and Nanotechnology, Center for Nanostructured Graphene, Technical University of Denmark — We have created nanoscale p- and n-doped graphene regions side by side, by partially removing the oxygen between the graphene and the Cu foil growth substrate intercalated upon elongated air exposure. The Cu foil surface is almost exclusively (100) oriented, and the removal of intercalated oxygen is by thermal annealing. Scanning tunneling microscopy (STM) reveals a 0.72 × 0.72 nm square superlattice in the single layer (1L) graphene/O/Cu(100) structure, assigned to be Cu(2√2 × 2√2)R45°-O, which has not been reported so far. Graphene with intercalated oxygen underneath is p-doped while the surrounding graphene areas, directly in contact with the copper surface, are n-doped. Comparing the scanning tunneling spectra (STS) of the two types of regions, we show a charge transfer-induced shift of the electronic structure. Such a shift is also observed between p- and n-doped twisted bilayer (2L) graphene regions, where the van Hove singularity (vHS) peaks are used as markers to precisely determine the energy shift. Across the boundaries between the p- and n-doped regions, the shift of the electronic structure is spatially resolved, showing the vanishing and reappearance of the vHS peaks. The experimental observations are consistent with first-principles calculations.

12:15PM B1.00006 Symmetry protected zero modes in graphene grain boundaries. MADELEINE PHILLIPS, E.J. MELE, University of Pennsylvania — We study electronic states in graphene grain boundaries using topological band theoretic arguments. Using bulk eigenstates, we calculate a geometric phase that counts the number of zero modes in projected bulk gaps. We argue that these localized zero modes are protected by a hidden chiral symmetry. We apply our topological theory to various grain boundary geometries and corroborate our results using numerical calculations on a tight binding lattice.

12:27PM B1.00007 Conserved Bonding Sequences and Atomic Strain Fields of Graphene Grain Boundaries. HAIDER RASOOL, UC Berkeley, COLIN OPHUS, Lawrence Berkeley National Laboratory, ZIANG ZHANG, Rice University, MICHAEL CROMMIE, UC Berkeley, BORIS YAKOBSON, Rice University, ALEX ZETTLUC Berkeley — Grain boundaries in polycrystalline materials have significant impact on their bulk mechanical properties. The detailed arrangement of atoms and bonding at the boundary dictate these properties and their differences from bulk single crystal behavior. In this work, we use aberration corrected high resolution transmission electron microscopy imaging to study the structure of graphene grain boundaries. By mapping the exact atomic positions of the carbon lattice, we visualize atomic scale strain organization in the material. We find that grain boundaries are comprised of conserved bonding sequences that can appear as periodic or aperiodic building blocks that give rise to similar strain behavior at the boundary. Using molecular dynamics fracture simulations, we predict that experimentally observed grain boundary structures will maintain strengths that are comparable to ideal theoretical grain boundaries.

12:39PM B1.00008 Scattering properties of extended structural defects in graphene. DANIEL GUNLYCZE, CARTER WHITE, Naval Research Laboratory — A challenge preventing widespread use of graphene in nanoelectronic devices is the absence of a band gap at the Fermi level. Without a practical band gap, other ways to make electronic transport switchable are needed. One promising possibility is to use parallel graphene transport barriers to generate a transport gap. This approach requires transport barriers that are penetrable and fairly reflective. Such barriers could be formed by extended structural defects such as grain boundaries or line defects. Herein, we present scattering properties in the specular regime of a generic transport barrier described by an effective barrier coupling, an effective barrier potential, and an asymmetry parameter. We also show that these scattering properties could be probed without the need for lateral transport measurements. Instead, we suggest the use of scanning probe techniques measuring the undulations in the local density of states. That the transmissivity could be probed in equilibrium when no current flows through the barrier is a manifestation of quantum interference at the barrier.

2This work was supported by the Office of Naval Research, directly and through the Naval Research Laboratory.
12:51PM B1.00009 Effect of defects produced by electron irradiation on the electrical properties of graphene

**ADRIAN BALAN, JULIO ALEJANDRO RODRIGUEZ-MANZO, MATTHEW PUSTER, MARUA DRNDIC**, Univ of Pennsylvania — We present a study of the effects of the defects produced by electron irradiation on the electrical and crystalline properties of graphene. We realized back or side gated electrical devices from monolayer graphene crystals suspended on a 50nm SiNx. The devices are exposed to electron irradiation inside a 200kV transmission electron microscope (TEM) and we perform in situ conductance measurements. The number of defects and the quality of the crystalline network obtained by diffraction are correlated with the observed decrease in mobility and conductivity of the devices. We observe a different behavior between type of monolayer materials, and try to associate with different conduction with defect models. [1] Towards sensitive graphene nanoribbon-nanopore devices by preventing electron beam induced damage. M. Puster, J. A. Rodriguez-Manzo, A. Balan, M. Drndic. ACS Nano,10.1021/nn405112m.

1:03PM B1.00010 Magnetic Defects in Graphene Quantum Dots

**SRINIVASA RAO SINGAMANENI**, North Carolina State University, JOHAN VAN TOL, National High Magnetic Field Laboratory, Florida State University, 1800 E. Paul Dirac Drive, Tallahassee, Florida 32310, USA, RUQUAN YE, JAMES M. TOUR, Department of Chemical Engineering and Materials Science, 65malley Institute for Nanoscale Science and Technology, Rice U — Spin-coherence time in graphene quantum dots (GQDs), which are highly sought-after spintronics materials is controlled by defects. To that end, the nature of the (spin) defect centers in these GQDs is important. Electron spin resonance (ESR) spectroscopy is an ideal local probe to investigate the spin properties of GQDs. ESR investigations are carried out on GQDs [1] as a function of temperature (6-290 K) at two distinct microwave high frequencies 292.2 and 336 GHz. The ESR signal does not show power dependence at 292.2 GHz, 6K, could be adequately described with three distinct components using Lorentzian line shape. From the experimental findings together with computer-aided simulations, we have identified them as one broad (700 Gauss) and narrow (60 Gauss) carbon-centered paramagnetic defect centers and the third one as Mn$^{2+}$ signal, which is an extrinsic impurity. The temperature dependence of carbon-derived spin centers in GQDs resembles to that of conduction electrons, in contrast to the localized spins observed by us earlier [2-5] in graphene nanoribbons.


**BI RU WU**, Department of Natural science, Center for General Education, Chang Gung University, CHIH-KAI YANG, Graduate Institute of Applied Physics, National Chengchi University — We investigated a variety of configurations of hydrogen-vacancy (HV) chains in graphane with density functional theory. We found the configurations that each of zigzagged HV chains separated by one or more H chains exhibit nonmagnetic conductor or has a tiny gap. Once as the neighbored zigzag HV chains blocked by isolated H atoms, the structure transformed from a nonmagnetic conductor into a magnetic semiconductor. If the HV chains are continuously distributed, it looks like a graphene nanoribbon embedded in graphane. The zigzag edged embedded graphene nanoribbons also show antiferromagnetic. An additional H atom on the ribbon can tune the band gap and generate magnetic moment; moreover, if bare C atoms are present outside the nanoribbon also have similar effect. The results will be helpful for designing graphane-based nanoelectronic devices.

1:27PM B1.00012 Characterizing Defects Generated in Graphene by Scanning Probe Microscopy

**JONATHON DAVID WHITE**, Yuan Ze University, Taiwan, HSIAO-MEI CHIEN, MIN-CHIANG CHUANG, HUNG-CHIEH TSAI, National Central University, Taiwan, HUNG-WEI SHUI, LO-YUEH CHANG, CHIA-HAO CHEN, National Synchrotron Radiation Research Center, Taiwan, SHENG-WEI LEE, WEI-YEN WOON, National Central University, Taiwan — Graphene was prepared by chemical vapor deposition (CVD). Defects with differing topographical and tribological properties were then created by scanning probe lithography (SPL) under ambient conditions. The nature of these defect structures was then investigated by micro-Raman ($\mu$-RS) and micro-X-ray photoelectron ($\mu$-XPS) spectroscopy. Investigation of these structures suggests that, despite their physical differences, similar defects are present in both structures. In particular, $\mu$-RS indicated that the ratio of the defect Raman peaks and the effective $\alpha_g$, in stark contrast to the atomic case where $\alpha_g \approx 170$ is experimentally inaccessible. However due to the significant screening in graphane, attaining the supercritical regime is challenging. We will report on a new method to create charge centers within the graphene layer whose charge, Z, can be tuned to exceed the critical value. Using low temperature scanning tunneling microscopy and spectroscopy we study the evolution in the local electronic structure of graphene as a function of Z, from charge neutrality to the supercritical regime, which is identified by comparing to numerical simulations.

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1Supported by the Ministry of Science and Technology of the Republic of China

1:39PM B1.00013 Supercriticality of charge centers in graphene probed with scanning tunneling microscopy

**YUHANG JIANG, JINHAI MAO, GUOHONG LI, Rutgers University, Department of Physics and Astronomy, 136 Frelinghuysen Road, Picataway, NJ 08855 USA, D. MOLDOVAN, M. RAMEZANI MASIR, F. M. PEETERS, Departement Fysica, Universiteit Antwerpen Groenenborgerlaan 171, B-2020 Antwerpen, Belgium, EVA Y. ANDREI, Rutgers University, Department of Physics and Astronomy, 136 Frelinghuysen Road, Picataway, NJ 08855 USA — The massless Dirac fermion carriers in graphene, with their effective fine structure constant, $\alpha_g$, being of order unity, provide fertile ground for exploring the physics of ultra-relativistic particles in the strong coupling limit.In particula, positive charge $Z$ embedded in graphene is expected to exhibit supercricital behavior already for $Z>Z_c=-5/\alpha_g$, in stark contrast to the atomic case where $Z_c \approx 170$ is experimentally inaccessible. However due to the significant screening in graphane, attaining the supercritical regime is challenging. We will report on a new method to create charge centers within the graphene layer whose charge, Z, can be tuned to exceed the critical value. Using low temperature scanning tunneling microscopy and spectroscopy we study the evolution in the local electronic structure of graphene as a function of Z, from charge neutrality to the supercritical regime, which is identified by comparing to numerical simulations.

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1Work supported by DOE-FC02-99ER45742 and NSF DMR 1207108

1:51PM B1.00014 Supercriticality and screening effects in graphene. JINHAI MAO, YUHANG JIANG, GUO-HONG LI, Rutgers University, Department of Physics and Astronomy, 136 Frelinghuysen Road, Piscataway, NJ 08855 USA, D. MOLDOVAN, M. RAMEZANI MASIRI, F.M. PEETERS, Departement Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium, EVA Y. ANDREI, Rutgers University, Department of Physics and Astronomy, 136 Frelinghuysen Road, Piscataway, NJ 08855 USA — The chiral nature of charge carriers in graphene prohibits backscattering and prevents confinement by electrostatic potentials, resulting in high electronic mobility and unusual phenomena such as Klein tunneling. This picture breaks down in the presence of charge impurities exceeding a critical value $Z_{c}$, whereas qualitative change in behavior leads to the capture of electrons akin to atomic collapse in 3D atoms. Although in graphene $Z_{c}$ is substantially lower than in 3D atoms, attaining the supercritical regime is difficult because screening can significantly reduce the effective charge of the impurity. We have devised a method of inducing a controllable amount of localized charge whose strength can be tuned by adjusting screening through a gate voltage or a magnetic field. The effect of the impurity on the local electronic structure was monitored with low temperature scanning tunneling microscopy and spectroscopy and with Landau level spectroscopy. By following the evolution of the spectra as a function of the induced charge and comparing with numerical simulations, we are able to pinpoint the onset of atomic collapse and beyond, providing new insights into the physics of supercriticality.

1Work supported by DOE- FG02-99ER45742 and NSF DMR 1207108.

2:03PM B1.00015 Observation of vacancy-induced suppression of electronic cooling in defected graphene. XIAOSONG WU, QI HAN, YI CHEN, GERUI LIU, DAPENG YU, Peking Univ — Previous studies of electron-phonon interaction in impure graphene have found that static disorder can give rise to an enhancement of electronic cooling. We investigate the effect of dynamic disorder and observe over an order of magnitude suppression of electronic cooling compared with clean graphene. The effect is stronger in graphene with more vacancies, confirming its vacancy-induced nature. The dependence of the coupling constant on the phonon temperature implies its link to the dynamics of disorder. Our study highlights the effect of disorder on electron-phonon interaction in graphene. In addition, the suppression of electronic cooling holds great promise for improving the performance of graphene-based bolometer and photo-detector devices.

2This work was supported by National Key Basic Research Program of China (No. 2012CB933404, 2013CBA01603) and NSFC (project No. 11074007, 11222436, 11234001).


11:15AM B2.00001 Improved Performance in MoS$_2$ Field-Effect Transistors Contacted by Highly Doped Graphene Electrodes and Passivated by Hexagonal Boron Nitride. HSUN-JEN CHUANG, ZHIXIAN ZHOU, Wayne State University — A major challenge for developing semiconducting transition-metal-dichalcogenide (TMD)-based electronic devices is that TMDs tend to form a substantial tunneling or Schottky barrier (SB) with most metals commonly used for making electrical contacts, while low resistance Ohmic contacts are needed for exploring intrinsic transport properties of the channel material, and performance limits of realistic devices. We have fabricated low-resistance contacts to MoS$_2$ field-effect transistors by using graphene as work function tunable electrode material. To minimize the Schottky barrier height at the MoS$_2$/graphene junction and the contact resistance, both electrostatic and surface charge transfer doping methods were used to selectively dope the graphene electrodes. Substantial improvement of device performance was observed in devices with highly n-doped graphene electrodes. Four-probe electrical transport measurement was performed on MoS$_2$ devices with the active channel stacked between atomically flat hexagonal boron nitride (hBN) to further investigate the intrinsic performance limit of MoS$_2$ as a channel material.

1This work was supported by NSF (DMR-1308436).

11:27AM B2.00002 Electrical and optical properties of chemically doped p-type MoS$_2$. JOONKI SUH, University of California, Berkeley, TAE-EON PARK, Korea Institute of Science and Technology, DER-YUH LIN, National Chianghua University of Education, SEFAATTIN TONGAY, Arizona State University, JUNQIAO WU, University of California, Berkeley — Molybdenum disulfide is a model example of two-dimensional semiconductors, holding promise for applications in optoelectronic devices and field-effect transistors. So far, however, its practical use has been exclusively restricted to native, n-type doping. Here we experimentally demonstrate stable p-type conduction in molybdenum disulfide substitutionally doped with niobium. This chemical doping leads to a degenerate hole density of $\sim 1.8 \times 10^{14}$ cm$^{-2}$ and enables gate-tunable van der Waals p-n homojunctions. Also, the p-type monolayer molybdenum disulfide exhibits a greatly enhanced and broadened photoluminescence compared to that acquired from undoped monolayers. Our study demonstrates the stable p-type doping in molybdenum disulfide, and also reveals an effective way to tailor optical and electrical properties of two-dimensional semiconductors with extrinsic dopants.

11:39AM B2.00003 Electrostatic control of polarity of $\alpha$-MoTe$_2$ transistors with dual top gates. SHU NAKAHARAI, MAHITO YAMAMOTO, Natl Inst for Materials Sci, KEIJI UENO, Saitama Univ, YEN-FU LIN, SONG-LIN LI, KAZUHITO TSUKAGOSHI, Natl Inst for Materials Sci — Transition metal dichalcogenides have been expected for future applications in nanoelectronics due to their unique features of the atomically-thin structure. Using semiconducting $\alpha$-molybdenum ditelluride ($\alpha$-MoTe$_2$), we realized field effect transistors (FETs) in which the polarity (n- or p-type) can be electrostatically controlled without impurity doping. The fabricated device had a pair of top gates (aluminum electrode on silicon dioxide) attached in series with a gap length of 100 nm in between. We experimentally performed transistor operations in both n-FET and p-FET modes in a single device by changing the voltage applied to one of the two top gates, which determined the transistor polarity, and sweeping the bias of the other gate. The demonstrated reversibility of the transistor polarity will contribute to the renovated architecture of logic circuits with lower numbers of transistors and hence the lower power consumption than the conventional technology.
11:51AM B2.00004 Field-Effect Transistors Based on Few-Layered Ambipolar MoSe$_2$ and α-MoTe$_2$. DANIEL RHODES, Florida State University, NIHAR PRADHAN, NHMFL, SIMIN FENG, Pennsylvania State University, BYOUNG-HEE MOON, VAN XIN, NHMFL, SHARHRIAR MEMANDAN, MUNANDIS NCHIDUMA, LAKSHMI BHASKARAN, PSU, STEPHEN HILL, NHMFL, HUMBERTO TERRONES, Rensselaer Polytechnic Institute, MAURICIO TERRONES, PSU, AJAYAN PULICKEL, Rice University, LUIS BALICAS, NHMFL. We report a room temperature study on the electrical responses of field-effect transistors (FETs) based on few-layered MoSe$_2$ and MoTe$_2$, grown by chemical vapor transport, mechanically exfoliated onto SiO$_2$. MoSe$_2$ FETs electrically contacted with Ti display ambipolar behavior with current on/off ratios up to $10^6$ for both hole and electron channels. For both channels the Hall effect indicates Hall mobilities $\mu_H \approx 250$ cm$^2$/Vs, which are comparable to the corresponding field-effect mobilities, $\mu_{FE} \sim 175$ cm$^2$/Vs, evaluated through two-terminal field-effect configuration. MoTe$_2$ field-effect transistors are observed to be hole-doped, displaying on/off ratios of $\sim 10^8$ and subthreshold swings of $\sim 140$ mV per decade. Our results suggest that MoSe$_2$ is a good candidate for single atomic layer p-n junctions and for low-power, complementary logic applications, with MoTe$_2$ having similar properties. However, in MoTe$_2$ we observe a field-effect mobility of only $\mu_{FE} \sim 20$ cm$^2$/Vs in a bilayer device and $\sim 27$ cm$^2$/Vs in seven layers.

$^3$This work was supported by the U.S. Army Research Office MURI Grant No. W911NF-11-1-0362. The NHMFL is supported by NSF through NSF-DMR-0084173 and the State of Florida.

12:03PM B2.00005 ABSTRACT WITHDRAWN

12:15PM B2.00006 Conduction and Valence Band Offsets in WSe$_2$-Graphene Heterostructures. KOYOUNGHWA KIM, STEFANO LARENTIS, BABAK FALLAHAZAD, KAYOUNG LEE, JIAMIN XUE, DAVID DILLEN, CHRIS CORBET, EMANUEL TUTUC, Univ of Texas, Austin. We investigate the electron transport in graphene-WSe$_2$ heterostructures realized using a layer-by-layer transfer technique. Lateral electron transport shows ambipolar behavior characteristic of graphene, with a marked saturation at high positive (negative) gate bias, associated with the population of the conduction (valence) band in WSe$_2$. The graphene carrier density dependence on gate bias was extracted from magneto-transport measurements. Using WSe$_2$ as a top dielectric in dual-gate graphene field-effect transistors, we determine the WSe$_2$ dielectric constant along the c-axis. By combining the graphene density dependence on gate bias in back-gated graphene-WSe$_2$ heterostructures with the WSe$_2$ dielectric constant, we determine the offset between the graphene charge neutrality point and the WSe$_2$ conduction and valence bands.

This work was supported by NRI, NSF and Intel.

12:27PM B2.00007 Strain induced change in electronic and thermoelectric properties in few layers of MoS$_2$. TRIBHUWAN PANDEY, SWASTIBRATA BHATTACHARYYA, ABHISHEK K. SINGH, Materials Research Centre, Indian Institute of Science, Bangalore. The sensitivity of the electronic and thermoelectric properties of MoS$_2$ on application of strain can open up a variety of applications in the emerging area of straintronics. Using first principles calculations, we investigate the effect of normal compressive (NC), bi-axial compressive (BC), and bi-axial tensile (BT) strain on the electronic properties of few layered MoS$_2$. Regardless of the manner of strain, a reversible semiconductor-to-metal transition is observed in this material. We further show that under NC strain, the inter-layer interactions between Mo-$d_{yz}$ and S-$p_y$ causes the S-M transition, whereas under BC and BT strain it is caused by the strong hybridization of the intra-layer Mo-$d_{x^2-}z^2$ and S-$p_z$ orbitals and Mo-$d_{z^2}$ and S-$p_y$ orbitals, respectively. We also study number of layer (nL) and strain dependent transport properties using Boltzmann transport theory. Our study reveals that the 3L and 2L-MoS$_2$ emerge as the most efficient thermoelectric materials under NC and BT strain, respectively. The concept proposed from our study can also be extended to other semiconducting TMDs owing to similar crystal structure and electronic properties.

12:39PM B2.00008 Tuning the Schottky barrier heights at MoS$_2$metal contacts: a first-principles study. MOJTABA FARMANBAR, GEERT BROCKS, MESA+ Institute for Nanotechnology, University of Twente, The Netherlands. The nature of the Schottky barrier at metal contacts with the two-dimensional semiconductor MoS$_2$ is controversial. Using first-principles DFT calculations we show that the Schottky barrier height (SBH) for high work function (> 4.7 eV) metals typically obeys the Schottky-Mott limit, provided that a potential step that arises at the metal-MoS$_2$ interface is taken into account. It suggests that selecting a metal with an appropriate work function may reduce the SBH to zero. However, we find that for low work function metals the Fermi level is pinned below the conduction band edge of MoS$_2$, leading to SBHs of 0.1-0.3 eV. We attribute the pinning to the metal-MoS$_2$ interaction at the interface perturbing the electronic structure of MoS$_2$, and causing a broadening of the MoS$_2$ conduction band edge. Inserting a monolayer of boron nitride (BN) between the metal surface and the MoS$_2$ layer disrupts this interaction. In addition the BN layer effectively decreases the work function, thereby enabling a line-up of the Fermi level with the MoS$_2$ conduction band with a vanishing SBH.

12:51PM B2.00009 Structural and transport properties of finite length grain boundaries in two-dimensional materials. YUHANXI WANG, VINCENT CREPSI, Pennsylvania State University. Grain boundaries in two dimensional materials such as graphene and monolayer transition metal dichalcogenides are a fundamental issue of the material growth from a monocrystalline ground state. We show that when 2D materials are grown on substrates with curved surfaces, grain boundaries produced are self-intersections are in fact the ground state. They screen out the curvature imposed by the substrate and form finite length grain structures, terminating with cone and saddle shapes of partial disclinations. The structural stability and transport properties of finite length grain boundaries are studied at the tight-binding level. Every dislocation in the grain boundary contributes an intrinsic pseudo-flux and induces loop currents during transport. We further show that transport properties depend sensitively on the number of dislocations in the grain boundary.

1:03PM B2.00010 Intrinsic Electron and Hole Transport in Channel Passivated WSe$_2$ Field-Effect Transistors with Graphene Contacts. HSUN JEN CHUANG, Wayne State University, NIRMAL JEEVI GHIMIRE, JIAQIANG YAN, DAVID MANDRU, The University of Tennessee, Knoxville and Oak Ridge National Laboratory, ZHIHUI ZHOU, Wayne State University. We report electrical transport measurement of high-quality WSe$_2$ field-effect transistors. As a nearly intrinsic semiconductor with a relatively large bandgap, WSe$_2$ tends to form substantial Schottky barriers with common contact metals for both electron and hole channels, which obstructs the charge injection especially at low temperatures. In this work, we use highly n- and p-doped graphene as an electrode material to form low resistance electrical contacts to the electron and hole channels, respectively. To minimize surface and interface scattering, hexagonal boron nitride was used to passivate both the top and bottom surfaces of the WSe$_2$ channel. Four-terminal transport measurement was carried out for a wide temperature range to understand the intrinsic transport properties of atomically thin WSe$_2$. Field-effect transport and effective mobility for both electron and hole channels as well as their temperature dependence will be discussed.

This work was supported by NSF (DMR-1308436).

1:29PM B2.00011 Electronic and Optical Properties of MoS$_2$ and its Heterostructures. JUN JUN LIU, TSUYOSHI TAKAMA, Masayuki URASHIMA, Jun-roy KIM, Masaaki NAKAI, Tatsuo MIYASAKA, Hiroyuki NAKAJIMA, and Toyoki KITAO. University of Tokyo, Japan. Using angle-resolved photoemission spectroscopy, we study carrier mobility in few-layer MoS$_2$. We show that carrier mobility can be enhanced by the interface interaction between MoS$_2$ and MoO$_3$. It is found that the carrier mobility is improved when the interface interaction is strengthened under the in-plane tension. The enhancement of the carrier mobility is attributed to the interface interaction between MoS$_2$ and MoO$_3$.
1:15PM B2.00011 The Effect of Substrate on the Electron Transport Properties of MoS₂ Field-Effect Transistors¹ — BHIM CHAMALAGAIN, HSUN-JEN CHUANG, MEEGHAGE MADUSANKA PERERA, ZHIXHRAN ZHOU. Wayne State University — Substrate plays an important role in the performance of field-effect transistors (FETs) with two-dimensional transition metal dichalcogenide (TMD) channels. In this work, we systematically study the transport properties of few-layer MoS₂ FETs consistently fabricated on various substrates including SiO₂, Al₂O₃, SiO₂ modified by octadecyltrimethoxysilane (OTMS) self-assembled monolayers (SAMs), and hexagonal boron nitride (hBN). Standard four-probe electrical transport measurement was carried out at temperatures ranging from 77 K to room temperature to understand the scattering mechanism. Surprisingly, the room temperature mobility extracted from devices on different substrates is nearly the same. In contrast, a substantially higher mobility is observed in MoS₂ devices on clean hBN substrates at low temperatures. The results of various sources of scattering originating from the substrate and the channel/substrate interface such as charged impurities, charge traps, surface roughness, and remote surface optical phonons will be discussed.

¹This work was supported by NSF (No. ECCS-1128297) and Thomas C. Rumble Fellowship Award.

1:27PM B2.00012 Enhanced mobility electrons at the monolayer / multilayer MoS₂ homo-interface¹ — Y. JIA, E.J. LENFERINK, T. STANEV, N.P. STERN. Department of Physics and Astronomy, Northwestern University, Evanston, IL, US 60208 — Energy band alignment at interface of heterostructures can give rise to non-trivial local electronic structure and charge states with low dimensionality. In transition metal dichalcogenides (TMDcS), the optical band gap depends on the number of 2D crystal layers, transitioning from 1.29 eV in bulk to 1.88 eV for 60208 — Energy band alignment at interface of heterostructures can give rise to non-trivial local electronic structure and charge states with low dimensionality. In transition metal dichalcogenides (TMDcS), the optical band gap depends on the number of 2D crystal layers, transitioning from 1.29 eV in bulk to 1.88 eV for a monolayer of MoS₂, for example, and providing the possibility to create unusual charge state at the monolayer/multilayer homo-interface. Here, we examine the boundaries between MoS₂ monolayers and multilayers using scanning photocurrent microscopy and gate-dependent transport. Enhanced photocurrent and conductance were observed at the 1D homo-interface, which can be explained as accumulated carriers in the bent-band region of the junction. Our heterojunction modeling suggests a high local carrier density and enhanced mobility at the homo-interface. Our work presents an opportunity to achieve a 1D electron state in a homojunction and a pathway to break the mobility limit of TMDC monolayer transistors.

¹This work was supported by the Institute for Sustainability and Energy at Northwestern and the U.S. Department of Energy (DE-SC0012130). N.P.S. acknowledges support as an Alfred P. Sloan Research Fellow.

1:39PM B2.00013 High Powerfactor in single and few-layer MoS2 — YING WANG, YU YE, KEDAR HIPPAL-GAONKAR, YUAN WANG, XIANG ZHANG, University of California, Berkeley — The thermoelectric effect enables conversion between thermal and electrical energy, and provides one way to extract energy from waste heat. The efficiency of a thermoelectric device can be defined by a dimensionless figure of merit given by $ZT = S^2σT/k$. In order to achieve efficient thermoelectric devices, $S^2σ$ needs to be kept high by optimizing the interplay between the $S$ and $σ$. The thin layered transition-metal dichalcogenide semiconductor MoS₂ has attracted great interest because of its two dimensional density of states and relatively high mobility, which could give a large $S$ and $σ$. Here we study on pristine exfoliated 1L-, 2L- and 3L MoS₂ samples by simultaneous measurement of the Seebeck coefficient$(S)$ and two probe electrical conductivity using nano-fabricated heater and thermometer. It firstly shows that atomic thin MoS₂ which has a large effective band masses $(m^*)$ as well as high mobilities $(μ)$, increases the powerfactor $S^2σ/τ$ as high as 8.5 mWm⁻¹K⁻² at room temperature (twice as high as commercially usedBi₂Te₃). Further, we show for the first time that the confined two-dimensional density of states of the conduction band can be studied in monolayer MoS₂ by measuring the gate-dependent Seebeck voltage.

1:51PM B2.00014 Carrier injection in van der Waals multilayer systems — MARCELO KURODA, CHRISTOPHER COGER, Auburn University — Carrier injection is critical for the use of two-dimensional material systems like transition metal dichalcogenides (TMD) or graphene in electronic devices. Here we use first principles calculations (within the density functional theory) to quantify and classify the contact formed between metals and TMD multilayer systems. In particular we study the cases of multilayer MoS₂ and MoSe₂ with different metal electrodes (e.g. Pd, Au, Ti). We find different behaviors depending on the choice of metal, thickness and electric field. An analytical model is produced accounting for the Fermi level pinning and the layer quantum capacitance. This atomistic description also sheds light on the ambipolar behavior observed in these systems and the gate-dependent contact resistance in field effect transistors.

2:03PM B2.00015 Ambipolar conduction in MoS₂/WSe₂ hetero-bilayers — HEMA CHANDRA PRAKASH MOVVA, SANGWOO KANG, AMRITESH RAI, SANJAY BANERJEE, Microelectronics Research Center, The University of Texas at Austin — Recent interest in layered semiconductors, and the ability to assemble them into artificial heterostructures with atomically sharp interfaces has opened up new avenues for the design of future electronic devices. In this work, we fabricated vertical heterostructures of exfoliated monolayer MoS₂ and monolayer WSe₂ using a facile flake pick-up-and-place technique, and studied their optical and electrical properties. Photoluminescence measurements showed evidence of indirect excitons at ~1.55 eV, indicating a clean interface between the two layers. We observed back-gate tunable, layer-selective ambipolar conduction in field effect transistors (FETs) made using these hetero-bilayers, with e-transport occurring through the MoS₂, and h-transport through WSe₂. The addition of a top-gate using a thin hBN dielectric further enabled selective operation of the hetero-bilayer FET as an n-FET/p-FET depending on the back-gate bias.

Monday, March 2, 2015 11:15AM - 1:39PM — Session B3 FIP: Invited Session: Condensed Matter Physics in Latin America I 002AB - Alex de Lozanne, University of Texas at Austin

11:15AM B3.00001 An overview of Experimental Condensed Matter Physics in Argentina by 2014, and Oxides for Non Volatile Memory Devices: The MeMOSat Project — PABLO LEVY, CNEA +CONICET — In the first part of my talk, I will describe the status of the experimental research in Condensed Matter Physics in Argentina, biased towards developments related to micro and nanotechnology. In the second part, I will describe the MeMOSat Project, a consortium aimed at producing non-volatile memory devices to work in aggressive environments, like those found in the aerospace and nuclear industries. Our devices rely on the Resistive Switching mechanism, which produces a permanent but reversible change in the electrical resistance across a metal-insulator-metal structure by means of a pulsed protocol of electrical stimuli. Our project is devoted to the study of Memory Mechanisms in Oxides (MeMO) in order to establish a technological platform that tests the Resistive RAM (ReRAM) technology for aerospace applications. A review of MeMOSat's activities is presented, covering the initial Proof of Concept in ceramic millimeter sized samples; the study of different oxide-metal couples including (LaPr)₂/3Ca₁/3MnO, La₂/3Ca₁/3MnO₃, YBa₂Cu₃O₇, TiO₂, HfO₂, MgO and CuO; and recent miniaturized arrays of micrometer sized devices controlled by in-house designed electronics, which were launched with the BuzzSat01 satellite in June2014 by the argentinian company Satellogic.
We also discuss the effects of the framing anomaly on linear responses of non-Abelian FQH states. The framing anomaly which fixes the value of thermal Hall conductivity and generates a "finite size correction" to the Hall viscosity of the FQH states on a sphere. This phenomenon is known as the framing anomaly. It is shown that accounting for the framing anomaly of the manifold through the path integral measure.

The Effects of Quantum Dots and Surface Nanotexturization on Solar-Cell Performance

Monday, March 2, 2015 11:15AM - 1:45PM

Session B4 FIAP: Meet Your Future: Industrial Careers for Physicists: An Interactive Workshop

Mayor Cockrell Room 004 -

11:15AM B4.00001 Workshop —

Monday, March 2, 2015 11:15AM - 2:15PM

Session B5 FIAP DCMP: Fractional Quantum Hall Effect II

Juan Gorman Room 005 - Johannes Pollanen, California Institute of Technology

11:15AM B5.00001 Using Composite Fermions to Probe a Wigner Solid in 2D Hole Systems

INSUN JO, YANG LIU, H. DENG, M. SHAYEGAN, L. N. PFIEFFER, K. W. WEST, K. W. BALDWIN, Dept. of Electrical Engineering, Princeton University, Princeton, NJ 08544 — We have studied a GaAs double-quantum-well structure that hosts an interacting, bilayer two-dimensional hole system with a large density difference between the two layers. At very low temperatures and large perpendicular magnetic field, we expect the two layers to exhibit distinct many-body states of holes: The high-density layer develops a Fermi sea of composite fermions when its last Landau Level is half-filled, while the holes in the low-density layer in the same magnetic field range are at very small fillings and should condense into a Wigner crystal. Via measuring the magneto-resistance of the bilayer system, we monitor signatures of the Wigner crystallization and melting.

11:27AM B5.00002 ABSTRACT WITHDRAWN —

11:39AM B5.00003 Framing Anomaly in the Effective Theory of Fractional Quantum Hall Effect

ANDREY GROMOV, ALEXANDER ABANOV, Stony Brook University, GIL YOUNG CHO, YIZHI YOU, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — While the classical Chern-Simons theory is topological, its quantum version is not as it depends on the metric of the base manifold through the path integral measure. This phenomenon is known as the framing anomaly. It is shown that accounting for the framing anomaly of the quantum Chern-Simons theory is essential to obtain the correct gravitational linear response functions of fractional quantum Hall systems (FQH). In the lowest order in gradients the effective action includes Chern-Simons, Wen-Zee and gravitational Chern-Simons terms. The latter term has a contribution from the framing anomaly which fixes the value of thermal Hall conductivity and generates a “finite size correction” to the Hall viscosity of the FQH states on a sphere. We also discuss the effects of the framing anomaly on linear responses of non-Abelian FQH states.
11:51AM B5.00004 Evaluation of Quantum Scattering Time in Ultra-High Quality GaAs Quantum Wells. QI QIAN, SUMIT MONDAL, GEOFFREY C. GARDNER, JOHN D. WATSON, MICHAEL J. MANFRA, Purdue Univ — We present a critical analysis of the extraction of quantum scattering time from Shubnikov-de Haas oscillations in ultra-high quality GaAs quantum wells. In the regime of temperature and magnetic field study here (T~0.3K, B~0.3T) we find the canonical method for determination of quantum scattering time yields unreliable results (cf. Coleridge, Phys. Rev. B 44, 3793). We elaborate a formalism that allows extraction of the quantum scattering time in a regime in which the normalized modulation of the density of states $\Delta g/|g_0|$ is greater than unity. This approach describes well low-field data for samples that display very large excitation gaps for fragile fractional quantum Hall states at large magnetic field.

12:03PM B5.00005 Quantized coefficients for the Chern-Simons terms in bosonic and fermionic symmetry protected topological states in $2n+1$D with $U(1)$ symmetry. CHAO-MING JIAN, Stanford Univ, PENG YE, Perimeter Institute for Theoretical Physics, XIAO-LIANG QI, Stanford Univ — The study of symmetry protected topological (SPT) phases has led to many fruitful results. The classification of SPT states shows a big difference between bosonic systems and fermionic systems even when they share the same symmetry. In this talk, I will focus on SPT states with $U(1)$ symmetry. In $2n+1$ dimensions, when we gauge the $U(1)$ symmetry, the effective actions of the gauge field contain Chern-Simons term (and its generalization in higher dimensions) with quantized coefficients. The quantization of these coefficients is different between bosonic and fermionic systems. I will derive, using different methods, the quantization of coefficients for bosonic systems using general gauge invariance principle. I use Dirac fermions in $2n+1D$ coupled to $U(1)$ gauge field to show the quantization for fermionic systems. I find that the bosonic and fermionic systems have a factor of $(n+1)!$ difference in the quantization unit of the quantized coefficients.

12:15PM B5.00006 An investigation of orienting mechanisms of the quantum Hall stripe phases. J. POLLANEN, S. BRANDSEN, J.P. EISENSTEIN, Institute for Quantum Information and Matter and Department of Physics, California Institute of Technology, Pasadena, California 91125, USA, L.N. PFIEFFER, K.W. WEST, Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544, USA — At high magnetic field, two-dimensional electron systems (2DES) exhibit collective states possessing broken rotational symmetry. These states, known as the quantum Hall stripe phases (QHSP), are examples of electronic nematic liquid crystals. Experiments consistently show that the stripes are oriented relative to the GaAs crystal axes, but the exact nature of the native symmetry-breaking field remains unknown. We report here on an extensive study of the QHSPs in a series of high mobility single quantum well samples. These samples all have the same electron density, but differ systematically in the symmetry of the 2DES confinement potential and the distance between the 2DES and the sample surface. Tilted field magneto-transport measurements are used to observe the stripe phases and to assess the strength of the native symmetry-breaking field. We find that the stripes remain oriented in the same way in all our samples. Furthermore, our measurements show that the strength of the orienting potential does not depend on the distance to the sample surface but does exhibit an intriguing dependence on the symmetry of the 2DES confinement potential. We discuss these results in the light of recent suggestions that strain and/or spin-orbit effects may determine the stripe orientation.

12:27PM B5.00007 Numerical characterization of non-Abelian Moore-Read state in the microscopic lattice boson model. WEI ZHU, SHOUSHU GONG, California State University, Northridge, F. D. M. HALDANE, Princeton University, D. N. SHENG, California State University, Northridge — Identifying the interacting systems that host the non-Abelian (NA) topological phases has attracted intense attention in physics. Theoretically, it is possible to realize the NA Moore-Read (MR) state in bosonic system or double-layer system by coupling two Abelian fractional quantum Hall (FQH) states together. Here, based on the density matrix renormalization group and exact diagonalization calculations, we study two such examples in the microscopic lattice models and investigate their NA nature. In the first example, we provide a thorough characterization of the universal properties of MR state on Haldane honeycomb lattice model, including both the edge spectrum and the bulk anyonic quasiparticle statistics. By inspecting the entanglement spectral response to the $U(1)$ flux, it is found that two of Abelian ground states can be adiabatically connected through a charge unit quasiparticle pumping from one edge to the other. In the second example, we study a double-layer bosonic FQH system built from the $\pi$-flux lattice model. Some evidences of NA nature has been identified, including the groundstate degeneracy and finite drag Hall conductance. The numerical methods we developed here provides a useful and practical way for detecting the full information of NA topological order.

1 This research is supported by the U.S. Department of Energy, Office of Basic Energy Sciences under grant No. DE-FG02-06ER46305

12:39PM B5.00008 Fractional quantum Hall and nematic liquid crystal phases in a variable density two-dimensional electron system. S. BRANDSEN, J. POLLANEN, J.P. EISENSTEIN, Institute for Quantum Information and Matter and Department of Physics, California Institute of Technology, Pasadena, California 91125, L.N. PFIEFFER, K.W. WEST, Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544 — At high magnetic field, Coulomb interactions in a two-dimensional electron system (2DES) lead to a wide variety of collective phases, including the fractional quantum Hall fluids and the nematic liquid crystals found at high Landau level occupancy. In order to examine the density dependence of these quantum states, we have developed a new sample architecture consisting of a highly doped, yet transparent, conducting cap layer grown atop a conventional modulation-doped heterojunction where the 2DES resides. Separate contacts to the 2DES and the cap layer allow the latter to function as a gate for tuning the 2DES density both before and after low temperature illumination. After illustrating the basic functioning of this structure, we will report results on the density dependence of various quantum Hall and nematic liquid crystal phases of the 2DES.

1 This work was supported by the Institute for Quantum Information and Matter, an NSF Physics Frontiers Center with support of the Gordon and Betty Moore Foundation through Grant GBMF1250.

12:51PM B5.00009 Accessing topological order in fractionalized liquids with gapped edges. THOMAS IADECOLA, Boston University, TITUS NEUPERT, Princeton University, CLAUDIO CHAMON, Boston University, CHRISTOPHER MUDRY, Paul Scherrer Institue — We consider manifestations of topological order in time-reversal-symmetric fractional topological liquids (TRS-FTLs), defined on planar surfaces with holes. We derive a formula for the topological ground state degeneracy of such a TRS-FTL, which applies to cases where the edge modes on each boundary are fully gapped by appropriate backscattering terms. The degeneracy is exact in the limit of infinite system size, and is given by $q^{-N_{fl}}$, where $N_{fl}$ is the number of holes and $q$ is an integer that is determined by the topological field theory. When the degeneracy is lifted by finite-size effects, the holes realize a system of $N_{fl}$ coupled spin-like $q$-state degrees of freedom. In particular, we provide examples where $Z_{q}$ quantum clock models are realized on the low-energy manifold of states. We also investigate the possibility of measuring the topological ground state degeneracy with calorimetry.
1:03PM B5.00010 Topology and interactions in a frustrated slab: tuning from Weyl semimetal to $C > 1$ fractional Chern insulators\(^1\). ZHAO LIU, Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544, USA, EMIL BERGHOLTZ, MAXIMILIAN TRESCHER, Dahlem Center for Complex Quantum Systems and Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany, RODERICH MOESSNER, Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, D-01187 Dresden, Germany, MASAFUMI UDAWAGA, Department of Applied Physics, University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo 113-8656 — We show that a [111] slab of spin-orbit coupled pyrochlore lattice can become a Weyl semi-metal phase with exotic surface states called as Fermi arcs, i.e., these states are localized to different surfaces depending on their quasi-momentum. Remarkably, in this model, these Fermi arcs persists even when there is no Weyl point in the bulk. Considering interacting electrons in slabs of finite thickness, we find a plethora of known fractional Chern insulating phases, including a new discovered higher Chern number state which is likely a generalization of the Moore-Read fermionic fractional quantum Hall state. By contrast, in the three-dimensional limit, we argue for the absence of gapped states of the flat surface band due to a topologically protected coupling of the surface to gapless states in the bulk. We comment on generalizations as well as experimental perspectives in thin slabs of pyrochlore iridates.

\(^1\)Zhao Liu was supported by DOE Grant DE-SC0002140.

1:15PM B5.00011 Detecting fractional statistics in anyon interferometry employing thermal excitation. CHEOLHEE HAN, HEUNG-SUN SIM, KAIST — In this work, we propose an interferometry setup of anyons, a setup slightly modified from a usual Fabry-Perot interferometry. In this interferometry, there appears anyon braiding between thermally excited anyons and an anyon injected from a source of the setup. This braiding process, which has unnoticed before and does not exist in bosons and fermions, results in a temperature dependent phase shift of the interference pattern of the setup. Experimental observation of the phase shift will provide a direct evidence of fractional statistics.


1:27PM B5.00012 Reordering Fractional Chern Insulators into Stripes of Fractional Charges Using Long-Range Interactions\(^1\). MENGSIU CHEN, VITO SCAROLA, Virginia Tech — Long-range interactions contribute to the rich phenomenology of quasiparticle collective states in the fractional quantum Hall regime. We test for analogues in models of fractional Chern insulators derived from a screened Coulomb interaction. We project the interaction to the lowest band and numerically diagonalize it. We find that the uniform fractional Chern liquid is surprisingly robust to long-range interactions but gives way to a unidirectional charge density wave fractionally charged quasiparticles with increased screening length. Our results show that fractional Chern insulators offer a robust and important platform for studying quasiparticles collective states.

\(^1\)We acknowledge support from ARO (W911NF-12-1-0335), AFOSR (FA9550-11-1-0313), and DARPA-YFA.

1:39PM B5.00013 Composite Fermions with a Warped Fermi Contour\(^1\). M.A. MUEED, DOBROMIR KAMBUROV, YANG LIU, MANSOUR SHAYEGAN, LOREN PFIEFFER, KEN WEST, KIRK BALDWIN, Princeton Univ, ROLAND WINKLER, Northern Illinois Univ — Composite fermions (CFs), quasi-particles formed by attaching an even number of flux quanta to each charged carrier in high perpendicular magnetic fields ($B$), capture many phenomena exhibited by an interacting system of two-dimensional carriers. The flux attachment cancels out the external $B$ at a half-filled Landau level, enabling CFs to occupy a Fermi sea and possess a Fermi contour, similar to their $B = 0$ carrier counterparts. Because the CFs are primarily a manifestation of interaction, one might argue that they should retain no memory of the $B = 0$ particles, including their energy band properties. We present tantalizing evidence through commensurability measurements that the composite fermions can be strongly influenced by the characteristics of the Landau level in which they are formed. In particular, the composite fermions have a warped Fermi contour when their Landau level originates from a hole band with significant warping.

\(^1\)We acknowledge support through the DOE (DEFG02-00-ER45841) for measurements, and the Gordon and Betty Moore Foundation (Grant No. GBMF4420), Kec Foundation, and the NSF (DMR-1305691 and MRSEC DMR-0819860) for sample fabrication.

1:51PM B5.00014 Flat Chern Bands and Edge States in the Hofstadter Model Near to Rational Flux. FENNER HARPER, STEVEN SIMON, University of Oxford, RAHUL ROY, University of California, Los Angeles — We present a perturbative approach to the study of the Hofstadter model for when the amount of flux per plaquette is close to a rational fraction [Phys. Rev. B 90, 075104 (2014)]. Within this approximation, the eigenstates of the system connect smoothly to the Landau levels of the continuum, but in general develop an additional species (or colour) degree of freedom. Using the formalism of Haldane pseudopotentials, we describe the fractional quantum Hall-like wavefunctions that arise when interactions are turned on. We also discuss the form and energy spectrum of the bosonic edge excitations that would occur in the presence of a confining harmonic trap, making connections to the recent experimental realizations of the Hofstadter model using ultracold atoms.

2:03PM B5.00015 Topological textures and metal-insulator transition in Reentrant Integer Quantum Hall Effect: role of disorder\(^1\). YULI LYANDA-GELLER, GEORGE SIMION, Department of Physics and Astronomy, Purdue University, West Lafayette, IN 47907 USA — We investigate a ground state of the two-dimensional (2D) electron liquid in the presence of disorder for Landau level filling factors, for which the re-entrant integer quantum Hall effect is observed. Our particular interest is the range of filling factors, which in a clean 2D system is favorable to formation of the two-electron (2e) bubble crystal. For the smooth random potential due to charged impurities placed far away from the 2D gas, the ground state is a lightly distorted 2e bubble crystal. However, for positively or negatively charged residual impurities located approximately within about three magnetic lengths from the 2D electrons, the ground state contains charged 2e complexes formed either by positively charged impurity and 3e defect bubble, or negatively charged impurity and 2e defect bubble. In the vicinity of 1e and 3e defect bubbles, the 2e bubbles of the crystal change their shape from round to elongated forming hedgehog (for 1e defect) or vortex (for 3e defect) textures. The topological textures due to these complexes interact with vortex and hedgehog excitations, generated as temperature increases that are not bound by residual impurities. The temperature of insulator to metal transition calculated with both bound and unbound defects agrees with experiment.

\(^1\)Research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0010544.

Monday, March 2, 2015 11:15AM - 2:15PM – Session B6 DMP DCOMP: Focus Session: Proper and Improper Ferroelectrics 006A - Manfred Fiebig, ETH Zurich
11:15AM B6.00001 Ferroelectric Transition in Compressively Strained Epitaxial SrTiO$_3$, AMIT VERMA, Electrical Engineering, Univ. of Notre Dame, SANTOSH RAGHAVAN, SUSANNE STEMMER, Materials Dept., Univ. of California, Santa Barbara, DEBBIE JENA, Electrical Engineering, Univ. of Notre Dame — Strontium titanate (SrTiO$_3$) is a transition metal oxide semiconductor that crystallizes in the cubic perovskite crystal structure and exhibits incipient ferroelectricity. The dielectric constant of bulk unstrained SrTiO$_3$ crystals saturates at temperatures below 4K while above ~ 50K, its dielectric constant decreases following the Curie-Weiss law of ferroelectricity [Muller et al., Phys. Rev. B 19, 3593 (1979)]. Based on the Landau-Ginzburg-Devonshire theory of ferroelectrics, it is theoretically predicted that under biaxial compressive or tensile strain, SrTiO$_3$ thin films should become ferroelectric [Perstew et al., Phys. Rev. B 61, R255 (2000)]. Heteroepitaxial growth on lattice-mismatched substrates was used earlier to demonstrate near room temperature in-plane ferroelectricity in tensile strained SrTiO$_3$ thin films [Haeurn et al., Nature 390, 758 (2004)]. In this work, we have epitaxially grown compressively strained SrTiO$_3$ thin films on (001) LSAT substrates, fabricated Pt/SrTiO$_3$ Schottky diodes, and performed temperature-dependent capacitance-voltage (CV) measurements of these diodes. As predicted by the theory, the out-of-plane dielectric constant of SrTiO$_3$ extracted from these CV measurements shows a divergence, implying a ferroelectric transition in compressively strained SrTiO$_3$.

11:27AM B6.00002 Structural Stability of Nano-scale SrTiO$_3$ Under Pressure, HAN ZHANG, TREvor TYSOn, New Jersey Institute of Technology, XINGUO HONG, MEGAN SCOFIELD, STANISLAUS WONG, State University of New York at Stony Brook — The bulk phase of SrTiO$_3$ (STO) is paraelectric and exhibits a structural phase transition near ~ 6 GPa under hydrostatic pressure. It has recently been found that nano-scale STO is polar under ambient conditions. We have conducted pressure dependent structural measurements on monodispersed nano-scale samples with 10 nm and 83 nm particle size. The structures of both samples were explored and the results are compared with the reported studies of bulk STO. This work is supported by DOE Grant DE-FG02-07ER46402.

11:39AM B6.00003 Hybrid Improper Ferroelectricity, S.-W. CHEONG, YOON SEOK OH, Rutgers University, XUAN LUO, Pohang University of Science and Technology, FEI-TING HUANG, YAZHONG WANG, Rutgers University — Utilizing trilinear coupling of two types of octahedron rotations, hybrid improper ferroelectricity has been theoretically predicted in double layered compounds such as (Ca,Sr,Ba)$_2$MnTi$_2$O$_6$. On the other hand, there exists little theoretical prediction on practical properties of the potentially ferroelectric compounds such as ferroelectric transition temperature, switchability of polarization, and chemical phase stability. We have attempted to fabricate single crystals of some of these compounds, and examined the physical properties of the crystals with the aim of discovering new bulk ferroelectrics with switchable polarization at room temperature. We will report the results of our comprehensive experimental investigation.

11:51AM B6.00004 Experimental Demonstration of Hybrid Improper Ferroelectric in the Layered Ruddlesden-Popper Compounds , YOON SEOK OH, Department of Physics, Ulsan National Institute of Science and Technology (UNIST) — Geometric ferroelectrics are called as improper ferroelectrics where geometric structural constraints, rather than typical cation-anion paring, induce proper ferroelectric polarization. Hybrid improper ferroelectricity, one kind of geometric ferroelectricity, results from the combination of two or more non-ferroelectric structural order parameters. In recent, hybrid improper ferroelectricity has been theoretically predicted in ordered perovskites and the Ruddlesden-Popper compounds. However, the ferroelectricity of these compounds has never been experimentally confirmed and even their polar nature has been under debate. In this talk, we report our experimental results of exploring switchable electric polarization and domain structures in the single crystals of the $n = 2$ layered Ruddlesden-Popper compounds. In collaboration with Xuan Luo, Laboratory for Pohang Emergent Materials, Postech; Fei-Ting Huang, Department of Physics & Astronomy, Rutgers University; Yazhong Wang, Department of Physics & Astronomy, Rutgers University; and Sang-Wook Cheong, Department of Physics & Astronomy, Rutgers University.

12:27PM B6.00005 Single crystal ternary oxide ferroelectric integration with Silicon, SAIDUR BAKAUL, CLAUDY SERRAO, LONG YOUN, ASIF KHAN, SAYEEF SALAHUDDIN, University of California, Berkeley — Integrating single crystal, ternary oxide ferroelectric thin film with Silicon or other arbitrary substrates has been a holy grail for the researchers since the inception of microelectronics industry. The key motivation is that adding ferroelectric materials to existing electronic devices could bring into new functionality, physics and performance improvement such as non-volatile memory, sub-threshold swing of field effect transistor (FET) below 60 mV/decade in FET [Salahuddin, S, Datta, S. Nano Lett. 8, 405(2008)]. However, fabrication of single crystal ferroelectric thin film demands stringent conditions such that lattice matched single crystal substrate and high processing temperature which are incompatible with Silicon. Here we report on successful integration of Pb$_{2/3}$Ti$_{1/3}$O$_3$ in single crystal form with by using a layer transfer method. The lattice structure, surface morphology, piezoelectric coefficient d$_{33}$, dielectric constant, ferroelectric domain switching and spontaneous and remnant polarization of the transferred PZT are as good as these characteristics of the best PZT films grown by pulsed laser deposition on lattice matched oxide substrates. We also demonstrate Si based, FE gate controlled FET devices.

12:39PM B6.00006 Optical second-harmonic characterization of ferroelectricity in double perovskites Ca$_{2-x}$Mn$_x$Ti$_2$O$_6$, YUJIN CHO, FARBOD SHAFIEI, Department of Physics, University of Texas at Austin, ZONGYAO LI, JIANSHI ZHOU, Department of Mechanical Engineering, University of Texas at Austin, MICHAEL DOWNER, Department of Physics, University of Texas at Austin — Perovskite-type ferroelectric oxides such as BaTiO$_3$ are used widely as actuators and memory storage devices. Recently ferroelectricity was demonstrated in the double perovskite CaMnTi$_2$O$_6$, which represents a fundamental new class of ferroelectrics in which dipoles from Mn$^{2+}$ at the A-site and Ti$^{4+}$ at the B site are cooperatively coupled [1]. However, synthesis of CaMnTi$_2$O$_6$ from CaTiO$_3$-MnTiO$_3$ required pressure as high as 7GPa. We are developing spark plasma sintering (SPS) methods to synthesize Ca$_{2-x}$Mn$_x$Ti$_2$O$_6$ at pressures as low as 50 MPa, and using Second Harmonic Generation (SHG) microscopy to characterize the strength of ferroelectricity. Preliminary SHG results show that ferroelectric CaMnTi$_2$O$_6$ can be synthesized at low pressure with stronger ferroelectricity. Higher pressure SPS-synthesized sample present comparative SHG results for SPS-synthesized and high-pressure-synthesized CaMnTi$_2$O$_6$ and relate them to the underlying origins of ferroelectricity. [1] A. Aimi et al., Chem. Mat. 26, 2601 (2014).

12:51PM B6.00007 Local Structure Study of the Diffuse Phase Transitions in 0.75Pb(Mg$_{1/3}$Nb$_{2/3}$)$_2$O$_3$-0.25PbTiO$_3$, HIROYUKI TAKE NAKA, ILYA GRINBERG, ANDREW M. RAPPE, University of Pennsylvania, THE MAKINENI THEORETICAL LABORATORIES TEAM — Relaxor ferroelectrics have been of scientific interest and importance due to their fascinating properties such as a giant piezoelectric response, high permittivity over a broad temperature range, and unique dielectric response with frequency dispersion with the diffuse phase transitions. The experimental results undoubtedly explain the transitions with the widely accepted model of polar nanoregions (PNRs), appear at $T_b$, in a non-polar matrix. Local structure distortions using diffuse scattering (DS) technique had been reported already. Intensities of DS raise below the intermediate temperature $T_a$, a few degrees below $T_b$, and can be seen even at low temperature where system undergoes the frozen phase. Formations of local dipoles which give rise to the DS intensities are still unclear. We study DS by performing molecular dynamics simulations with the first-principle-based potential for 0.75Pb(Mg$_{1/3}$Nb$_{2/3}$)$_2$O$_3$-0.25PbTiO$_3$ without invoking the PNRs. Our results show that DS patterns form the experimentally reported shapes and integrated DS intensities as a function of temperature reveal a similar trend to the experimental results. Our results indicate that the local structure correlations in lead-based relaxors can arise from local random fields without PNRs. Instead, we find that the DS patterns are due to formations of slush-like dipole multidomains.
1:03PM B6.00008 Relative Stability of FE and AFE States in (Na0.5Bi0.5)TiO3-based Solid Solutions , V.L. SOBOLEV, South Dakota School of Mines & Technology, Rapid City, SD 57701, USA, V.M. ISCHCHUK, L.G. GUSAKOVA, N.G. KISEL, D.V. KUZENKO, N.A. SPIRIDONOV, Science & Technology Center “Reactivelectron” of the Nat. Acad. of Sci. of Ukraine, 83049 Donetsk, Ukraine — Changes of the relative stability of antiferroelectric (AFE) and ferroelectric (FE) phases in the [(Na0.5Bi0.5)0.80Ba0.20]Ti1−xByO3 system of solid solutions with the B-site ion substitutions have been studied. Ions of zirconium and tin along some ions complexes such as (InNb), (FeNb) and several others were used for substitutions. The increase in the substituent ion content leads to nearly linear variation of the crystal cell size along with changes of the relative stability of the AFE and FE phases according to the tolerance factor variation. Substituent ions with ionic radii larger than the ionic radius of original ion evoke a decrease of the FE-AFE phase transition temperature. The substituent ions with smaller ionic radii have the opposite effect. Our results demonstrate that the size of the substituent ion causes a predominant influence on the relative stability of the FE and AFE states in (Na0.5Bi0.5)TiO3-based solid solutions. Our studies also indicate the way to raise the FE-AFE phase transition temperature.

1:15PM B6.00009 Negative Capacitance transients in a ferroelectric capacitor , ASIF KHAN, KOROK CHATTERJEE, BRIAN WANG, STEVEN DRAPCHO, LONG YOU, CLAUDY SERRAO, SAIDUR BAKAUL, RAMAMOORTHY RAMESH, SAYEEF SALAHUD-DIN, University of California, Berkeley — The Boltzmann distribution of electrons poses a fundamental barrier to lowering energy dissipation in conventional electronics, often termed as Boltzmann Tyranny [1,2]. Negative capacitance in ferroelectric materials, which stems from the stored energy of phase transition, could provide a solution, but a direct proof of negative capacitance has so far been elusive. Here we demonstrate the negative differential capacitance in a thin, single crystalline ferroelectric film, by constructing a simple R-C network and monitoring the voltage dynamics across the ferroelectric capacitor. When a voltage pulse is applied, the voltage across the ferroelectric capacitor is found to be decreasing with time—in exactly the opposite direction to which voltage for a regular capacitor should change. The results are analyzed on the basis of the Landau-Khalatnikov equation, which shows that as the ferroelectric polarization switches its direction, it passes through the unstable negative capacitance region resulting in the characteristic “negative capacitance transients”. Analysis of this “inductance”-like behavior from a capacitor allows us to calculate the value of the negative capacitance directly and presents an unprecedented insight into the intrinsic energy profile of the ferroelectric material.


1:27PM B6.00010 Double hysteresis in BaTiO3/PbZr0.2Ti0.8O3 ferroelectric bilayer thin film , PAVEL SALEV, ALEXEI GRIGORIEV. The University of Tulsa — We observed two hysteresis loops in BaTiO3/PbZr0.2Ti0.8O3 (BTO/PZT) bilayer thin film. The first loop with polarization of 27 μC/cm2 was measured in the applied voltage of ±5V. The second hysteresis loop with polarization of 76 μC/cm2 was measured in the applied voltage of ±55V. Both hysteresis loops showed characteristic shape with concave region followed by saturation region in the broad range of applied voltage frequencies providing strong evidence for ferroelectric origin of both loops. We performed computational analysis of BTO/PZT bilayer based on Landau-Ginzburg-Devonshire model including contributions of electronic band structure. We found an increased concentration of free charge carriers at the interface between BTO and PZT which provides compensation for the bound charge due to polarization mismatch of the layers. Moreover, as the free charge effectively screens polarization in one layer from another, polarization switching of individual layers can be possible. This leads to the conclusion that two hysteresis loops can be a result of polarization switching of the individual layers.

1:39PM B6.00011 Ferroelectric Field Effect in Ultrathin Epitaxial Sm0.5Nd0.5NiO3 Films , LE ZHANG, H. JEFFREY GARDNER, VIJAY RAJ SINGH, XIA HONG, University of Nebraska - Lincoln — We report the study of ferroelectric field effect modulation of the metal-insulator transition in ultrathin Sm0.5Nd0.5NiO3 (SNO) films. We have fabricated high quality epitaxial SNO thin films and Pb(Zr,Ti)O3 (PZT)/SNO heterostructures on (001) LaAlO3 substrates using off-axis RF magnetron sputtering. X-ray diffraction and atomic force microscopy studies reveal (001) oriented films with high crystallinity and surface roughness of 3-4 Å. Thin SNO films (4-6 nm) typically have the transition temperature TMI around 230 K, showing thermally activated transport below TMI followed by 3D variable range hopping at low temperature. Hall effect measurements reveal p-type conduction with ~4 holes/uc in the metallic phase. Working with films one to two unit cells thicker than the electrical dead layer thickness (~4 nm), we have demonstrated nonvolatile, reversible ferroelectric field effect modulation of TMI in SNO by up to 10 K. The maximum resistance ratio Rhigh/Rlow is 1.7 at 140 K, which is in the thermally activated regime. In the metallic phase, the carrier density has been modulated by 1x1015 cm−2, corresponding to the polarization field of PZT of 80 μC/cm2.

1:51PM B6.00012 Electrical Properties of Tetragonal-PZT Thin Film Capacitors from 5 K to 300 K, D.R. DAUGHTON, Lake Shore Cryotronics, J.T. EVANS, S.P. CHAPMAN, Radiant Technologies, Inc — Rapid assessment of ferroelectric device characteristics is critical to improving ferroelectric materials processing as well as developing accurate ferroelectric device models. Here, we demonstrate automated electrical testing of thin PZT and Nb-doped PZT thin film devices at temperatures ranging from 300 K down to 5 K in a cryogenic probing environment. In this configuration, temperature-dependent dielectric constant, remanent polarization, coercive voltage, switching speed, and leakage are measured in a single pass on a single sample. From these measurements, it appears that tetragonal PZT does not have a phase boundary from room temperature down to 5 K. Retention tests conducted on several capacitors while transitioning from room temperature to 200 K, 100 K, and 6.5 K showed no loss of remnant polarization indicating 20/80 PZT and its niobium-doped cousins remain fully functional as memory devices down to 5 K.

2:03PM B6.00013 ABSTRACT WITHDRAWN

Monday, March 2, 2015 11:15AM - 2:15PM
Session B7 DMP DCMP: Focus Session: Majorana Fermions 006 -

11:15AM B7.00001 Engineering Majorana fermions in atomic chains with collinear magnetic order , PANAGIOTIS KOTETES, ANDREAS HEIMES, DANIEL MENDLER, GERD SCHÖN, Karlsruhe Institute of Technology — We propose new mechanisms for engineering Majorana fermions (MFs) based on atomic chains with collinear magnetic order, on top of a conventional superconductor. For antiferromagnetic ordering, we show [1] that a weak Zeeman field and a supercurrent convert the preexisting topologically-protected Shiba states into MFs, without the requirement of Rashba spin-orbit coupling (SOC). Remarkably, the electronic spin-polarization of the arising edge MF wavefunctions depends solely on the parity of the number of magnetic moments, which can serve as a unique signature of the MFs. Instead, if Rashba SOC is present, both ferro- and anti-ferromagnetic orders can lead to topological phases which are reflected in the spatial profile of the MF wavefunctions. Our findings connect to the recent observations of MFs in atomic chains [3] and can open alternative routes for confirming the emergence of MFs. [1] A. Heimes, P. Kotetes, and G. Schö,PRB 90, 060507(R) (2014). [2] A. Heimes, D. Mendler, and P. Kotetes, arXiv:1410.6367. [3] S. Nadj-Perge et al., Science 346, 602 (2014).
11:27AM B7.00002 Majorana Fermions in Quantum Wires with Helical Magnetic Textures1, GEOFFREY FATIN, ALEX MATOS-ABIAIQUÉ, BENEDIKT SCHARF, IGOR ZUTIC, University at Buffalo - SUNY — Magnetic textures can lead to the formation of Majorana states in a quantum wire located nearby an s-wave superconductor [1-3]. We investigate theoretically the formation of Majorana fermions in quasi-one-dimensional quantum wires in the presence of different kinds of helical-like magnetic textures. Our calculations reveal that finite-size effects as well as non-trivial helical magnetic configurations can lead to the formation of multiple Majorana states. Under some specific conditions it is possible to localize some of the Majorana modes at certain points within the wire. The positions of these points can be controlled by properly tuning the system parameters. The conditions governing the transitions from the trivial to the topological state are found and the different Majorana modes are characterized according to their local spin polarization. The possibility of experimentally realizing the proposed models in actual physical systems is also discussed.


1This work has been supported by ONR Grant N000141310754.

11:39AM B7.00003 Interplay of Majorana and Kondo modes in an interacting quantum dot coupled to a topological quantum wire1, DAVID A. RUIZ-TIJERINA, Instituto de Física, Universidade de São Paulo, EDSON VERNEK, Instituto de Física, Universidade Federal de Uberlândia, LUIS G. V. DIAS DA SILVA, Instituto de Física, Universidade de São Paulo, J. CARLOS EGUES, Instituto de Física de São Carlos, Universidade de São Paulo — We investigate the low-temperature conductance of an interacting quantum dot (QD) coupled to a topological quantum wire. Our realistic model includes the Rashba spin-orbit interaction, proximity s-wave superconductivity, an applied magnetic field, and an Anderson-type interacting QD. Using recursive Green’s function techniques we find a QD conductance of $0.5e^2/h$, associated with the emergent Majorana end mode in the wire “leaking” into the QD. This signature is robust, appearing in the presence of Zeeman fields and even when the QD is deep in the Coulomb blockade. We further study the Kondo regime using the numerical renormalization group. Our results indicate a strong interplay between Majorana & Kondo physics. The Kondo effect can be quenched by Zeeman fields, revealing a persistent $0.5e^2/h$ conductance coming from the Majorana mode leaking into the QD. These properties can be used for the experimental identification of Majorana-Kondo physics in these systems. Our results here corroborate and extend those of Phys. Rev. B 89, 165314 (2013) by showing that the Majorana resonance pinned to the Fermi level arising in the QD is robust and survives even in the presence of Coulomb effects within the QD.

1Supported by: CNPq, CAPES, FAPERJ, PRP/USP and FAPEMIG.

11:51AM B7.00004 Topological superconductivity and Majorana fermions in chains of magnetic atoms on the surface of a superconductor1, ALI YAZDANI, Princeton University — Chain of magnetic atoms on the surface of a BCS superconductor is a versatile platform for the realization of one-dimensional superconductors with Majorana bound states that lends itself to high-resolution scanning tunneling microscopy studies [1,2]. In this talk, I will describe experimental efforts to realize this platform using self-assembled chains of Fe atoms on the surface of Pb (110) and to directly visualize Majorana quasi-particle bound states at their edges [2]. Using spin-polarized STM studies, we show that Fe chains are ferromagnetic while tunneling into Pb’s substrate demonstrates signatures of strong spin-orbit interaction at its surface. Comparison of experimental measurements of structure and normal state electronic structure with DFT calculations suggest that these are triple zigzag chains with an odd number of band-crossings at the Fermi level. The onset of superconductivity in the Pb strongly modifies the low energy density of states of the Fe chains and induces a zero energy state at their ends. I will describe how these observations are consistent with the formation of a topological superconducting phase with Majorana edge states.


1Work supported by ONR, NSF-DMR, NSF-MRSEC, ARO-MURI, and LPS-ARO grants.

12:27PM B7.00005 Topological phase transitions of interacting Majorana fermions in an array of vortices, JIANSHENG WU, South University of Science and Technology of China, Shenzhen, China, HSIANG-HSUAN HUNG, University of Texas at Austin, Austin, Texas 78712-1192, USA, CHING-KAI CHIU, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z1, KUIE SUN, The University of Texas at Dallas, Richardson, Texas 75080-3021, USA — We study a vortex array in a p-wave superconducting thin film that produces ladder-like lattices with interacting Majorana fermions. We construct a model Hamiltonian with parameters which are tunable via the deformation of the vortex array. We explore topological phase transitions of the system and compute phase diagrams using the density-matrix-renormalization-group method. We further investigate transport properties for experimental detection. Our results have potential application on building devices to engineer strongly correlated Majorana fermions.

12:39PM B7.00006 Majorana Fermions in Chiral Topological Ferromagnetic Nanowires1, EUGEN DUMITRESCU, BRENDBEN ROBERTS2, SUMANTA TEWARI, Clemson University, JAY D. SAU, University of Maryland — Motivated by a recent experiment in which zero-bias peaks have been observed in STM experiments performed on chains of magnetic atoms on a superconductor, we show that a multichannel ferromagnetic wire deposited on a spin-orbit coupled superconducting substrate can realize a non-trivial chiral topological superconducting state with Majorana bound states localized at the wire ends. The non-trivial topological state occurs for generic parameters requiring no fine tuning, at least for very large exchange spin splitting in the wire. We theoretically obtain the signatures which appear in the presence of an arbitrary number of Majorana modes in multi-wire systems incorporating the role of finite temperature, finite potential barrier at the STI tip, and finite wire length. These signatures are presented in terms of spatial profiles of STI differential conductance which clearly reveal zero energy Majorana end modes and the prediction of a multiple Majorana based fractional Josephson effect.

1Co-author: S. Das Sarma. Work supported by AFOSR (FA9550-13-1- 0045) at Clemson University and by LPS-CMTC and JQI-NSF-PFC at the University of Maryland
2Now at California Institute of Technology

12:51PM B7.00007 ABSTRACT WITHDRAWN —
1:03PM B7.00008 Majorana bound states without topological superconductivity, PABLO SAN-JOSE, JORGE CAYAO, Consejo Superior de Investigaciones Científicas (CSIC) - Spain, ELSA PRADA, Universidad Autónoma de Madrid (UAM) - Spain, RAMÓN AGUADO, Consejo Superior de Investigaciones Científicas (CSIC) - Spain — Recent experimental efforts towards the detection of Majorana bound states have focused on creating the conditions for topological superconductivity. Here we demonstrate an alternative route, which achieves fully localised zero-energy Majorana bound states when a topologically trivial superconductor is opened to a normal region. The emergence of Majorana states is a consequence of non-hermitian degeneracies of the resulting open quantum system, while arbitrarily large Majorana lifetimes follow from high junction transparency and helicity of the normal side. At these degeneracies, also known as “exceptional points,” both the eigenvalues and the eigenstates coalesce, and acquire Majorana properties (zero-energy, self-conjugation, 1r-periodic braiding...) despite the trivial band topology. Exceptional Majoranas are thus the open-system counterparts of conventional Majorana bound states, to which they are continuously connected, and exhibit all their phenomenology while not requiring topological superconductivity.

1:15PM B7.00009 Disorder-induced phase transitions in a quasi 1-D Majorana wire, MARIA-THERESA RIEDER, PIET W. BROUWER, Freie Universität Berlin, JINANC ADADIGELI, Sabanci University, Istanbul — In a strictly 1D spinless p-wave superconductor, disorder is known to induce a phase transition between a topologically nontrivial phase and a trivial insulating phase when the mean free path l becomes of the order of the superconducting coherence length ξ. We show that, in constrast, a multichannel spinless p-wave superconductor goes through a series of phase transitions alternating between topologically trivial and nontrivial phases upon increasing the disorder strength. The number of phase transitions equals the channel number N and each phase transition is accompanied by a Dyson singularity in the density of states v(ε) ∝ ε−1/2. The observed behavior is the result of an effective chiral symmetry allowing us to analytically investigate the phase boundaries and the density of states. The latter displays a power-law singularity v(ε) ∝ εα−1 for small energies ε away from the critical points. Using the concept of “superuniversality,” we relate the exponent α to the wire’s transport properties at zero energy and, hence, to the mean free path and the superconducting coherence length.

1:27PM B7.00010 Parity crossings of Shiba states and Majorana-like zero bias anomalies in hybrid superconductor-normal nanowire systems with quantum dot behavior, RAMON AGUADO, CSIC - Madrid, ROK ZITIKO, Jozef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia, ROSA LOPEZ, IFISC (UIB-CSIC), Palma de Mallorca, Spain, JONG SOO LIM, School of Physics, Korea Institute for Advanced Study, Seoul, Korea. — Although recent experiments with semiconducting nanowires are partially consistent with the existence of Majorana bound states (MBS) at normal-superconductor junctions, other mechanisms cannot be completely ruled out. In this talk, I will focus on short nanowires with quantum dot behavior and discuss the magnetic field dependence of Shiba states [1] as well as novel Kondo features induced by the weak coupling to a normal lead [2]. Our results are based on the phase diagram of an Anderson impurity in contact with superconducting and normal-state leads. This phase diagram is obtained by means of the numerical renormalization group technique and is valid for arbitrary ratio of the superconducting gap to the Kondo temperature. Overall, we find a very rich behavior of spectral functions with zero-bias anomalies which can emerge irrespective of whether the ground state is a doubllet or a singlet. This phenomenon originates from crossings of the ground state fermionic parity and mimics that of MBS. [1] E. J. H. Lee, X. Jiang, M. Houzet, R. Aguado, C. M. Lieber, and S. De Franceschi, Nature Nanotechnology, 9, 79 (2014). [2] R. Zitko, J. S. Lim, R. Lopez and R. Aguado, arXiv:1405.6084 (2014).

1:39PM B7.00011 Helical Majorana surface states of strongly disordered topological superconductors with time-reversal symmetry, RAQUEL QUEIROZ, ANDREAS SCHNYDER, Max Planck Institute for Solid State Physics — Noncentrosymmetric superconductors with strong spin-orbit coupling and the B phase of 3He are possible realizations of topological superconductors with time-reversal symmetry. The nontrivial topology manifests itself at the material’s surface in terms of linearly dispersive helical Majorana modes protected by symmetry from disorder weaker than the superconducting gap. Using extensive numerical simulations, we investigate the stability and properties of these Majorana states under strong disorder, which influences both bulk and surface states. A critical crossover from weak to strong disorder is observed in both two and three dimensions, through which an extended state exactly at zero energy always persists. The localization properties of the ingap states are studied through the distribution of the local density of states and level repulsion statistics.

1:51PM B7.00012 Floquet Majorana Modes in Graphene Quantum Dots, YANTAO LI, Sun Yat-sen Univ. & Indiana Univ - Bloomington, ARJIT KUNDU, BABA SERADJHEH, Indiana Univ - Bloomington — We propose a possible way to realize Floquet Majorana fermions in graphene quantum dots connected by a superconducting island. The effective crossed Andreev reflection and hopping amplitudes between the dots are calculated as a function of system parameters. It is shown that the spin degeneracy is broken when the dots are driven out of phase. This all-electric, highly tunable device could be a realistic platform for uncovering dynamically generated Majorana fermions in graphene systems.

2:03PM B7.00013 Exploring signatures of Majorana fermions in Fe chains on Pb using a dilution refrigerator scanning tunneling microscope, BENJAMIN E. FELDMAN, ILYA K. DROZDOV, MALLIKA T. RANDERIA, JIAN LI, B. ANDREI BERNEVIG, ALI YAZDANI, Princeton University — Recently, it was shown that Majorana fermions can be realized by depositing chains of magnetic atoms on a superconductor if the spins are non-colinear or if they are ferromagnetic and subject to large spin-orbit coupling. Scanning tunneling microscopy (STM) studies of Fe chains on a Pb(110) surface revealed zero-energy states localized to the ends, and a spin-polarized tip was used to show ferromagnetism in the chains as well as spin-orbit coupling on the Pb surface, providing strong evidence for Majorana fermions. These measurements were performed at 1.4 K, and the width of the zero-energy mode was limited by thermal broadening. In this talk, I will present subsequent measurements in which we extend these results to temperatures below 250 mK using a dilution refrigerator STM. The low temperature allows us to obtain significantly higher energy resolution, and I will discuss our results in the context of Majorana fermions.

Monday, March 2, 2015 11:15AM - 2:15PM
Session B8 DCMP: From Single Molecules to Molecular Assemblies on Surfaces

11:15AM B8.00001 Long Range Modification of a Metal Surface Electronic Structure by an Organic Semiconductor, JINGYING WANG, DANIEL DOUGHERTY, North Carolina State Univ — In an organic spintron device the interaction between electrode surface and organic semiconductor layer plays an important role in spin injection at this interface. The antiferromagnetic material Cr(001) is known to have a spin-polarized state near Fermi level that could potentially hybridize with organic molecules. Here we report our STM/STS study of electronic structure at interface between an organic semiconductor, PTCDA, and Cr(001) surface. The study shows that the surface state at Fermi level of Cr(001) can be broadened by PTCDA molecules deposited on the surface due to hybridization of PTCDA molecular orbital and conduction sp band of Cr(001). This indirect modification is not only localized at molecular adsorption sites, but also extends several nm to bare surrounding Cr(001) surface and decays with distance away from PTCDA molecules.
11:27 AM B8.00002 Accurate Energy Level Alignment at Physisorbed Molecule-Metal Interfaces from a Density Functional Theory-Based Approach, DAVID A. EGGER, Weizmann Institute of Science, ZHENFEI LIU, Molecular Foundry, Lawrence Berkeley National Laboratory, JEFFREY B. NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, and Department of Physics, UC-Berkeley, LEEROR KRONIK, Weizmann Institute of Science — A highly relevant physical quantity for nanostructured molecule-metal interfaces is the energy level alignment of the molecular electronic states with respect to the Fermi level of the metal. Here, we introduce an efficient theoretical method that is based on density functional theory, but in contrast to common approximations fulfills physically motivated criteria for exchange-correlation interactions and can therefore yield quantitatively accurate energy level alignment information for physisorbed metal-molecule interfaces. We validate our approach by a detailed comparison with experimental and theoretical reference data for several prototypical interfaces of this kind: benzene on graphite (0001), and 1,4-benzenediamine, Cu-phthalocyanine, and 3,4,9,10-perylene-tetracarboxylic-dianhydride on Au(111). Our results indicate that obtaining quantitatively accurate energy level alignment information from density functional theory is possible.

11:39 AM B8.00003 Rethinking chemisorption: New insights into the factors controlling the binding energy1, MARISOL ALCANTARA ORTIGOZA, SERGEY STOLBOV, University of Central Florida — Chemisorption of atomic and molecular species on a substrate induces electronic redistribution upon which substrate nuclei respond by adjusting their positions. This lattice distortion has been linked to the binding energy $E_B$ of the adsorbed species and attributed to the so-called surface relaxation energy, $E_{rx}$. We have found, however, that for transition metals the energy associated with the mere charge redistribution $E_{elec}$ is much larger than $E_{rx}$ and thus both contributions must be considered [1]. In this work, we quantify the electronic and structural perturbation energy $E_P$ brought by various adsorbates on surfaces to understand anomalous adsorbate binding energies, i.e., those in which $E_B$ strongly influences the magnitude of $E_{rx}$. For example, for O adsorption on Au(111), while $E_{rx}$ is only 0.25 eV, the overall perturbation energy $E_P$ affecting $E(B,O) \sim 1$ eV [1]. This indicates that $E_P$ cannot be ignored but also that local bonds may not be as weak as portrayed by $E_{elec}$, even though $E_B$ is significantly reduced. We expose cases in which $E_P$ is really dominated by the lattice distortion energy, as well as a rationale for its trends as a function of the substrate and adsorbate. We discuss the implications of the fact that $E_B$ is not always predominately controlled by the bond-strength on heterogeneous catalysis, as well as the applications of the same fact. M. Alcántara Ortigoza and S. Stolbov; “The Perturbation Energy: The missing key to understand gold ‘nobleness.’” Submitted in October 2014

1 This work was supported the NSF under Grant CBET-1249134.

11:51 AM B8.00004 ABSTRACT WITHDRAWN

12:03 PM B8.00005 Surface-Mediated Self-Assembly Controlled by Interfacial Charge-Transfer1, OLIVER MONTI, NAHID ILYAS, BRET MAUGHAN, Univ of Arizona, PERCY ZAHL, ROCIO CORTES-RODRIGUEZ, PETER SUTTER, Brookhaven National Laboratory — Precise control of molecular self-assembly is desirable and essential to understand electronic structure and dynamics at organic semiconductor interfaces. Self-assembly into ordered supramolecular structures for such pi-conjugated molecules is determined by a subtle balance between surface-molecule and molecule-molecule interactions, and a predictive mechanistic understanding has remained a substantial challenge for most commonly used organic semiconductors. Here we show by a combination of low-temperature scanning tunneling microscopy and two-photon photoemission spectroscopy for the model system of chloro-boron subphthalocyanine on Cu(111) that interfacial charge-transfer results in fundamentally different self-assembly mechanisms for different molecular orientations on the surface. We uncover a novel mechanism that controls thin film growth for an important class of organic semiconductors. We conclude that the adsorption geometry may be exploited in self-assembly to control electronic structure and dynamics at organic semiconductor interfaces.

1 NSF CHE-1213243 and DOE DE-AC02-98CH10886

12:15 PM B8.00006 Photo-Activation of Single Molecules and Assemblies on Au{111}, YUXI ZHAO, MOONHEE KIM, NATCHA WATTANATORN, Department of Chemistry and Biochemistry, University of California, Los Angeles, JEFFREY SCHWARTZ, Department of Physics & Astronomy, University of California, Los Angeles, HONG MA, ALEX JEN, Department of Materials Science and Engineering, University of Washington, PAUL WEISS, Department of Chemistry and Biochemistry, University of California, Los Angeles — Understanding electron transfer at the molecule-surface interface is critical to the rational design and improvement of organic optoelectronics and photovoltaics. The behavior of photoactive molecules depends critically on their local environment and defects present in the surface. Here, we use a custom-built, laser-assisted scanning tunneling microscope to probe the photocurrent of isolated anthracene derivates on Au(111). The photocurrent originates from charge-transfer transitions of anthracene into an excited state when illuminated by an evanescent field. The influence of the image potential states on terraces and at defects in the gold surface on photo-induced charge transfer will be discussed.

12:27 PM B8.00007 Anchoring and Bending of Pentacene on Aluminum (001), GUIDO FRATESI, ETSF, CNISM, Dip. di Fisica, Università di Milano, Via Celoria 16, I-20133 Milano, Italy, and Dip. di Scienza dei Materiali, Milano-Bicocca, ANU BABY, Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Via Cozzi 55, I-20125 Milano, Italy, SHITAL R. VAIDYA, LAERTE E. PATERA, CNR-IOM, Lab TASC, Dep. of Physics, and Grad. School of Nanotechnology, Univ. of Trieste, Via Valerio 2, I-34127 Trieste, Italy, CRISTINA AFRICH, LUCA FLOREANO, CNR-IOM, Laboratorio TASC, Basovizza SS-14, Km 163.5, I-34149 Trieste, Italy, CRISTINA AFRICH, LUCA FLOREANO, CNR-IOM, Laboratorio TASC, Basovizza SS-14, Km 163.5, I-34149 Trieste, Italy — We study the structural, electronic, and spectroscopic properties of pentacene adsorbed on Al(001) surface, combining density functional theory (DFT) methods including van der Waals interactions with x-ray photoemission spectroscopy (XPS), near-edge x-ray absorption fine structure (NEXAFS), and scanning tunneling microscopy (STM). We find a major change of the molecular backbone resulting into a peculiar V-shape conformation, as driven by the link of the central carbon atoms of pentacene to a pair of slightly displaced Al atoms. Remarkably, V-shape bending, due to the direct anchoring of the two central carbons atop two Al atoms underneath. In the most stable adsorption configuration, pentacene V-shape conformation, as driven by the link of the central carbon atoms of pentacene to a pair of slightly displaced Al atoms.

12:39 PM B8.00008 Pentacene thin films on flat and vicinal Au(111) surfaces, M. FATIH DANIMAN, Middle East Technical University, ERSEN METE, Balikesir University, EROL ALBAYRAK, Ahi Evran University — Here we present a structural study of pentacene thin films on flat and vicinal Au(111) surfaces by He atom diffraction measurements and dispersion corrected density functional theory (DFT) calculations. Though experimentally investigated parameter space was limited, no significant difference between the films prepared by different deposition energies was observed. Completion of monolayer coverage was confirmed by simultaneous helium scattering and quartz crystal resonance frequency shift measurements during pentacene film growth on the gold electrode of a quartz resonator. Monolayer films were found to adopt a (6x3) unit cell which was also observed for pentacene monolayers on Ag(1 1 1). However no ordered multilayer film structure could be observed which is in contrast with the previous Ag(1 1 1) studies. DFT calculations were performed with and without dispersion correction. Adsorption site of isolated pentacene molecules, crystal and electronic structure of monolayers and multilayers (up to 4 ML) were studied. The most stable monolayer structure was found to be the (6x3) unit cell in agreement with the experimental findings.
Conducted at Oak Ridge National Laboratory is sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. DOE.

Molecular ordering and orientation at the hetero-interface with the silicon substrate to be tuned accordingly. This mechanism provides new control over the development of organic and molecular electronics. Combining scanning tunneling microscopy and density functional theory, we show that by appropriately extending the site preferences of benzenes substituted with various activating and deactivating functional groups has been explored.

Choosing the coordinated transition-metal ion in metal phthalocyanine, the strength of the molecule-substrate interaction can be tailored, allowing for the substrates can lead to desired transport properties such as charge transfer, charge injection, exciton diffusion, etc., at the hetero-interface, which is crucial to understanding of the structure of such interfaces can potentially guide nanoscale modifications for improved electrical transport and energy-conversion efficiency in future devices.

1:03PM B8.00010 Layer resolved evolution of α-sexithiophene films: Correlation between PEEM and optical reflectance, EBRAHIM GHANBARI, THORSTEN WAGNER, PETER ZEPPENFELD, Johannes Kepler university — α-sexithiophene (α-6T) is a well-known organic dye pigment which represents a model system to study the photo-physical properties of π-conjugated molecules. We apply a combination of Differential Reflectance Spectroscopy (DRS) and Photo Electron Emission Microscopy (PEEM) to follow the growth of α-6T on Cu(111) surfaces in real time. The deposition of the molecules changes the density of states at the surface as well as the actual photoelectron emission barrier. Therefore, the lateral variation of the electron yield can be used to follow the growth of layers and 3D crystallites. Upon opening of the shutter, the PEEM intensity rises uniformly across the entire field of view (145 µm) until the first layer is closed. The following drop of the electron yield is terminated when the wetting layer is completed and the nucleation of 3D islands sets in. The DRS and the PEEM are synchronized and both signals are recorded simultaneously. The evolution of different features in the normalized differential optical reflectance can be attributed to the formation of the first layer, the second layer, the nucleation and growth of 3D crystallites. Therefore, we can make a direct correlation between the PEEM and the transients of the spectral reflectance.

1:15PM B8.00011 Spatially-resolved molecular Quantum Dots at the Surface of a Gated Graphene Device, HSIN-ZON TSAI, SEBASTIAN WICKENBURG, UC Berkeley physics/ LBNL, JIONG LU, UC Berkeley physics/ NUS Graphene Research Centre, ARASH A. OMRAI, SINISA COH, HAN SAE JUNG, DILLON WONG, JOHANNES LISCHNER, RAMIN KAHEJ, UC Berkeley physics, ALEXANDER RISS, UC Berkeley physics/ TU Wien applied physics, AARON J. BRADLEY, UC Berkeley physics, ERIK PIATTI, Politecnico di Torino DI SAT, ALEX ZETTL, STEVEN G. LOUIE, MARVIN L. COHEN, MICHAEL F. CROMMIE, UC Berkeley physics/ LBNL MSD — The ability to modify the electronic properties of monolayer graphene via charge-donating or charge-accepting molecules creates new opportunities for fabricating nano-scale hybrid devices. Understanding the charge transfer process at the single molecule level is essential for tuning the electronic and magnetic characteristics of such hybrid devices. We have used scanning tunneling microscopy (STM) to locally probe how different molecular assemblies (including single molecules, molecular chains, and 2D molecular islands) exchange charge with a graphene substrate as the device backgate voltage is varied. Different molecular configurations exhibit substantially different charging behavior - some are permanently charged while others can be controllably ionized using the device backgate. Electrostatic interactions lead to charge heterogeneity at the molecular level. Single-chemical-bond-resolved atomic force microscopy allows us to correlate chemical structure and adsorption geometry of the molecules with their electronic properties.

1:27PM B8.00012 Tailored Organic Molecular Growth on Silicon Studied by STM and DFT*, SEAN WAGNER, Michigan State University, BING HUANG, CHANGWON PARK, Oak Ridge National Laboratory, JIAJUI FENG, Michigan State University, MINA YOON, Oak Ridge National Laboratory, PENGPENG ZHANG, Michigan State University — Control of highly ordered organic molecular thin films with extended π systems is currently of intense interest for integrating molecules into modern electronics due to their tunable nature. Selection of molecules and substrates can lead to desired transport properties such as charge transfer, charge injection, exciton diffusion, etc., at the hetero-interface, which is crucial to the development of organic and molecular electronics. Combining scanning tunneling microscopy and density functional theory, we show that by appropriately choosing the coordinated transition-metal ion in metal phthalocyanine, the strength of the molecule-substrate interaction can be tailored, allowing for the molecular ordering and orientation at the hetero-interface with the silicon substrate to be tuned accordingly. This mechanism provides new control over the deliberately balanced molecule-substrate and intermolecular interactions, opening a route towards well-ordered molecular organic growth. *Experimental work is funded by the U.S. DOE Office of Science Early Career Research Program (DE-SC0006400) through the Office of Basic Energy Sciences. Theory work conducted at Oak Ridge National Laboratory is sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. DOE.

1:39PM B8.00013 Bonding at the Metal-Organic Interface, EVA ZUREK, University at Buffalo, SUNY — We present the results of density functional theory calculations that account for dispersion, which systematically study the perturbations of the electronic structure of various organic molecules physisorbed or weakly chemisorbed to the (111) surfaces of the coinage metal surfaces copper, silver and gold. The molecules considered include: benzene, substituted benzenes, 4-fluorostyrene, tetr phenyl porphyrin, a quinonoid zwitterion, croconic acid and rhodzonic acid. We have employed a frontier orbital perspective to analyze the bonding between the substrate and the adsorbate, studied the charge redistribution at the organic-metal interface, and analyzed how this affects the self-assembly. Our theoretical studies have helped to explain the experimental observations of STM (scanning tunneling microscopy) groups by showing that: tetr phenyl-porphyrin forms attractive networks on the Ag(111) surface and repulsive ones on Cu(111) because of the larger amount of charge transfer on Cu(111); the 10 D dipole of a quinonoid zwitterion changes substantially upon adsorption to the coinage metal surfaces Cu(111), Ag(111) and Au(111) as a result of donation of charge from the molecular HOMO to the surface and back donation to the LUMO; the charge transfer which occurs between the quinonoid zwitterion and Au(111) has been studied as a function of surface coverage; 4-fluorostyrene molecules form clusters of “magic” sizes that depend on the metal surface and can be understood in terms of a balance between attractive H-bonding and van der Waals interactions as well as Coulomb repulsion between the molecules; the topological organic ferroelectric molecule croconic acid forms chiral honeycomb networks on the Ag(111) surface. Moreover, our calculations have illustrated that classic activating groups generally increase and prototypical deactivating groups decrease the amount and direction of charge transferred from a substituted benzene derivative to the Cu(111) and Ag(111) surfaces. The effect of functionalization on the binding site preferences of benzenes substituted with various activating and deactivating functional groups has been explored.

1:39 PM B8.00013 Bonding at the Metal-Organic Interface, EVA ZUREK, University at Buffalo, SUNY — We present the results of density functional theory calculations that account for dispersion, which systematically study the perturbations of the electronic structure of various organic molecules physisorbed or weakly chemisorbed to the (111) surfaces of the coinage metal surfaces copper, silver and gold. The molecules considered include: benzene, substituted benzenes, 4-fluorostyrene, tetr phenyl porphyrin, a quinonoid zwitterion, croconic acid and rhodzonic acid. We have employed a frontier orbital perspective to analyze the bonding between the substrate and the adsorbate, studied the charge redistribution at the organic-metal interface, and analyzed how this affects the self-assembly. Our theoretical studies have helped to explain the experimental observations of STM (scanning tunneling microscopy) groups by showing that: tetr phenyl-porphyrin forms attractive networks on the Ag(111) surface and repulsive ones on Cu(111) because of the larger amount of charge transfer on Cu(111); the 10 D dipole of a quinonoid zwitterion changes substantially upon adsorption to the coinage metal surfaces Cu(111), Ag(111) and Au(111) as a result of donation of charge from the molecular HOMO to the surface and back donation to the LUMO; the charge transfer which occurs between the quinonoid zwitterion and Au(111) has been studied as a function of surface coverage; 4-fluorostyrene molecules form clusters of “magic” sizes that depend on the metal surface and can be understood in terms of a balance between attractive H-bonding and van der Waals interactions as well as Coulomb repulsion between the molecules; the topological organic ferroelectric molecule croconic acid forms chiral honeycomb networks on the Ag(111) surface. Moreover, our calculations have illustrated that classic activating groups generally increase and prototypical deactivating groups decrease the amount and direction of charge transferred from a substituted benzene derivative to the Cu(111) and Ag(111) surfaces. The effect of functionalization on the binding site preferences of benzenes substituted with various activating and deactivating functional groups has been explored.

11:15AM B9.00001 Evidence for phononic pairing in extremely overdoped “pure” d-wave superconductor Bi2212, YU HE, Department of Applied Physics, Stanford University, Stanford, CA, MAKOTO HISHIMOTO, Stanford Synchrotron Radiation Lightsource, SLAC, CA, DONGJOON SONG, HIROSHI EISAKI, AIST, Japan, ZHI-XUN SHEN, Department of Applied Physics, Stanford University, Stanford, CA — Recent advancement in High Tc cuprate superconductor research has elucidated strong interaction between superconductivity and competing orders. Therefore, the mechanism behind the ‘pure’ d-wave superconducting behavior becomes the next stepping stone to further the understanding. We have performed photoemission study on extremely overdoped Bi2212 single crystal synthesized via high pressure method. In this regime, we demonstrate the much reduced superconducting gap and the absence of pseudogap. Clear gap shifted bosonic mode coupling is observed throughout the entire Brillouin zone. Via full Eliashberg treatment, we find the electron-phonon coupling strength capable of producing a transition temperature very close to Tc. This strongly implies bosonic contribution to cuprate’s superconductivity’s pairing glue.

11:27AM B9.00002 Spectral moment sum rules for electron-phonon coupled superconductors in equilibrium and nonequilibrium, KHADIJEH NAJAFI, JAMES FREERICKS, Georgetown University — Recent developments in high-resolution time- and angle-resolved photoemission spectroscopy (trARPES) has opened a new path to study the dynamics of quantum materials in nonequilibrium. Several experimental studies have used trARPES to characterize the dynamics of the energy gap in superconductors. One experiment from the Lanzara group indicates that the fluence dependence of the photoemission signal is consistent with a weakening of the electron-phonon coupling in the superconducting state that increases with increasing fluence. The normal state sum rules shows that the integrated spectral weight in the normal state is constant if the phonon fluctuations are unchanged. Here we discuss the extension of these sum rules to the superconducting state.

11:39AM B9.00003 RIXS Study on the Doping Dependence of Elementary Excitations across AFM-SC Phase Boundary in Electron-doped Cuprates1, WEI-SHENG LEE, SIMON GERBER, SLAC National Accelerator Lab., USA, Y. B. HUANG, Paul Scherrer Institut, Switzerland, GUICHUAN YU, University of Minnesota, USA, BRIAN MORTIZ, SLAC National Accelerator Lab., USA, H. Y. HUANG, R. P. WANG, W. B. WU, NSRRC, Taiwan, V. N. STROCov, Paul Scherrer Institut, Switzerland, E. M. MOTOYAMA, Stanford University, USA, C. T. CHEN, D. J. HUANG, NSRRC, Taiwan, MARTIN GREVEN, THORSTEN SCHMITT, University of Minnesota, USA, Z. X. SHEN, T. P. DEVEREAUX, SLAC National Accelerator Lab., USA — Tracking the doping dependence of elementary excitations in cuprates is an important approach to gain further insight into the high temperature superconductivity. Recently, RIXS measurements have revealed two surprising behaviors in the electron-doped cuprates: (i) the bandwidth of magnetic excitation increases, and (ii) an unexpected branch of collective modes emanating from the zone center was found in superconducting compounds, indicating the existence of a quantum phase distinct from superconductivity. Yet, a detailed doping dependence study of these two behaviors in the phase diagram, especially near the antiferromagnetic-superconductivity phase boundary, is still lacking. Here we report RIXS measurements on electron-doped cuprates, Nd$_{2-x}$Ce$_x$CuO$_4$. Doping dependence of magnetic and these zone-center excitations will be presented.

1  This work is supported by the SLAC LDRD program.

11:51AM B9.00004 Terahertz nano-spectroscopy and imaging of superfluid surface plasmons in conventional and anisotropic superconductors, H. T. STINSON, J. S. WU, B. Y. JIANG, Z. FEI, University of California San Diego, A. S. RODIN, Boston University, B. CHAPLER, A. S. MCLEOD, University of California San Diego, A. CASTRO NETO, National University of Singapore, Y. S. LEE, Soongsil University, M. M. FOGLER, D. N. BASOV, University of California San Diego, H. T. STINSON, J. S. WU, B. Y. JIANG, Z. FEI, University of California San Diego — We numerically model terahertz plasmonics experiments on conventional and unconventional superconductors in the infrared and terahertz regime. Our modeling shows that near-field spectroscopy can measure the magnitude of the superconducting gap in Bardeen-Cooper-Schrieffer superconductors with nanoscale spatial resolution. We demonstrate how the same technique can measure the c-axis plasma frequency, and thus the c-axis superfluid density, of layered unconventional superconductors such as cuprates and pnictides with identical spatial resolution. We discuss the development of a cryogenic terahertz near-field microscope designed to perform these proposed experiments.

12:03PM B9.00005 The fate of quasiparticles in the superconducting state, S.V. DORDEVIC, The University of Akron, D. VAN DER MAREL, Universite de Geneve, Switzerland, C.C. HOMES, Brookhaven National Laboratory — Quasiparticle properties in the superconducting state are masked by the superfluid and are not directly accessible to infrared spectroscopy. We show how one can use a Kramer-Kronig transformation to separate the quasiparticle from superfluid response and extract intrinsic quasiparticle properties in the superconducting state. We also address the issue of a narrow quasiparticle peak observed in microwave measurements, and demonstrate how it can be combined with infrared measurements to obtain unified picture of electrodynamics properties of cuprate superconductors.

12:15PM B9.00006 Broken time reversal symmetry states in superconductors using the ultrafast pump-probe method, CHANDAN SETTY, JIANGPING HU, Purdue Univ — The excitation of vibrational modes by ultrafast optical pulses can be a useful probe of the electronic ground state in a solid through the electron-phonon interactions. In this work, we show that the phase of the oscillations of reflectivity/transmissivity as a function of the delay time can contain signatures of broken time reversal symmetry (BTRS) in the superconducting ground state. To illustrate this, we consider a simple Hamiltonian consisting of a two band electronic part and a phononic part; additionally, we include terms which couple electrons to phonons and light. In the absence of dissipation, we show that entry into the BTRS superconducting state, the phase of the reflectivity oscillations deviates from the normal state values of $\pm \pi/2$ in a continuous fashion. We will also comment on the effects of dissipation and the dependence of our result on the opacity of the superconductor.

12:27PM B9.00007 Reduction of dissipative nonlinear conductivity of superconductors by static and microwave magnetic fields, ALEXANDER GUREVICH, Old Dominion University — A theory of dissipative nonlinear conductivity, $\sigma_1(\omega, H)$, of s-wave superconductors under strong electromagnetic fields at low temperatures and frequencies $\hbar \omega \ll k_B T$ is proposed. Closed-form expressions for $\sigma_1(H)$ and the surface resistance $R_s(\omega, H)$ are obtained in the nonequilibrium dirty limit for which $\sigma_1(H)$ has a significant minimum as a function of the amplitude of magnetic field $H$. The calculated microwave suppression of $R_s(\omega, H)$ is in good agreement with recent experiments on alloyed Nb resonator cavities. It is shown that superimposed dc and ac fields, $H = H_0 + H_0 \cos \omega t$, can be used to reduce dc dissipation in thin film nanostructures by tuning $\sigma_1(H_0)$ with the dc field, consistent with experiments performed in the sixties.

1Supported by DOE HEP under grant No. DE-SC0010081.
12:39PM B9.00008 The non-linear response of a superconductor to a few-cycle THz pulse\(^1\). G.L. CARR, XIAOXIANG XI\(^2\). Photon Sciences, Brookhaven National Laboratory — We present a time-domain analysis of the response of a BCS superconductor (in the low temperature limit) to a few cycle THz pulse whose spectral content may span the absorption threshold for pair breaking. The analysis is based on the finite-difference time-domain (FDTD) approach, in combination with a model susceptibility for a superconductor that includes an explicit dependence on the energy gap\(^1\). The FDTD approach allows us to calculate the THz induced current density, from which we determine the modified energy gap at each instant of time during the THz wave’s passage. The resulting non-linear susceptibility causes up-conversion of the incident THz wave into odd harmonics. The model results are compared with experiment for thin NbN films in both linear\(^2\) and non-linear\(^3\) regimes. [1] Xiaoxiang Xi and G.L. Carr, Supercon. Sci. & Technol. 26, 114001 (2013). [2] T. Hong et al., J. Appl. Phys. 114, 243905 (2013). [3] R. Matsunaga et al., Science 345, 1145 (2014).

\(^1\)Research supported by the U.S. Dept. of Energy under contract DE-AC02-98CH10886

\(^2\)Present address: Dept. of Physics, the Pennsylvania State University

12:51PM B9.00009 What does resonant inelastic x-ray scattering at the Cu L-edge measure? CHUNJING JIA, BRIAN MORITZ, THOMAS DEVEREAUX, Stanford Institute for Materials and Energy Sciences, SLAC National Laboratory and Stanford University, Menlo Park, CA 94025, USA, KRZYSZTOF WOHLFELD, 1) SLAC and Stanford University; 2) Institute of Theoretical Physics, University of Warsaw — Recent resonant inelastic x-ray scattering (RIXS) experiments at the transition metal L-edge of copper oxides suggest that this technique can be regarded as one of the best momentum-resolved probes of low energy excitations. However, the theoretical understanding of this technique remains incomplete \([1]\). Here we show, using both numerical studies and analytical approaches, which low energy excitations are probed by RIXS in both undoped and doped cuprates, as modeled by the Hubbard Hamiltonian. We conclude on a qualitative level that (i) RIXS is sensitive to the spin dynamical structure factor in the cross-polarized geometry, whereas (ii) RIXS is sensitive primarily to the \(A_{1g}\) projected charge dynamical structure factor, i.e. to both charge excitations and the two-spin excitations (including e.g. bimagrons) in the parallel scattering geometry. 

\([1]\) C. J. Jia et al., Nature Communications 5, 3314 (2014).

1:03PM B9.0010 Terahertz transient photoconductivity of insulating cuprates, J. STEVEN DODGE, JESSE PETERSEN, AMIR FARAHANI, DEREK SAHOTA, Simon Fraser University, RUIXING LIANG, University of British Columbia — We establish a detailed phenomenology of photoconductivity and transient THz transport in the copper oxide plane by studying the terahertz transient photoconductivity of \(\text{Sr}_2\text{CuO}_2\text{Cl}_2\) and \(\text{YBa}_2\text{Cu}_3\text{O}_6\). We observe a common dependence on time, fluence, and temperature. We infer an intrinsic photocarrier mobility from the peak photoconductivity, and show that this description fails. The pump-probe signal saturates at a characteristic fluence that depends on pump wavelength. In all three materials, the saturation fluence reaches a minimum at a pump photon energy 0.6 eV above the optical absorption peak associated with the charge transfer gap. We associate both the pump-probe spectrum and its saturation behavior with the thermalization of the initial photoexcitations, indicating a lack of interaction among photoexcitations. We observe a crossover with time, to a thermalized regime characterized by hopping conductivity with a low activation energy.

1:15PM B9.00011 Pump-probe excitation spectroscopy of insulating cuprates, DEREK SAHOTA, Department of Physics, Simon Fraser University, HANNA DABKOWSKA, Brockhouse Institute for Materials Research, McMaster University, GRAEME LUKE, Department of Physics and Astronomy, University of British Columbia, RUIXING LIANG, Department of Physics and Astronomy, University of British Columbia — We examine the transient optical response of optically thick single crystals of the Department of Physics and Astronomy, McMaster University, RUIXING LIANG, Department of Physics and Astronomy, University of British Columbia, J. STEVEN DODGE, Department of Physics, Simon Fraser University — We examine the transient optical response of optically thick single crystals of the insulating cuprates \(\text{La}_2\text{CuO}_4\), \(\text{YBa}_2\text{Cu}_3\text{O}_6\), and \(\text{Sr}_2\text{CuO}_2\text{Cl}_2\), as a function of probe wavelength, pump excitation wavelength, and pump fluence. At pump-probe time delay \(t > 1\) ps, the transient reflectance spectrum mimics a change in temperature, while for \(t < 1\) ps we observe a non-thermal response for which this description fails. The pump-probe signal saturates at a characteristic fluence that depends on pump wavelength. In all three materials, the saturation fluence reaches a minimum at a pump photon energy 0.6 eV above the optical absorption peak associated with the charge transfer gap. We associate both the pump-probe spectrum and its saturation behavior with the thermalization of the initial photoexcitations, and argue that the saturation spectrum indicates a relaxation bottleneck just above the charge transfer gap.

1:27PM B9.00012 Effect of pressure on the Fermi-surface reconstruction in the cuprate superconductor \(\text{YBa}_2\text{Cu}_3\text{O}_7\), SVEN BADOUX, OLIVIER CYR-CHONIERE, SOPHIE DUFOUR-BEAUSEJOUR, NICOLAS DOIRON-LEYRAUD, LOUIS TAILLEFER, University of Sherbrooke, Sherbrooke, Canada, DAVID VIGNOLLES, MARC NARODNE, CYRIL PROUST, LNCMI, Toulouse, France, DOUGLAS BONN, WALTER HARDY, RUIXING LIANG, University of British Columbia, Vancouver, Canada — Quantum oscillations and transport measurements have shown that the Fermi surface of cuprate superconductors undergoes a reconstruction near optimal doping \([1-5]\). It has recently become clear that charge-density-wave order and Fermi-surface reconstruction in the copper oxide plane by studying the terahertz transient photoconductivity of \(\text{Sr}_2\text{CuO}_2\text{Cl}_2\) and \(\text{YBa}_2\text{Cu}_3\text{O}_6\). We observe a common dependence on time, fluence, and temperature. We infer an intrinsic photocarrier mobility from the peak photoconductivity, and show that this description fails. The pump-probe signal saturates at a characteristic fluence that depends on pump wavelength. In all three materials, the saturation fluence reaches a minimum at a pump photon energy 0.6 eV above the optical absorption peak associated with the charge transfer gap. We associate both the pump-probe spectrum and its saturation behavior with the thermalization of the initial photoexcitations, and argue that the saturation spectrum indicates a relaxation bottleneck just above the charge transfer gap.

1:39PM B9.00013 Magnetic excitations in the superconducting and pseudogap states of the slightly underdoped high-temperature superconductor \(\text{HgBa}_2\text{CuO}_4+\delta\), MUN CHAN, Los Alamos National Laboratory, C. J. DOROW, Y. TANG, M. J. VEIT, Y. GE, M. GREVEN, University of Minnesota, L. MANGIN-THRO, Y. SIDIS, P. BOURGES, Laboratoire Léon Brillouin, France, X. ZHAO, Jilin University, China, D. L. ABERNATHY, Oak Ridge National Laboratory — We present an inelastic neutron scattering study of the magnetic excitations in slightly underdoped cuprate high-temperature superconductor \(\text{HgBa}_2\text{CuO}_4+\delta\) \((\text{Hg}2101, \rho=0.117, T_c = 88 \text{ K})\). Unlike more underdoped \(\text{Hg}1201\), the magnetic spectrum exhibits an X-shaped hourglass dispersion with an incommensurate low energy response and a clear resonance mode in the superconducting state. At temperatures above \(T_c\), the low energy incommensurate excitations disappear, replaced by a commensurate Y-shaped spectrum characteristic of the pseudogap state. The magnetic excitations become weaker with increasing temperature and are no longer discernable above the pseudogap temperature \(T^*\). The temperature evolution of the magnetic spectrum across \(T_c\) is consistent with models based on excitations of itinerant spins with a d-wave superconducting order parameter. Our work suggests that itinerant carriers should play an integral part for the understanding of the pseudogap state as well.

1:51PM B9.00014 Quasiparticle mass enhancement approaching optimal doping in \(\text{YBa}_2\text{Cu}_3\text{O}_6+\delta\) \(x\). BRAD RAMSHAW, Los Alamos National Laboratory, SUCHITRA SEBASTIAN, Cambridge University, ROSS MCDONALD, Los Alamos National Laboratory, JAMES DAY, University of British Columbia, BENG TAN, Cambridge University, ZENGWEI ZHU, JON BETTS, Los Alamos National Laboratory, RUIXING LIANG, DOUG BONN, WALTER HARDY, University of British Columbia, NEIL HARRISON, Los Alamos National Laboratory — Unconventional superconductivity is almost always found in proximity to other broken-symmetry states. The high-Tc cuprates exhibit a rich phase diagram that includes both spin and charge order. Previous quantum oscillation studies on \(\text{YBa}_2\text{Cu}_3\text{O}_6+\delta\) \(x\) have addressed how broken symmetry reconstructs the Fermi surface, but the evolution of the Fermi surface toward optimal doping was missing due to the high upper-critical fields. We use magnetic fields approaching 100 tesla to measure quantum oscillations in \(\text{YBa}_2\text{Cu}_3\text{O}_6+\delta\) \(x\) at three new doping levels with Tcs of 75, 81, and 91 K. We find that the quasiparticle effective mass is strongly enhanced approaching a hole doping of \(p=0.18\) — the same doping where experimental signatures of broken symmetry terminate and superconducting properties are enhanced. This is suggestive of a quantum critical point underlying the superconducting dome near optimal doping.
2:03PM B9.00015 Photo-induced Ultra-fast Carrier Dynamics in a Mott Insulator with Antiferromagnetic Long-range Order, SUMIO ISHIHARA, Department of Physics, Tohoku University, EIKI IVODA, Department of Basic Science, The University of Tokyo — We study transient dynamics of conduction carriers injected into a Mott insulator with antiferromagnetic long-range order, motivated from the recent optical pump-probe experiments in high-Tc superconductors. This is termed ?dynamical hole doping? in contrast to the chemical hole doping. The theoretical framework for the transient carrier dynamics is presented based on the two-dimensional t-J model [1]. The time dependencies of the optical conductivity spectra, as well as the one-particle excitation spectra, are calculated based on the Keldysh Green’s function formalism, associated with the self-consistent Born approximation. In the early stage, the Drude component only appears, and then incoherent components originating from hole-magnon scattering start to grow. Fast oscillatory behavior owing to coherent magnon and slow relaxation dynamics are confirmed in the spectra. The time profiles are interpreted as doped bare holes being dressed by magnon clouds and relaxed into spin polaron quasiparticle states. Implications for recent pump-probe experiments are discussed. [1] E. Iyoda, and S. Ishihara, Phys. Rev. B 89, 125126 (2014).

Monday, March 2, 2015 11:15AM - 2:15PM — Session B10 DCMP: Topological Insulators - Materials and Structures (Theory) 007A - Arijit Kundu, University of Indiana, Bloomington

11:15AM B10.00001 Numerical studies on the robustness of the topological surface modes of the topological insulator nanostructures, HSU-JUAN HSU, AJIT COIMBATORE BALRAM, JAINENDRA JAIN, CHAOXING LIU, The Pennsylvania State University, DEPARTMENT OF PHYSICS TEAM — It has been found experimentally that the magnetoconductance oscillates as a function of the magnetic flux with a period of $\phi_0$ ($\phi_0 = \hbar/e$, one flux quantum) in strongly disordered topological insulator (TI) nanotubes. In an effort to understand the origin of the oscillation, we calculate the magnetoconductance of TI nanowire and nanotube within the Landauer formalism at different disordered strengths and Fermi levels. We found unambiguous oscillation features of the magnetoconductance which survive even in extreme disordered regime. The oscillation is attributed to the occurrence of gapless helical surface modes when the surface encloses a magnetic flux of integer multiples of $\phi_0/2$. These features demonstrate a robust transport signature of the helical surface mode(s) of the TI nanostructures.

11:27AM B10.00002 Wire deconstructionism of two-dimensional topological phases1, RONNY THOMALE, Wuerzburg University, TITUS NEUFURT, Princeton University, CLAUDIO CHAMON, Boston University, CHRISTOPHER MUDRY, PSI Zurich — A scheme is proposed to construct integer and fractional topological quantum states of fermions in two spatial dimensions. We devise models for such states by coupling wires of non-chiral Luttinger liquids of electrons, that are arranged in a periodic array. Which inter-wire couplings are allowed is dictated by symmetry and the compatibility criterion that they can simultaneously acquire a finite expectation value, opening a spectral gap between the ground state(s) and all excited states in the bulk. First, with these criteria at hand, we reproduce the tenfold classification table of integer topological insulators, where their stability against interactions becomes immediately transparent in the Luttinger liquid description. Second, we construct an example of a strongly interacting fermionic topological phase of matter with short-range entanglement that lies outside of the tenfold classification. Third, we expand the table to long-range entangled topological phases with intrinsic topological order and fractional excitations.

1This work is supported by the European Research Council (ERC) through ERC-StG-Thomale-336012.


11:51AM B10.00004 Magnetic Susceptibility and Quantum Oscillations in a Buckled Honeycomb Lattice, CALVIN TABERT, University of Guelph, JULES CARBOTTE, McMaster University, ELISABETH NICOL, University of Guelph — We calculate the magnetic response of a low-buckled honeycomb lattice with intrinsic spin-orbit coupling which is described by the Kane-Mele Hamiltonian (a model which would describe the low-energy physics of a material like silicene). Included in the Hamiltonian, is a sublattice potential difference term which may be induced by a perpendicular electric field; this field can tune the system from a topological insulator (TI), through a valley-spin polarized metal, to a trivial band insulator (BI). In an external magnetic field, a distinct signature of the phase transition is seen in the derivative of the magnetization with respect to chemical potential; this gives the quantization of the Hall plateaus through the Streda relation. The results are compared with the zero-frequency conductivity obtained from the Kubo formula. The magnetic susceptibility also displays signatures of the different topological phases. We also explore the de-Haas van-Alphen effect. At the transition point between the TI and BI, magnetic oscillations exist for any value of chemical potential. Away from the critical point, the chemical potential must be larger than the minimum gap. For large chemical potential (or small but finite sublattice potential difference), there is a strong beating pattern.

12:03PM B10.00005 Properties of interacting 2D chiral tensor network states, BARRY BRADLYN, Yale University, JEROME DUBAIL, CNRS Nancy, NICHOLAS READ, Yale University — In a recent paper, Dubail and Read [1] gave a construction for free fermion tensor network states [2] (TNSs) in the chiral $p + ip$ and $\nu = 1$ Chern insulator topological phases in two dimensions, and gave a generalization to Laughlin-like states. However, on general principles these free fermion states must be ground states of gapless local Hamiltonians. In this talk, we address the issue of the energy gap in the interacting states, with a particular focus on the $\nu = 1/2$ bosonic Laughlin-like TNS. Through a combination of analytic and numerical arguments, we will show that these states too have gapless local parent Hamiltonians. Nevertheless, we will explore to what degree they can be used as numerical approximations to gapped phases.

12:15PM B10.00006 Exactly soluble 3D lattice models and the braiding statistics of their loop excitations, CHIEN-HUNG LIN, MICHAEL LEVIN, University of Chicago — We construct two exactly soluble 3D lattice models that belong to distinct topological phases in the sense that they cannot be smoothly connected without an intervening phase transition. What is interesting is that the two models have very similar physical properties: both are gapped and both support particle-like and loop-like excitations with non-trivial mutual statistics similar to that of charges and vortex lines in a $Z_2 \times Z_2$ gauge theory. The only difference between the two models lies in the braiding statistics of their loop excitations. As an application of these results, we construct two other closely related spin models with $Z_2 \times Z_2$ global symmetry. We show that one of these spin models realizes a $Z_2 \times Z_2$ symmetry protected phase with protected surface states while the other realizes a trivial phase without a protected surface.

12:27PM B10.00007 Topological phases in Iridium oxide superlattices: quantized anomalous charge or valley Hall insulators, HAE-YOUNG KEE, YIGE CHEN, University of Toronto — Designing materials is one of the hottest topics in modern condensed matter physics. Recently, how to achieve a topological insulator in transition metal oxides with strong spin-orbit coupling became an interesting subject. We have investigated possible topological phases in orthorhombic perovskite Ir oxide superlattices grown along the $[001]$ crystallographic axis. We found that bilayer Ir oxide superlattices exhibit quantized anomalous Hall effects in magnetic topological insulating phases. We also found, depending on the stacking of two layers, a valley Hall insulator with nontrivial valley dependent surface modes and a topological crystalline insulator with the crystal symmetry protected edge states can be realized. Experimental tools to detect such topological phases are also discussed.

12:39PM B10.00008 Surface States of Perovskite Iridates $\alpha$Al$\text{IrO}_3$: Signatures of Topological Crystalline Metal with Nontrivial $Z_2$ Index, HEUNG-SIK KIM, YIGE CHEN, HAE-YOUNG KEE, Department of Physics, University of Toronto — There have been increasing efforts in realizing topological metallic phases with nontrivial surface states, including a topological crystalline metal phase with flat surface states suggested recently. Here we perform first-principles electronic structure calculations for epitaxially stabilized orthorhombic perovskite iridates with $P\text{mmm}$ symmetry. Remarkably, two types of distinct topological surface states are found depending on the surface direction. On the side surfaces, flat surface states protected by the mirror symmetry emerge manifesting the topological crystalline character. On the top surface where mirror symmetry is broken, a Dirac cone appears indicating a non-trivial topology of the nodal metal. There, we find a well-defined two dimensional topological $Z_2$ index associated with time reversal symmetry. Transitions to weak and strong topological insulators and implications of different surface states in light of angle resolved photoemission spectroscopy are also discussed.

12:51PM B10.00009 Topological phase transitions in TiBiS$_2$ and TiSbS$_2$ under strain, QINGYUN ZHANG, YINGCHUN CHENG, UDO SCHWINGENSCHEIDL, Physical Sciences and Engineering, King Abdullah University of Science and Technology, COM-PUTATIONAL PHYSICS AND MATERIALS SCIENCE TEAM — Using first-principles calculations, we investigate the band structure evolution and topological phase transitions in TiBiS$_2$ and TiSbS$_2$ under hydrostatic pressure as well as uniaxial and biaxial strain. For TiBiS$_2$ topological transitions occur around 0 and 5 GPa, the system remaining a direct gap semiconductor up to 8 GPa. On the other hand, for TiSbS$_2$ the transitions occur around 2 and 5 GPa and the system transform from a direct gap semiconductor to a semimetal around 2 GPa. Biaxial and uniaxial strains are compared to each other. The phase transitions are identified by parity analysis and by calculating the surface states. Zero, one and four Dirac cones are found for the $(111)$ surfaces of both TiBiS$_2$ and TiSbS$_2$ when increasing the pressure, which confirms the trivial-nontrivial-trivial phase transitions. The Dirac cones at the $M$ points are anisotropic with a large out-of-plane component and inversely related in-plane spin and momentum direction. By examining the states on different surfaces we show that TiBiS$_2$ under 8 GPa pressure is a topological crystalline insulator. This finding makes the thallium-based III-V-VI$_2$ ternary chalcogenides candidates for studies on topological crystalline phase.

1:03PM B10.00010 A Novel Quasi-One-Dimensional Topological Insulator in Bismuth Iodide $\beta$-Bi$_4$I$_4$: Theoretical Prediction and Experimental Confirmation, OLEG V. ZAYZEV, GABRIEL AUTÉS, EPFL, ANNA ISAEVA, TU Dresden, LUCA MORESCHINI, LBNL, JENS C. JOHANNSSEN, ANDREA PISONI, EPFL, TATISCHI G. FILATOVA, ALEXEY N. KUZNETSOV, MSU, ŁAŚZLÓ FORRÓ, EPFL, WOUTER VAN DEN BROEK, LUL University, YEONGKwan KIM, JONATHAN D. DENLINGER, ELI TROETENBERG, AARON BOSTWICK, LBNL, MARCO GRIONI, EPFL — A new strong $Z_2$ topological insulator is theoretically predicted and experimentally confirmed in the $\beta$-phase of quasi-one-dimensional bismuth iodide Bi$_4$I$_4$. According to our first-principles calculations the material is characterized by $Z_2$ invariants $\{1;110\}$ making it the first representative of this topological class. Importantly, the electronic structure of $\beta$-Bi$_4$I$_4$ is in proximity with both the weak topological insulator phase $(0;000)$ and the trivial phase $(0;000)$, suggesting that a high degree of control over the topological electronic properties of this material can be achieved. Experimentally produced samples of this material appears to be practically defect-free, which results in a low concentration of intrinsic charge carriers. By using angle-resolved photoemission spectroscopy (ARPES) on the $(001)$ surface we confirm the theoretical predictions of a highly anisotropic band structure with a small band gap hosting topological surface states centered at the $M$ point, at the boundary of the surface Brillouin zone.

1We acknowledge support from Swiss NSF, ERC project “TopoMat”, NCCR-MARVEL, DFG and US DoE, G.A., A.I., L.M. and J.C.J. contributed equally to this work.

1:15PM B10.00011 ABSTRACT WITHDRAWN —

1:27PM B10.00012 Topological phases in SnTe thin films with a periodic array of defects and charge doping, MINSUNG KIM, JISOON IHAM, Dept. of Physics and Astronomy, Seoul Natl Univ — In this study, we investigate the topological phases of two-dimensional SnTe thin films with defect superstructures and charge doping. We find that the Sn-Te bilayer is a two-dimensional normal insulator, but can be transformed into a topological insulator by introducing an appropriate array of defects. Also, the topological phases of the films can be further controlled by charge doping due to the narrow bandwidth of the topologically nontrivial defect-induced bands. The results could be useful for the realization and control of the topological phases in nano-scale thin films.

1:39PM B10.00013 Topological states of non-Dirac electrons on $\text{Si}[111]$ surface, RUI YU, International Center for Materials Nanoarchitectonics (WPI-MANA) National Institute for Materials Science, Tsukuba 305-0044, Japan, QIFENG LIANG, Department of Physics, Shaoxing University, Shaoxing 312000, China, XIAO HU, International Center for Materials Nanoarchitectonics (WPI-MANA) National Institute for Materials Science, Tsukuba 305-0044, Japan — In the present work, we demonstrate the possibility of nontrivial topology of non-Dirac electrons. In particular, we show that, in two dimensional systems with $C_4$ crystal symmetry and time reversal symmetry, multiple $p$-orbitals exhibit a degeneracy and quadratic non-Dirac band dispersions at $\Gamma$ point. When the atomic spin-orbit coupling (SOC) is taken into account, a gap is opened at $\Gamma$ point and a quantum spin Hall effect state is realized. We construct a $k\cdot p$ model to reveal the nontrivial topology which is associated with a meron structure with double vorticity in the pseudo spin texture, a mechanism different from that on honeycomb lattice and the band inversion. We propose that $\text{Si}[111]$ surface with $1/3$ regular coverage of Bi atoms is a realization of our idea. First-principles calculations show that this system takes a quantum spin Hall phase with topological gap as large as $0.15eV$.

2This work is supported by WPI Initiative on Materials Nanoarchitectonics, MEXT, Japan.
topologically nontrivial. This can occur when either spatial inversion (P) or time-reversal (T) symmetry is broken, and spin-orbit is present. Taking ferromagnetic iron as a prototypical T-broken metal, we determine the Chern indices of all the Fermi sheets, starting from a census of the isolated band touchings in the Brillouin zone. Although there are many band touching points carrying a topological charge, the Chern index vanishes for most Fermi sheets. The reason is that they surround different Fermi arcs in the (010) surface bandstructure. We map out the phase diagram as a function of both nearest- and next-nearest-neighbor interaction strengths for an infinite cylinder geometry and find different charge-ordered phases but no sign of the interaction driven Chern insulator phase.

Monday, March 2, 2015 11:15AM - 2:15PM
Session B11 DCMP: Cuprate Superconductivity

11:15AM B11.00001 Intra unit cell electronic structure of the d-symmetry form factor density wave in the underdoped cuprates – Part I

KAZUHIRO FUJITA, MOHAMMAD HAMIDIAN, STEPHEN EDKINS, Cornell University, CHUNG KOO KIM, Brookhaven National Laboratory, ANDY MACKENZIE, University of St. Andrews, HIROSHI EISAKI, Brookhaven National Laboratory, JOHANNES MOTRUK, ADOLFO G. GRUSHIN, FRANK POLLMANN, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Mean field calculations in the literature have suggested the existence of an interaction-induced Chern insulator (CI) phase in a tight-binding model of spinless fermions on a honeycomb lattice with nearest- and next-nearest-neighbor interactions. The CI phase is an example of a state that breaks time-reversal symmetry and possesses a quantized Hall conductance. However, it has been proven elusive in exact diagonalization (ED) studies of this system. Since ED is limited to small system sizes, the fate of this phase in the thermodynamic limit still remains unclear. Using the infinite density matrix renormalization group (iDMRG) algorithm we reach system sizes exceeding those accessible in ED calculations while keeping track of quantum fluctuations neglected in mean field studies. We map out the phase diagram as a function of both nearest- and next-nearest-neighbor interaction strengths for an infinite cylinder geometry and find different charge-ordered phases but no sign of the interaction driven Chern insulator phase.

11:27AM B11.00002 Intra unit cell electronic structure of the d-symmetry form factor density wave in the underdoped cuprates – Part II

STEPHEN EDKINS, University of St Andrews, Cornell University, KAZUHIRO FUJITA, Cornell University, CMPMS Brookhaven National Lab, University of Tokyo, MOHAMMAD HAMIDIAN, Cornell University, CHUNG KOO KIM, CMPMS Brookhaven National Lab, Cornell University, ANDREW MACKENZIE, MIFI PFNS, University of St. Andrews, HIROSHI EISAKI, Institute of Advanced Industrial Science and Technology, SHINICHI SHIGETA, University of Tokyo, MICHAEL LAWLER, Binghamton University, Cornell University, EUN-AH KIM, Cornell University, SUBIR SACHDEV, Harvard University, SEAMUS DAVIS, Cornell University, KAZUHIRO FUJITA, Cornell University

In this talk we report on the electronic structure of Pb-Bi-2201. We develop a technique of sub-lattice phase-resolved electronic structure visualization within each CuO$_2$ unit-cell, we discovered a d-symmetry form factor density wave within the cuprate pseudogap state. In this talk, part I, we demonstrate that d-symmetry is the predominant form factor in the density wave within pseudogap states and show how this situation evolves upon doping.

11:39AM B11.00003 Decoding Spatial Complexity of Local Charge Modulations in Superconducting Pb-Bi-2201

ERICA CARLSON, Purdue University, CAN-LI SONG, ELIZABETH MAIN, Harvard University, SHUO LIU, BENJAMIN PHILLABABUM, Purdue University, KARIN DAHMEN, University of Illinois, Urbana-Champaign, ERIK HUDSON, Pennsylvania State University, JENNIFER HOFFMAN, Harvard University

In unconventional superconductors, real-space orders such as charge density modulations can coexist with superconductivity. In the cuprate superconductors, it has recently been recognized that local charge modulations are a ubiquitous feature and likely important for understanding the superconductivity in these materials. However, there are still open issues surrounding the dimensional profile of these charge modulations, including whether the modulation wavevector is unidirectional or bidirectional, and also whether the charge modulations extend beyond the surface of the material into the bulk. In bismuth-based cuprates, material disorder is a severe enough effect so as to preclude understanding the charge modulations through bulk scattering techniques. In order to resolve these issues, we use a local technique, scanning tunneling microscopy, to image the static charge modulations in Pb-Bi-2201. We find that the charge modulations are more consistent with an underlying tendency to a unidirectional charge density wave than a bidirectional charge density wave. Using recently developed cluster analysis techniques, we show that these locally 1D structures are more than surface deep, extending into the bulk of the material throughout the doping range.

11:51AM B11.00004 Resonant x-ray scattering study of charge order in the electron-doped cuprate Nd$_2$Ce$_{1-x}$CuO$_4$

EDUARDO DA SILVA NETO, RICCARDO COMIN, University of British Columbia, FEI ZHUO HE, RONNY SUTARTO, Canadian Light Source, YEPING JIANG, RICHARD GREENE, UNIVERSITY OF MARYLAND, GEORGE SAWATZKY, ANDREA DAMASCHELL, University of British Columbia

In cuprate high-temperature superconductors, an antiferromagnetic Mott insulating state can be destabilized toward unconventional superconductivity by either hole- or electron-doping. In hole-doped (p-type) cuprates a charge ordering (CO) instability competes with superconductivity inside the pseudogap state. In this talk we report resonant x-ray scattering measurements that demonstrate the presence of charge ordering in the n-type cuprate Nd$_2$Ce$_{1-x}$CuO$_4$ (NCCO) near optimal doping. We find that the CO in NCCO occurs with similar periodicity, and along the same direction as in p-type cuprates. However, in contrast to the latter, the CO onset in NCCO is higher than the pseudogap temperature, and is in the temperature range where antiferromagnetic fluctuations are first detected. Our discovery opens a parallel path to the study of CO and its relationship to antiferromagnetism and superconductivity. E.H. da Silva Neto, R.C. Comin et al. arXiv 1410.2253 (2014).
12:03PM B11.00005 Mapping the Striped Phase Diagram of La$_{2-x}$Ba$_x$CuO$_4$ with Resistance Fluctuation Spectroscopy, ADAM WEIS, AZTON WELLS, JUSTIN LANE, University of Illinois at Urbana-Champaign, SO RA CHUNG, Belmont University, PATHIKUMAR SELAPPAN, WALTRAUD KRIVEN, DALE VAN HARLINGEN, University of Illinois at Urbana-Champaign — La$_{2-x}$Ba$_x$CuO$_4$ (LBCO) is an exceptional high-temperature superconductor in which, near $x=1/8$ doping, superconductivity is suppressed and ‘striped’ charge order emerges. The charge stripes cause short-range conductance anisotropy that may be observed as fluctuations in resistance. In thin film LBCO devices grown by pulsed laser deposition, we measure time-resolved resistance as a function of bias current, temperature, and doping. As is consistent with charge stripes, the resistance noise exhibits a critical onset temperature and suppression at high currents. Combining resistance fluctuation spectroscopy with combinatorial laser deposition techniques, we are able to tune the doping of LBCO and map its phase diagram.

This research was supported by the DOE-BES under grant DE-FG02-07ER46453, through the Frederick Seitz Materials Research Laboratory at the University of Illinois at Urbana-Champaign. SRC was sponsored by NSF-REU 13-59126.

12:15PM B11.00006 Magnetic-field-driven superconductor-insulator transition in stripe-ordered La$_{1.48}$Nd$_{0.43}$Sr$_{0.12}$CuO$_4$, PAUL BAITY, ZHENZHONG SHI, DRAGANA POPOVIĆ, Dept. of Phys. & Natl. High Magnetic Field Lab., Florida State Univ., T. SASAGAWA, Tokyo Inst. of Tech. — The effects of the magnetic field ($H$) in underdoped cuprates, the nature of the $H$-driven superconductor-insulator transition (SIT), and the interplay with charge ordering are some of the key questions in high-temperature superconductivity. A recent study of the $H$-driven SIT in highly underdoped ($T_c \sim 4$ K) La$_{2-y}$Sr$_y$CuO$_4$ (LSCO) revealed an intermediate phase, with two quantum critical points separating the superconductor and the insulator. While charge distribution in highly underdoped LSCO seems to be inhomogeneous, its sister compound La$_{2-y}$No$_{0.4}$Sr$_{0.6}$CuO$_4$ (LNSCO) with $y = 0.12$ is known to have a charge-stripe order already in $H = 0$ at low enough temperatures ($T$). In order to address the above issues, we carry out detailed measurements of the in-plane and out-of-plane magnetoresistance with different $H$ orientations and over a wide range of $T$ on LNSCO single crystals with $y = 0.12$ and $T_c \sim 4$ K. The results will provide insight into the universality of the $H$-driven SIT in cuprates with different types or, at least, varying degrees of charge order.

Supported by NSF DMR-1307075 and NHMFL via NSF DMR-1157490 and the State of Florida.

12:27PM B11.00007 Pairing interaction near a nematic QCP of a 3-band CuO$_2$ model, THOMAS MAIER, Oak Ridge National Lab, DOUGLAS SCALAPINO, University of California, Santa Barbara — We calculate the pairing interaction and the k-dependence of the gap function associated with the nematic charge fluctuations of a CuO$_2$ model. We find that the nematic pairing interaction is attractive for small momentum transfer and that it gives rise to d-wave pairing. As the doping $\nu$ approaches a quantum critical point, the strength of this pairing increases and higher d-wave harmonics contribute to the k-dependence of the superconducting gap function, reflecting the longer range nature of the nematic fluctuations.

12:39PM B11.00008 Doping dependence of fluctuation diamagnetism in High Tc superconductors, SUBROTO MUKERJEE, KINGSHUK SARKAR, Indian Institute of Science, SUMILAN BANERJEE, Weizmann Institute of Science, T. V. RAMAKRISHNAN, Banaras Hindu University — Using a recently proposed Ginzburg-Landau-like energy functional due to Banerjee et. al. Phys. Rev. B 83, 024510 (2011), we calculate the fluctuation diamagnetism of high-Tc superconductors as a function of doping $x$ in addition to the magnetic field $H$ and temperature $T$ by employing classical Monte-Carlo simulations. We explicitly show that the doping dependence of our diamagnetism results are in good qualitative agreement and reasonable quantitative agreement with experimental data. Our calculations show that a model where the pairing scale increases and superfluid density decreases with underdoping produces features of the observed magnetization in the pseudogap region. In particular we show that the magnetization tracks the superconducting dome instead of the pseudogap temperature as seen in experiment and also comment on the determination of doping dependence of the upper-critical field.

12:51PM B11.00009 Fermi Arc Evolution and Doping Mechanism in High-Temperature Superconductors, DENIS K. SUNKO, DAMJAN PELC, MIROSLAV POŽEK, VITO DESPOJA, Department of Physics, Faculty of Science, University of Zagreb, Bijenčka cesta 32, HR-10000 Zagreb, Croatia, PREDRAG LAZIC, Theoretical Physics Division, Rudjer Boskovic Institute — We calculate realistic Fermi surface (FS) evolution of La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) with Sr doping within an extensive ab-initio framework including advanced band-unfolding techniques. We show that ordinary Kohn-Sham DFT+U can reproduce the observed metal-insulator transition and arc growth, when not restricted to the paramagnetic solution space. We elucidate both arc protection and the inadequacy of the rigid-band picture as consequences of a rapid change in orbital symmetry at the Fermi energy: the material undergoes a dimensional crossover along the Fermi surface, between the nodal (2D) and antinodal (3D) regions. In LSCO, this crossover accounts for FS arcs and the antinodal pseudogap, otherwise ubiquitous phenomena in high-Tc cuprates. The orbital transition is experimentally confirmed by replacing 4% of planar Cu in nearly optimally doped YBa$_2$Cu$_3$O$_{7-\delta}$ powder with $^{67}$Zn isotope, lowering $T_c$ to 57 K. The NQR spectrum of $^{67}$Zn, measured for the first time, shows that each Zn dopand surrounds itself with an insulating cluster. Zn destroys the SC metal by a Coulomb “domino effect” which reverts the orbital transition locally and pushes a significant number of surrounding sites back towards the parent-compound configuration.

1:03PM B11.00010 Andreev-Bragg reflection from an Amperian superconductor, PAUL BAIREUTHER, TIMO HYART, BRIAN TARASINKSI, CARLO BEENACKER, Instituut-Lorentz, Universiteit Leiden — We show how an electrical measurement can detect the pairing of electrons on the same side of the Fermi surface (Amperian pairing), recently proposed by Patrick Lee for the pseudogap phase of high-$T_c$ cuprate superconductors. Bragg scattering from the pair-density wave introduces odd multiples of $2\hbar \omega$ momentum shifts when an electron incident from a normal metal is Andreev-reflected as a hole. These Andreev-Bragg reflections can be detected in a three-terminal device, containing a ballistic Y-junction between normal and superconductor. The cross-conductance $\frac{dI_1}{dV_2}$ has the opposite sign for Amperian pairing than it has either in the normal state or for the usual BCS pairing.

1:15PM B11.00011 Shearconductivity as evidence for broken mirror symmetries, PATRIK HLOBIL, Karlruhe Institute of Technology, Stanford University, SRINIVAS RAGHU, AKASH MAHARAJ, PAVAN HOSUR, Stanford University — We propose the possible detection of broken mirror symmetries in highly correlated two-dimensional materials by elastotransport measurements. Using linear response theory we calculate the shearconductance $\Gamma_{xx,xy} = \sigma_{xx,xy}$, the linear change of the longitudinal conductivity $\sigma_{xx}$ due to a shear strain $\epsilon_{xy}$. This quantity can only be non-vanishing if the in-plane mirror symmetries are broken and we show that a square lattice with checkerboard charge and bond density wave shows a finite shearconductivity. This implies that a measurement of $\Gamma_{xx,xy}$ opens the possibility to verify broken mirror symmetry in the pseudogap regime of high-$T_c$ superconductors. Experimental setups to detect shearconductance are presented.
1:27PM B11.00012 Nanoscale phase separation in deep underdoped Bi$_2$Sr$_2$CuO$_{6+y}$ and Ca$_3$CuO$_2$Cl$_2$\textsuperscript{1} PETER MISTARK, ROBERT MARKIEWICZ, ARUN BANSIL, Northeastern University — We demonstrate that the tunneling spectra from deeply underdoped Bi$_2$Sr$_2$CuO$_{6+y}$ (Bi2201) and Ca$_3$CuO$_2$Cl$_2$ (CCOC) provide clear evidence for a nanoscale phase separation (NPS), which causes the gap to fill rather than close with doping. The phase separation extends from half-filling to a doping of $x \sim 0.09$. Assuming that the NPS is in the form of stripes, the nodal gap, which we model as a Coulomb gap, arises from impurity pinning of the charged stripes, and ultimately drives a metal-insulator transition.

\textsuperscript{1}This work is supported by the U.S.D.O.E.

1:39AM B11.00003 Enhancement of thermoelectric performance by phase separation of Ag$_2$Te in quaternary Ag$_x$Bi$_{0.5}$Sb$_{1.5-x}$Te$_3$\textsuperscript{*} YOO JANG SONG, JONG-SOO RHYEE, Kyung Hee Univ - Suwon Campus, BONG SEO KIM, Su DONG PARK, Korea Electrotechnology Research Institute, JAE HOON JUNG, Korea University, BYUNG-GIL RYU, JONG RAE LIM, LG Advanced Research Institute — Quaternary Ag–Bi–Sb–Te alloys with the general formula of Ag$_x$Bi$_{0.5}$Sb$_{1.5-x}$Te$_3$ are synthesized by solid state reaction for the high Ag doping $x=0.1, 0.2,$ and $0.3$. The powder x-ray diffraction analysis of the melted ingot shows the phase separation of AgSbTe$_3$ and Bi$_{0.5}$Sb$_{1.5}$Te$_3$ phases. After the hot press sintering at 350 $^\circ$C, we found Ag$_x$Te/Bi$_{0.5}$Sb$_{1.5}$Te$_3$ composite, instead of AgSbTe$_3$ phase separation, from the energy dispersive x-ray spectroscopy and x-ray diffraction measurements. The electrical conductivities of the Ag$_x$Te/Bi$_{0.5}$Sb$_{1.5}$Te$_3$ composite are significantly increased comparing with that of conventional p-type Bi$_{0.5}$Sb$_{1.5}$Te$_3$ composite, implying that the interface effect by phase separation can attribute to the increase of electrical conductivity. The maximum power factor and ZT values are reached up to 2.1 mW K$^{-2}$ m$^{-1}$ ($\sim 400$ K) and 1.1 (at 570 K), respectively, for $x = 0.1$ composite. Here we propose that the phase separation of Ag$_2$Te in Bi$_{0.5}$Sb$_{1.5}$Te$_3$ matrix can increase thermoelectric performance at mid-temperature temperature range.

1:51PM B11.00014 The insulator and pseudogap states coalescence beneath the superconductor dome . ALEJANDRO CABO MONTES DE OCA, ICMAT, La Habana, Cuba, ALEJANDRO CABO-BIZET, CEADEN, La Habana, Cuba, VICTOR MARTINEZ, YOANDRI VIELZA, Department of Physics, University of Pernambuco, Recife, Brasil, CONDENSED MATTER GROUP TEAM — The pseudogap effects and the expected quantum phase transitions (QPT) in cuprate materials are yet unclear in nature. A single band Tight-Binding (TB) model for the CuO planes of these materials had predicted the existence of definite pseudogap states at half-filling, after considering that a crystal symmetry breaking and non-collinear spin orientations of the single particle states are allowed. Here we show that after including hole doping in the model, a QPT which lies beneath the superconducting dome exists and is a second order one. In it, an insulator ground state (AFI), showing strong spin fluctuations at low doping, coalesce with an excited paramagnetic pseudogap (PPG) state, exhibiting a broken lattice symmetry at the critical hole density $x_c = 0.2$. Above this value the system becomes a paramagnetic metal. The band structures and Fermi surfaces with doping are evaluated and their evolution show a close resemblance with the experimental observations, including the topological change in structure for varying hole density.

2:03PM B11.0015 Charge Order in the Three-Band Model of Cuprate Superconductors\textsuperscript{2} BILL ATKINSON, Trent University, ARNO KAMPF, SINAN BULUT, Augsburg University — Numerous experiments have pointed to the widespread occurrence in underdoped high temperature superconductors of charge order with a strong intra-unit cell component. Motivated by this, we have performed theoretical calculations of charge instabilities in cuprate superconductors. First, we discuss a persistent discrepancy between theoretical predictions and experimental observations of the ordering wavevector $q^*$. We show that the correct direction and magnitude for $q^*$ can be obtained under the assumption that the charge order emerges from a pre-formed pseudogap. Second, we show that this type of long-range charge order reacts sensitively to dilute concentrations of strongly scattering impurities such as zinc, unlike the pseudogap which has been found to be robust against zinc doping. Taken together, these suggest that the pseudogap is a distinct phenomenon from charge order.

\textsuperscript{2}Supported by NSERC of Canada and Deutsche Forschungsgemeinschaft through TRR 80


11:15AM B12.00001 Investigation of InSb-In$_2$XTe (X=Ge & Sn) pseudo binary alloys as potential thermoelectric materials*, VIJAYABARATHI PONNAMBALAM, DONALD T. MORELLI, Dept. of Chemical Engineering and Materials Science, University of Michigan, Ann Arbor, MI, U.S.A. — We have fabricated high quality pseudo binaries InSb-In$_2$XTe (X=Ge & Sn) hold the promise of offering reduced thermal conductivity while maintaining the other thermoelectric properties intact. A series of InSb-In$_2$XTe type alloys has been synthesized. Thermal and electrical transport properties have been studied, and the results will be discussed with an emphasis on how the thermal conductivity is affected by the concentration of solute atoms. This work was supported as part of the Center for Revolutionary Materials for Solid State Energy Conversion, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001054.

11:27AM B12.00002 Study on thermoelectric performance by Na doping in nanostructured Mg$_{1-x}$Na$_x$Ag$_{0.97}$Sb$_{0.99}$, JING SHUAI, HEE SEOK KIM, YUCHENG LAN, SHUO CHEN, YUAN LIU, HUAIZHOU ZHAO, JIEHE SUI, ZHIFENG REN, Department of Physics and TsSUH, University of Houston, TX 77024 — MgAg$_{0.97}$Sb$_{0.99}$ was found to be potentially a new class of thermoelectric materials with ZT values above 1 in the temperature from 100 to 300 $^\circ$C. In this report, we systematically studied the effect of Na doping in Mg$_{1-x}$Na$_x$Ag$_{0.97}$Sb$_{0.99}$, on the thermoelectric properties and found Na was effective to increase the carrier concentration and power factor, especially below 180 $^\circ$C, which led to higher ZT values, a better self-compatibility factor, and ultimately a higher output power at the optimal Na concentration of $x = 0.005-0.0075$.

11:39AM B12.00003 Enhancement of thermoelectric performance by phase separation of Ag$_2$Te in quaternary Ag$_x$Bi$_{0.5}$Sb$_{1.5-x}$Te$_3$. YOO JANG SONG, JONG-SOO RHYEE, Kyung Hee Univ - Suwon Campus, BONG SEO KIM, SU DONG PARK, Korea Electrotechnology Research Institute, JAE HOON JUNG, Korea University, BYUNG-GIL RYU, JONG RAE LIM, LG Advanced Research Institute — Quaternary Ag–Bi–Sb–Te alloys with the general formula of Ag$_x$Bi$_{0.5}$Sb$_{1.5-x}$Te$_3$ are synthesized by solid state reaction for the high Ag doping $x=0.1, 0.2,$ and $0.3$. The powder x-ray diffraction analysis of the melted ingot shows the phase separation of AgSbTe$_3$ and Bi$_{0.5}$Sb$_{1.5}$Te$_3$ phases. After the hot press sintering at 350 $^\circ$C, we found Ag$_x$Te/Bi$_{0.5}$Sb$_{1.5}$Te$_3$ composite, instead of AgSbTe$_3$ phase separation, from the energy dispersive x-ray spectroscopy and x-ray diffraction measurements. The electrical conductivities of the Ag$_x$Te/Bi$_{0.5}$Sb$_{1.5}$Te$_3$ composite are significantly increased comparing with that of conventional p-type Bi$_{0.5}$Sb$_{1.5}$Te$_3$ composite, implying that the interface effect by phase separation can attribute to the increase of electrical conductivity. The maximum power factor and ZT values are reached up to 2.1 mW K$^{-2}$ m$^{-1}$ ($\sim 400$ K) and 1.1 (at 570 K), respectively, for $x = 0.1$ composite. Here we propose that the phase separation of Ag$_2$Te in Bi$_{0.5}$Sb$_{1.5}$Te$_3$ matrix can increase thermoelectric performance at mid-temperature temperature range.
2:27PM B12.00005 Nanostructured YbAgCu₄ for potential cryogenic thermoelectric cooling

MACHHINDRA KOIRALA, HUI WANG, Department of Physics and TcSÜH, University of Houston, Houston, TX, 77204, MANI POKHAREL, CYRIL OPEIL, Department of Physics, Boston College, Chestnut Hill, MA, 02467, ZHIFENG REN, Department of Physics and TcSÜH, University of Houston, Houston, TX, 77204 — We have studied thermoelectric properties of nanostructured YbAgCu₄ for cryogenic temperature range. Nanostructured YbAgCu₄ has been prepared using arc melting method followed by ball milling and hot pressing process. Thermal conductivity of the nanostructured samples has been reduced at 42 K by 30-50 % compared to the previously reported value. A high power factor of 131 µW m⁻¹ K⁻² has been obtained at 22 K. A peak dimensionless figure of merit ZT of 0.11 has been achieved at 42 K. With the variation of Cu-Ag composition, the temperature of peak ZT can be tuned, which could be useful for the preparation of segmented legs. The method of nanostructuring can be implemented with different fermen ions for obtaining high power factor with reduced thermal conductivity.

12:39PM B12.00006 Atomic Disorder in Tetrahedrite

JOHN ROBERT SALASIN, Univ of Tennessee, Knoxville, BRYAN CHAKOUMAKOS, Oak Ridge National Lab, CLAUDIA RAWN, Univ of Tennessee, Knoxville, ANDREW MAY, EDGAR LARA-CURZIO, MICHAEL MCGUIRE, HUIBO CAO, Oak Ridge National Lab — Thermoelectrics (TE) are materials which turn heat energy into electrical energy with applications spanning multiple disciplines including space exploration, Peltier cooling, and engine efficiency. Tetrahedrite is a copper sulfosalt with the general formula Cu₃₋ₓMₓ(Sb,As)₅S₁₃. Where M denotes a Cu²⁺ or Sb³⁻ site frequently replaced in natural tetrahedrite with Zn, Fe, Hg, or Mn. It has a cubic structure with an I-43m symmetry, c/a=10.4 Å, and only a handful of adjustable parameters. This structural study corroborates theoretical calculations on atomic disorder. Positional disorder of the trigonally coordinated Cu(2) site is suggested from the temperature dependence of the atomic displacement parameters determined from single-crystal x-ray and neutron diffraction. The displacements are extremely anisotropic for Cu(2) with a maximum rms static displacement of ~ 0.25 Å.

3 This research at ORNL’s High Flux Isotope Reactor and Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

12:51PM B12.00007 Exploring Materials Properties via Simulations and Experiments for Thermoelectricity

ARTEM KHABIBULLIN, LILIA WOODS, GEORGE NOLAS, University of South Florida — Thermoelectricity is an alternative route for energy conversion and suitable materials play an important role for enhanced efficiency of related applications. The optimization of the thermoelectric transport relies on the microscopic understanding of the materials internal properties, such as electronic structure characteristics. Simulations methods and effective medium theories are utilized to investigate advantageous features in materials composed of earth-abundant elements. Some general trends in the electronic structure influencing the transport are formulated for chalcopyrite and clathrate systems suitable for thermoelectricity. We emphasize the importance of theoretical and computational efforts not only to identify existing classes, but also predict new structures with desirable internal characteristics for effective materials design and optimization.

3 Financial support from NSF-DMR-1400957 is acknowledged.

1:03PM B12.00008 Novel Thermoelectric Materials Synthesis and Thermodynamics

XINFENG TANG, Wuhan University of Technology — No abstract available.

1:39PM B12.00009 Ab Initio Electron Relaxation Times and Computational Screening of Thermoelectric Materials

BORIS KOZINSKY, GEORGE SAMSONIDZE, Bosch Research, Cambridge MA — We report recent progress in development of an efficient approximation scheme for computing electron relaxation times in bulk crystalline materials from first principles. This technique takes into account electron-phonon coupling and opens up the possibility for ab initio calculations of electronic transport coefficients: electrical conductivity, the electronic part of thermal conductivity, and Seebeck coefficient. We find that electron relaxation times and transport coefficients are very sensitive to carrier concentration, and their accurate prediction is necessary for computational optimization of thermoelectric material composition. For a given thermoelectric material, we are able to determine the optimal carrier concentration which maximizes ZT at a target temperature. With this methodology at hand, systematic computational screening is performed in the compositional space of half-Heusler materials selected from materials databases and consisting of cheap earth-abundant elements. Good agreement is found with the available experimental data for previously synthesized half-Heusler compounds, and several new promising candidates for thermoelectric applications are identified, which have been synthesized and validated by experimental collaborators. Based on the results of our calculations, we also discuss the validity and applicability limits of the Wiedemann-Franz law for thermoelectric materials.

1:51PM B12.00010 NMR study of Cu₂Se and Cu₁₉₈Ag₄₂Se superionic conductors

ALI SIRUSI ARVJU, JOSEPH H. ROSS, JR., Department of Physics and Astronomy, Texas A&M University, SEDAT BALLIKAYA², CIRAD UHER, Department of Physics, University of Michigan — Cu₂Se and Cu₁₉₈Ag₄₂Se are well known as superionic conductors and recently as thermoelectric materials due to observation of high ZT. We will report NMR of these compounds. Our results include indications of glassy anharmonic behavior at low temperatures, Cu ion motion which becomes initiated near 90K, and motional narrowing near the phase transition at high temperatures as well as modified dynamics observed in the Ag-doped sample. NMR is particularly well suited to probe low frequency dynamics and at low temperatures the relaxation rate indicates anharmonic rattling behavior similar to what has been observed in other thermoelectric materials. A 90K change in the NMR spectra corresponds to the recently observed transport anomaly and indicates that the slow motion of Cu ions is initiated at this temperature and eventually becomes liquid-like at higher temperatures. We detect fast ion motion in Cu₂Se starting at 140K whereas in the Ag-doped compound this onset shifts to a higher temperature around 300K. At high temperatures the spectra become motional narrowed, and we will discuss the narrowing and shifts in terms of activated carrier density and ionic motion.

1 This work was supported by the Robert A. Welch Foundation.

2 Department of Physics, University of Istanbul
2:03PM B12.00011 Mechanical robust BiSbTe alloys with superior thermoelectric performance: A case study of stable hierarchical nanostructured thermoelectric materials. XIANLI SU, YUN ZHENG, XINFENG TANG, Wuhan University of Technology, CTIRAD UHER, University of Michigan, TANG’S GROUP TEAM, UHER’S GROUP TEAM — Poor machinability and susceptibility to brittle fracture of commercial ingots often impose significant limitations on the manufacturing process and durability of thermoelectric devices. In this study, melt spinning combined with plasma activated sintering (MS-PAS) method is employed with commercial p-type zone-melted (ZM) ingots of Bi$_{0.5}$Sb$_{1.5}$Te$_3$. This fast synthesis approach achieves hierarchical structures and in-situ nanoscale precipitates, resulting in the simultaneous improvement of thermoelectric performance and mechanical properties. Benefiting from a strong suppression of the lattice thermal conductivity, a peak ZT of 1.22 is achieved at 340 K in MS-PAS synthesized structures, representing about a 40% enhancement over that of ZM ingots. Moreover, MS-PAS specimens with hierarchical structures exhibit superior machinability and mechanical properties with an almost 30% enhancement in the fracture toughness, eightfold and a factor of six increase in the compressive and flexural strength respectively.


11:15AM B13.00001 Topological properties and correlation effects in oxide heterostructures, SATOSHI OKAMOTO, Oak Ridge National Lab — Transition-metal oxides (TMOs) have long been one of the main subjects of material science because of their novel functionalities such as high-$T_c$ superconductivity in cuprates and the colossal magnetoresistance effect in manganites. In recent years, we have seen tremendous developments in thin film growth techniques with the atomic precision, resulting in the discovery of a variety of electronic states in TMO heterostructures. These developments motivate us to explore the possibility of novel quantum states of matter such as topological insulators (TIs) in TMO heterostructures. In this talk, I will present our systematic theoretical study on unprecedented electronic states in TMO heterostructures. An extremely simple but crucial observation is that, when grown along the [111] crystallographic axis, bilayers of perovskite TMO form buckled honeycomb lattices of transition-metal ions, similar to graphene. Thus, with the relativistic spin-orbit coupling and proper band filling, two-dimensional TI states or spin Hall insulators are anticipated. Based on tight-binding modeling and density-functional theory calculations, possible candidate materials for TIs are identified. By means of the dynamical-mean-field theory and a slave-boson mean field theory, correlation effects, characteristics of TMO heterostructures, are also examined. I will further discuss future prospects in topological phenomena in TMO heterostructures and related systems.

The author thanks D. Xiao, W. Zhu, Y. Ran, R. Arita, Y. Nomura and N. Nagaosa for their fruitful discussions and collaboration.

1This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

11:51AM B13.00002 Effect of band filling and symmetry breaking on the electronic ground state in (La$_{1-x}$Sr$_x$)O$_3$/LaAlO$_3$ (111) (X = 3d) superlattices, DAVID DOENNIG, FMR II, TU Munich, WARREN E. PICKETT, University of California at Davis, ROSSITZA PENTCHEVA, University of Duisburg-Essen — Structural patterns, e.g., a buckled honeycomb lattice, realized in (111)-oriented perovskite bilayers may lead to exotic electronic ground states such as a Dirac-point Fermi surface. Based on density functional theory calculations including a Hubbard $U$ term, we explore systematically the effect of band filling in [111]-oriented (La$_{1-x}$Sr$_x$)O$_3$/LaAlO$_3$ superlattices with $X$ spanning the series of open shell $3d$ ions. The interplay of charge, spin, orbital, and lattice degrees of freedom reveals some regularities over the series, but also several unexpected symmetry lowering reconstructions that can guide the design of artificial materials of desired spin-charge-orbital order in conjunction with size of the energy gap and the possibility for emergent topological character.

11:51AM B13.00002 Effect of band filling and symmetry breaking on the electronic ground state in (La$_{1-x}$Sr$_x$)O$_3$/LaAlO$_3$ (111) (X = 3d) superlattices, DAVID DOENNIG, FMR II, TU Munich, WARREN E. PICKETT, University of California at Davis, ROSSITZA PENTCHEVA, University of Duisburg-Essen — Structural patterns, e.g., a buckled honeycomb lattice, realized in (111)-oriented perovskite bilayers may lead to exotic electronic ground states such as a Dirac-point Fermi surface. Based on density functional theory calculations including a Hubbard $U$ term, we explore systematically the effect of band filling in [111]-oriented (La$_{1-x}$Sr$_x$)O$_3$/LaAlO$_3$ superlattices with $X$ spanning the series of open shell $3d$ ions. The interplay of charge, spin, orbital, and lattice degrees of freedom reveals some regularities over the series, but also several unexpected symmetry lowering reconstructions that can guide the design of artificial materials of desired spin-charge-orbital order in conjunction with size of the energy gap and the possibility for emergent topological character.


1Financial support by DFG SFB/TR80, project G3.

12:03PM B13.00003 Raman Scattering in La$_{0.2}$Sr$_{0.8}$FeO$_{8-d}$ thin film: annealing-induced reduction and phase transformation, MOHAMMAD ISLAM, State University of New York at Oswego, YUJUN XIE, MARK SCAFETTA, STEVEN MAY, JONATHAN SPANIER, Drexel University — Raman scattering in thin film La$_{0.2}$Sr$_{0.8}$FeO$_{8-d}$ on MgO(001) collected at 300 K following different stages of annealing at selected temperatures (300 K < $T$ < 543 K, to 10 h.) and analysis reveal changes in spectral characteristics due to loss of oxygen, onset of oxygen vacancy-induced disorder, and activation of Raman-inactive modes that are attributed to symmetry transformation. The interpretation is further supported by carrier transport measurements under identical conditions showing orders of magnitude increase in the resistivity induced by oxygen loss. After prolonged annealing in air, evolution of the spectrum is consistent with the appearance of a topotactic transformation of the crystal structure from that of the rhombohedral ABO$_3$ perovskites to that of Brownmillerite-like structure consisting of octahedrally and tetrahedrally coordinated Fe atoms.

1We acknowledge the ONR (N00014-11-1-0664), the Drexel Centralized Research Facilities, the Army Research Office DURIP program, the Department of Education (GAANN-RETAI, Award No. P200A100117), and Leszek Wielunski at Rutgers University.

12:15PM B13.00004 Strain control of oxygen stoichiometry in epitaxial perovskites, HO NYUNG LEE, TRICIA MEYER, JONATHAN PETRIE, SHINBUHM LEE, JOHN NICHOLS, Oak Ridge National Laboratory, S.S. AMBROSE SEO, University of Kentucky, JOHN FREELEND, Argonne National Laboratory — Many physical properties of transition metal oxides (TMOs) are critically dependent upon the oxidation state of transition metals. Thus, a precise control of oxygen stoichiometry is critical to unambiguously understand many intriguing properties and functionalities. Based on a recent discovery of TMO-based oxygen sponges that can shed or absorb oxygen at highly reduced temperatures as low as 200 °C [Leeen et al., Nature Mater. 12, 1057 (2013) and Choi et al., Phys. Rev. Lett. 111, 097401 (2013)], we have explored various complex oxide materials to control the oxygen stoichiometry and, thereby, the critical physical properties. The latter include superconductivity in doped La$_2$CuO$_4$, metal-insulator transition in VO$_2$, and electronic and ionic conductivity as well as magnetism in SrCoO$_{3-d}$. In particular, by tuning strain systematically via lattice mismatching, we found that the epitaxial strain is a great tool to create functional defects that are critical in discovering new functionalities and/or improving the performance of materials especially for electronic and ionic conduction in complex oxides.

1The work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
12:27PM B13.00005 Epitaxial Growth of BaSnO₃ using Hybrid Molecular Beam Epitaxy¹
ABHINAV PRAKASH, TIANQI WANG, Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455, CHRISTIAN M. SCHLEPÜTZ, X-Ray Science Division, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, BHARAT JALAN, Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455 — Using co-deposition of a chemical precursor for Sn, a solid source for Ba and an RF plasma source for oxygen, we have extended the hybrid MBE approach for the growth of stoichiometric BaSnO₃. First, we present a detailed growth study of SnO₂ on r-plane sapphire as a function of Sn flux, oxygen pressure and substrate temperature. High-resolution x-ray diffraction (HRXRD) and AFM showed single-phase, epitaxial SnO₂ films and smooth surfaces, respectively. Three growth regimes were identified: reaction-, flux- and desorption-limited with increasing substrate temperature. Further study at constant substrate temperature revealed growth rate increases first and then becomes constant with increasing tin flux. We will then present a comprehensive study of the growth of phase-pure, smooth epitaxial BaSnO₃ films on SrTiO₃. HRXRD of 5nm BaSnO₃ on SrTiO₃ using synchrotron radiation suggest that films grow mostly coherent with out-of-plane lattice parameters of 4.20-4.25 Å for different cation flux ratios, remarkably similar to the calculated value of 4.26 Å using elastic tensors assuming BaSnO₃ grows coherent on SrTiO₃. Strain relaxation, stoichiometry control and their roles on the electronic transport will be discussed.

¹Work support by NSF (Grant No. DMR-1410888).

12:39PM B13.00006 Structure and Electronic Transport in BaSnO₃ Deposited via High Pressure Oxygen Sputtering
KOUSTAV GANGULY, PALAK AMBWANI, JONG SEOK JEONG, K. ANDRÉ MKHOYAN, PENG XU, CHRISTIAN M. SCHLEPÜTZ, BHARAT JALAN, University of Minnesota — We present structural and electronic transport properties of oxygen vacancy-doped BaSnO₃ films grown on SrTiO₃(001) and MgO(001) using the high pressure oxygen sputtering technique. High-resolution x-ray diffraction (HRXRD), combined with scanning transmission electron microscopy (STEM), confirms phase-pure epitaxial BaSnO₃(001) films on both substrates. The out-of-plane lattice parameter obtained from wide-angle x-ray diffraction is used as a sensitive probe for cation stoichiometry and strain relaxation. Irrespective of growth parameters, the out of plane lattice parameter remains unchanged, close to that of bulk (4.116 Å). A detailed thickness-dependent structural study using HRXRD and STEM suggests the formation of misfit dislocations as the primary mechanism for strain relaxation. We further show that as-grown, insulating BaSnO₃ films can be made conductive with n-type carriers (with typical room temperature concentrations and Hall mobilities being $10^{19}$ cm⁻¹ and 12 cm²/V·s) via high temperature (900 °C) vacuum annealing. Analysis of transport data from films with fixed density indicates a significant influence of film thickness, and thus strain relaxation, on the electron mobility. Temperature-dependent transport and magnetotransport studies will be described in detail as a function of annealing conditions, and will be correlated to strain relaxation. This work is supported by NSF through the UMN MRSEC.

12:51PM B13.00007 A Conductive Polar Interface with high mobility formed between LaInO₃ and BaSnO₃ perovskite oxides
USEONG KIM, CHULKWON PARK, Seoul Natl Univ, TAEWOO HA, YONSEI UNIV, YOUNG MO KIM, NAMWOOK KIM, CHANCHUNG JU, JAEJUN YU, Seoul Natl Univ, JAE HOON KIM, YONSEI UNIV, KOOKRN CHAR, SEOUL NATL UNIV — LaInO₃/BaSnO₃ (LIO/BSO) polar interface is the interface between BaSnO₃ (BSO), a non-polar perovskite oxide with high oxygen stability and electron mobility, and LaInO₃ (LIO), a polar perovskite oxide with the matched lattice parameters. Once the LIO/BSO interface forms, the conductance in the interface is significantly enhanced. The high oxygen stability of BSO enables dopant-controlled transport experiments by ruling out the involvement of oxygen vacancies in the transport phenomena. The conductance enhancement at the LIO/BSO interface was monitored while varying the doping rate of La dopants in the BSO layer. As a result, we found that the La doping rate was a dominant factor determining the extent to which the conductance was enhanced. It implies that the electronic reconstruction at the polar interface depends critically on the initial position of the Fermi level in the BSO side. The high electron mobility of BSO enables the exploitation of the conductive LIO/BSO interface at room temperature. We fabricated a field effect transistor utilizing such interface. At room temperature the device shows outstanding performances in terms of three key parameters: field effect mobility higher than 90 cm²/V·s, on/off ratio as high as 10⁷, and subthreshold swing as low as 0.65 V/dec.

1:03PM B13.00008 Enhanced electrical mobility in the (La,Ba)SnO₃ film grown on BaSnO₃ (001) substrate
KEE HOON KIM, Dept of physics and astronomy, CeNSCMR, Seoul Natl Univ, HYUNG JOON KIM, HYUNG-JHAE LEE, TAI HOON KIM, EGGON SOHN, JU-YOUNG PARK, KI-YOUNG CHOI, Seoul Natl Univ — Doped BaSnO₃ (BSO) systems with a perovskite structure are drawing increasing interests because of their high electrical mobility ($\approx 300$ cm²/V·s⁻¹), wide optical band gap ($\geq 3.1$ eV) and superior oxygen stability. In order to realize a semiconducting device with high speed based on the doped BSO films, an insulating substrate made of the BSO single crystal will be indispensable to the realization of truly epitaxial films without structural defects. Here, we report the successful growth of an insulating BSO single crystal by using the cupric-oxide-based flux growth method with an oxidizer. After preparing the BSO(001) substrate with one side polished, we deposited epitaxial La doped BSO films on the BSO substrate (BLSO/BSO(001)) by using the pulsed laser deposition. The electrical mobility ($\mu$) of BLSO/BSO(001) films are found to be $\approx 70$-$100$ cm²/V·s⁻¹ in the low ($10^{19}$ cm⁻³) to high ($10^{20}$ cm⁻³) doping ranges, which are clearly larger than those grown on SrTiO₃ (STO) substrate ($\approx 15$-$60$ cm²/V·s⁻¹). We’ll also show some of our recent efforts to realize the field effect transistor based on the BSO single crystal substrate. The present results show that the single crystal BSO substrate can offer various opportunities to realize practical electronic devices based on the doped BSO films.

1:15PM B13.00009 Interfacial engineering of optical absorption in epitaxial La(Cr,Ti)O₃SrTiO₃ superlattices
RYAN COMES, TIFFANY KASPAR, Pacific Northwest National Laboratory, STEVE HEALD, Advanced Photon Source, Argonne National Laboratory, MARK BOWDEN, SCOTT CHAMBERS, Pacific Northwest National Laboratory — SrTiO₃ (STO) is a wide-gap semiconductor well suited for photocatalytic H₂ production due to the alignment of its band edges with the half-cell reactions of the H₂O redox reactions. However, the wide optical gap of STO (3.3 eV) makes the material an inefficient light absorber in the visible spectrum, preventing formation of electron-hole pairs needed for photocatalysis. Superlattice films comprised of alternating layers of band insulator SrTiO₃ and Mott insulator LaCrO₃ (LCO) have been theoretically predicted to offer intriguing optical properties due to the broken symmetry between the unoccupied Ti dx²-y² and Ti dxz and dxy orbitals. In this work, we examine the properties of LCO-STO superlattices grown with various periodicities on (La,Sr)(Al,Ta)O₃ (LSAT) (001) substrates using oxide molecular beam epitaxy. Films were characterized via in situ x-ray photoelectron spectroscopy to measure valence band structure and interfacial band bending. Polarized Ti and Cr K-edge x-ray absorption near edge spectroscopy was used to examine the bonding anisotropy. Spectroscopic ellipsometry measurements show the presence of interfacially-induced visible light absorption not found in either STO or LCO.

1:27PM B13.00010 Tuning the physical properties in strontium iridate heterostructures
JOHN NICHOLS, TRICIA MEYER, HO NYUNG LEE, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — Strontium iridate operates as a high mobility, high Tc superconductor with a smooth surface. Lots of attention recently for its potential to reveal novel physical phenomena due to strong spin-orbital coupling with an interaction energy comparable to that of the on-site Coulomb interaction and crystal field splitting. The coexistence of fundamental interactions has created an exotic $J_{eff}$ = 1/2 antiferromagnetic insulating ground state in Sr$_2$IrO$_4$. In particular, it is known that this system can be driven into a metallic state with the simultaneous increase in dimensionality (n) and strain. We have investigated the effects of electron confinement by interfacing strontium iridium oxides with other perovskite oxides. We have synthesized thin film heterostructures, SrIrO₃/AMO$_3$ (A = Sr, La, B = Ti, Mn, Rh), layer-by-layer with pulsed laser deposition equipped with reflection high-energy electron diffraction. Based on investigations with x-ray diffraction, dc transport, SQUID magnetometry, and various spectroscopic measurements, we will present that the physical properties of the heterostructures are strongly dependent on spatial confinement and epitaxial strain. *This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division.
1:39PM B13.00011 Strain-controlled easy axis orientation of epitaxial CoFe₂O₄ films by He implantation, ANDREAS HERKLOTZ, ANTONY T. WONG, Oak Ridge National Laboratory, STEFANIA F. RUS, National Institute for Research and Development in Electrochemistry and Condensed Matter, THOMAS Z. WARD, Oak Ridge National Laboratory — Heteroepitaxial strain engineering is an essential tool in the strongly correlated systems for investigating fundamental coupling effects and for more practical control of thin film properties. Here, we use strain doping by He implantation as an alternative technique to control thin film functionalities. We demonstrate the tuning of the magnetic anisotropy of CoFe₂O₄ (CFO) films through He implantation. Compressively strained thin films of CFO are grown coherently on MgO substrates and show pronounced out-of-plane magnetic anisotropy. Successive doping of the CFO films with He using a commercial ion gun results in an expansion of the out-of-plane lattice parameter while maintaining in-plane epitaxial lock to the substrate. We observe a continuous rotation of the magnetic easy axis towards the film plane with increasing unit cell tetragonality. The results are in agreement with the strain-induced change of the magnetic anisotropy due to the large negative magnetostriction of CFO and demonstrate that strain doping via He implantation is an elegant path to tune desired characteristics of transition metal oxide thin films. This work was supported by the U. S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division.

1:51PM B13.00012 Atomic structure, electronic properties, and band offsets of SrRuO₃/TiO₂ heterojunctions, NAHEED FERDOUS, ELIF ERTEKIN, Univ of Illinois - Urbana — Photocatalytic water splitting by sunlight can in principle be an environmentally green approach to hydrogen fuel production, but at present photocatalytic conversion efficiencies remain too small. In titanium dioxide (TiO₂), the most commonly used photocatalyst, the biggest limitation arises from poor absorption of visible light. One way to increase the visible light absorption is to create a composite heterojunction by integrating TiO₂ with a strongly light absorbing material. Inspired by experimental results demonstrating good light absorption in the correlated metal oxide Strontium Ruthenate (SrRuO₃), as well as enhanced photocatalytic activity of SrRuO₃/TiO₂ heterojunctions [1], we have carried out electronic structure calculations based on density functional theory to explain and improve on the observed properties of such heterojunctions. Our calculations present that this heterojunction exhibits type-II band alignment which is necessary to transport optically excited electrons from the SrRuO₃ to the TiO₂, with calculated work functions in good agreement with experimental measurements. Also, DFT calculations help to explain the origin of large light absorption in this system, which is due to enhanced optical transitions leading to the observation of a zero-dimensional Fermi-liquid-like$^*$ quasiparticle states are suppressed at the metal-insulator transition observed in transport. We also will describe some recent unpublished work using epitaxial strain to drive a Lifshitz transition in atomically thin films of the spin-triplet ruthenate superconductor Sr₃Ru₂O₇, where we also can dramatically alter the quasiparticle scattering rates and drive the system towards non-Fermi liquid behavior near the critical point ($B$. Burganov, C. Adamo, in preparation).

2:03PM B13.00013 ABSTRACT WITHDRAWN —


008A - Divine Kumah, Yale University

11:15AM B14.00001 Atomic Scale Control of Competing Electronic Phases in Ultrathin Correlated Oxides$^*$, KYLIE SHEN, Cornell University — Ultrathin epitaxial thin films offer a number of unique advantages for engineering the electronic properties of correlated transition metal oxides. For example, atomically thin films can be synthesized to artificially confine electrons in two dimensions. Furthermore, using a substrate with a mismatched lattice constant can impose large biaxial strains of larger than 3% (Δa/a), much larger than can achieved in bulk single crystals. Since these dimensionally confined or strained systems may necessarily be less than a few unit cells thick, investigating their properties and electronic structure can be particularly challenging. We employ a combination of reactive oxide molecular beam epitaxy (MBE) and angle-resolved photoemission spectroscopy (ARPES) to investigate how dimensional confinement and epitaxial strain can be used to manipulate electronic properties and structure in correlated transition metal oxide thin films. We describe some of our recent work manipulating and studying the electronic structure of ultrathin LaNiO₃ through a thickness-driven metal-insulator transition between three and two unit cells (Nature Nanotechnology 9, 443, 2014), where coherent Fermi liquid-like quasiparticle states are suppressed at the metal-insulator transition observed in transport. We also will describe some recent unpublished work using epitaxial strain to drive a Lifshitz transition in atomically thin films of the spin-triplet ruthenate superconductor Sr₃Ru₂O₇, where we also can dramatically alter the quasiparticle scattering rates and drive the system towards non-Fermi liquid behavior near the critical point (B. Burganov, C. Adamo, in preparation).

$^*$Funding provided by the Office of Naval Research and Air Force Office of Scientific Research

11:51AM B14.00002 Extremely large electronic anisotropy caused by electronic phase separation in Ca₃(Ru₀.₉₇Ti₀.₀₃)O₇ single crystal, JING PENG, Tulane University and Nanjing University, XIAOSHAN WU, Nanjing University, ZHIQIANG MAO, Tulane University — Bilayered ruthenate Ca₃Ru₂O₇ exhibits rich electronic and magnetic properties. It orders at 56K, with FM bilayers antiferromagnetically coupled along c-axis (AFM-a). The AFM transition is closely followed by a first-order metal-insulator (MI) transition at 48K where spin directions switch to the b-axis (AFM-b). While this MI transition is accompanied by the opening of an anisotropic charge gap; small Fermi pockets survive from the MI transition, thus resulting in quasi-2D metallic transport behavior for T<30K. We previously showed such a quasi-2D metal with the AFM-b order composed of FM bilayers can be tuned to a Mott-insulating state with a nearest-neighbor AFM order via Ti doping [Ke et al, PRB 84, 201102(11)]. Ca₃(Ru₀.₉₇Ti₀.₀₃)O₇ is close to the critical composition for the AFM-b-to-IG-AFM phase transition. Our recent studies show the sample with this composition is characterized by an electronic phase separation between the insulating G-AFM phase (major) and the localized AFM-b phase (minor). The minor AFM-b phase forms a conducting path through electronic percolation within the ab-plane, but not along the c-axis, thus resulting in extremely large electronic anisotropy with 10⁷, which may be the largest among bulk materials.

12:03PM B14.00003 Separation of transport and Hall scattering rates in SrTiO₃/ReTiO₃ two-dimensional electron gases, EVGENY MIKHEEV, BRANDON ISAAC, TYLER CAIN, CHRISTOPHER FREEZE, SUSANNE STEMMER, Univ of California - Santa Barbara — ReTiO₃/SrTiO₃/ReTiO₃ (Re=Gd, Sm) quantum well structures that contain a high-density, two-dimensional electron gas (2DEG) exhibit phenomena that are reminiscent of the normal state behavior of unconventional superconductors, including a pseudogap, proximity to two-dimensional antiferromagnetism, and non-Fermi liquid behavior. Here we will discuss another transport anomaly, namely that scattering rates measured in the longitudinal and Hall conductivities are distinct and have different temperature dependences. We show that the two-scattering rate framework provides a remarkably simple, consistent, and accurate description for the dependencies of the Hall effect on temperature and quantum well thickness. This analysis reveals signatures of a spin density wave gap opening (Re=Sm) and a divergent Hall effect in the T=0 limit for an intermediate quantum well thickness (near 5 SrO layers), indicating a quantum critical point. Several theoretical proposals exist that may explain the two-lifetime separation. We discuss how the results in this system introduce a number of new, specific constraints and the need for a unifying microscopic theory.
12:15PM B14.00004 Odd frequency Density Waves1, YARON KEDEM, Nordic Institute for Theoretical Physics (NORDITA), Roslagstullsbacken 23, S-106 91 Stockholm, Sweden, ALEXANDER BALATSKY, Institute for Materials Science, Los Alamos National Laboratory, Los Alamos, NM 87545, Nordic Institute for Theoretical Physics (NORDITA), Roslagstull — A new type of hidden order in many body systems is explored. This order appears in states which are analogous to charge density waves, or spin density waves, but involve anomalous particle hole correlations that are odd in time and frequency. These states are shown to be inherently different from the usual states of density waves. We discuss a method to experimentally observe the new type of pairing by measuring the density-density correlation, both in time and space, where a clear distinction between odd and even correlations can be detected. An order parameter for these states is defined and calculated for a simple model, eliminating the physical nature of this phenomenon.

1Work supported by US DOE BES E 304, ERC DM 321031 and KAW

12:27PM B14.00005 Controlling Magnetism in Spin-Orbit-Driven Oxides with Epitaxial Strain, PATRICK CLANCY, University of Toronto — The layered perovskite iridates Sr$_2$IrO$_4$ and Ba$_2$IrO$_4$ are the prototypical spin-orbital Mott insulators, displaying a novel $j_{	ext{eff}} = 1/2$ ground state driven by strong 5d spin-orbit coupling effects. Efforts to understand, and ultimately control, this spin-orbit-induced ground state have led to the emergence of a new type of thin film iridates, which offer unique opportunities for the tuning of electronic and magnetic properties via epitaxial strain. We have performed complementary resonant magnetic x-ray scattering (RMXS) and resonant inelastic x-ray scattering (RIXS) measurements on epitaxial thin film samples of Sr$_2$IrO$_4$ and Ba$_2$IrO$_4$. By measuring 13 to 50 nm films grown on a variety of different substrates (PSO, GSO, STO, LSAT), we are able to investigate the impact of applied tensile and compressive strain on the magnetic structure, correlation lengths, and characteristic excitations of these materials. We find that the dispersion of the low-lying magnetic and orbital excitations is strongly affected by strain-induced structural changes, and show that epitaxial strain provides an effective method for tuning three distinct energy scales: the magnetic ordering temperature ($T_N$), the magnetic exchange interactions ($J$), and the non-cubic crystal field splitting ($\Delta_{\text{CEF}}$). Perhaps most strikingly, we demonstrate that hard x-ray RIXS can be used to perform detailed magnetic dispersion measurements on thin film samples of 13 nm (~5 unit cells) or less.


1:03PM B14.00006 Series of alternating states with unpolarized and spin-polarized bands in dimerized IrTe$_2$, V. KIRYUKHIN, G.L. PASCUT, T. BIROL, S.-W. CHEONG, K. HAULE, Rutgers U., M.J. GUTMANN, ISIS, J.J. YANG, Pohang U. — A series of states with different densities of stripes of Ir dimers is investigated using x-ray diffraction and density functional theory in layered nonmagnetic metal IrTe$_2$. With decreasing temperature, structures with and without inversion symmetry alternate. In non-centrosymmetric states, spin-orbit coupling splits the electronic energy bands into spin-polarized pairs. Factors affecting the stability of the observed dimerized states are established, and it is conjectured that an infinite series of alternating states with and without polarized bands is realized in IrTe$_2$. Switching dimerized states with different symmetries by changing temperature or strain enables control of band polarization, adding a new tool for spintronics and valleytronics research.

1:15PM B14.00007 Quantum Monte Carlo study of the nematic quantum critical point in a metal, YONI SCHATTNER, Weizmann Institute of Science, SAMUEL LEDERER, Stanford University, EREZ BERG, Weizmann Institute of Science, STEVEN A. KIVELSTON, Stanford University — The coupling of fermions to gapless collective modes can lead to interesting critical phenomena, non-Fermi-liquid behavior and/or superconductivity. As an example for such a system, we present a sign-problem free lattice model of quantum-critical Ising-nematic bosons coupled to fermions in two dimensions. Determinantal Quantum Monte-Carlo simulations show a second order nematic transition at low temperatures. As the transition is approached, we find evidence of non-Fermi-liquid behavior. At the temperature scales accessible to us, we find no traces of superconductivity.

1:27PM B14.00008 Itinerant density instability at classical and quantum critical points, YEJUN FENG, Argonne National Laboratory, JASPER VAN WEZEL, FELIX FLICKER, Univ. of Bristol, JIYANG WANG, D.M. SILEVITCH, P. B. LITTLEWOOD, T. F. ROSENBAUM, Univ. of Chicago — Itinerant density waves are model systems for studying quantum critical behavior. In both the model spin- and charge-density-wave systems Cr and NbSe$_2$, it is possible to drive a continuous quantum phase transition with critical pressures below 10 GPa. Using x-ray diffraction techniques, we are able to directly track the evolution of the order parameter vector Q across the pressure-temperature phase diagram. We find a non-monotonic dependence of Q on pressure. Using a Landau-Ginzburg theoretical framework developed by McMillan for CDWs, we evaluate the importance of the physical terms in driving the formation of ordered states at both the thermal and quantum phase transitions. We find that the itinerant instability is the deciding factor for the emergent order, which is further influenced by the quantum fluctuations in both the thermal and quantum limits.

1:39PM B14.00009 Emergence of charge density wave domain walls above the superconducting dome in 1T-TiSe$_2$, PETER ABBAMONTE, YOUNG IL JOE, XIAOQIAN CHEN, POUYAN GHAEMI, KEN FINKELSTEIN, GILBERTO DE LA PENA, YU GAN, University of Illinois, JAMES LEE, Lawrence Berkeley National Laboratory, SHI YUAN, University of Illinois, JOCHEN GECK, Leibniz Institut, GREG MACDOUGALL, TAI CHANG, LANCE COOPER, EDUARDO FRADKIN, University of Illinois — Superconductivity in so-called unconventional superconductors is nearly always found in the vicinity of another ordered state, such as antiferromagnetism, charge density wave (CDW), or stripe order. This suggests a fundamental connection between superconductivity and fluctuations in some other order parameter. To better understand this connection, we used high-pressure X-ray scattering to directly study the CDW order in the layered dichalcogenide TiSe$_2$, which was previously shown to exhibit superconductivity when the CDW is suppressed by pressure or intercalation of Cu atoms. We succeeded in suppressing the CDW fully to zero temperature, establishing for the first time the existence of a quantum critical point (QCP) at $P_c = 5.1 \pm 0.2$ GPa, which is more than 1 GPa beyond the end of the superconducting region. Unexpectedly, at $P \sim 3$ GPa we observed a reentrant, weakly first order, incommensurate phase, indicating the presence of a Lifshitz tricritical point somewhere above the superconducting dome. Our study suggests that superconductivity in TiSe$_2$ may be connected to the formation of CDW domain walls

1Supported by DOE grant DE-FG02-06ER46285

1:51PM B14.00010 Nanoscale Charge-order Dynamics in Stripe-phase Nickelates Probed via Ultrafast THz Spectroscopy1, GIACOMO COSLOVICH, SASCHA BEHL, BERNHARD HUBER, Lawrence Berkeley National Laboratory, WEI-SHENG LEE, ZHI-XUN SHEN, SIMES, SLAC National Accelerator Laboratory, Stanford University, TAKAO SASAGAWA, Tokyo Institute of Technology, HANS A. BECHTEL, MICHAEL C. MARTIN, ROBERT A. KAINDL, Lawrence Berkeley National Laboratory — Here we report ultrafast optical pump-THz probe spectroscopy of the model stripe-ordered system Li$_x$Sr$_{2}$Ir$_{2}$O$_{5}$NiO$_{2}$. Ultrafast experiments in the multi–THz spectral range show strong THz reflectivity variations around the phonon bending mode frequency ($\approx 11$ THz). At low temperatures this phonon mode exhibits a splitting directly related to the formation of long-range stripe-order, while the background conductivity is reminiscent of the opening of the mid-IR pseudogap due to charge localization. The transient THz probe response therefore captures both the electronic and structural dynamics in a single light pulse. The results reveal the dynamical interplay between charge localization and the bending mode folding, providing insight in the emergence of nanoscale charge-order in complex oxides.

1This work was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering,
can be used to map out local stress distributions, and also relate to thermal expansion and vibrational anharmonicity via the Gruneisen parameter.

4-point bending setup, and found a stress coefficient consistent with the simulations, in contrast to inconsistent previous results in the literature. These results
peak position proportional to stress. We then performed Raman experiments on an a-Si:H film deposited on a c-Si wafer, in which stress was applied with a
amorphous silicon as well, particularly for studying local stress and composition of nanostructured amorphous/crystalline devices. Toward that goal, we have
since the positions of vibrational peaks are sensitive to local stress. This method has been applied extensively for crystalline silicon, and would be useful for
Engineering, Massachusetts Institute of Technology — Raman microscopy has proven to be a very useful technique for inferring stress distributions in materials,

TONIO BUONASSISI, Dept. of Mechanical Engineering, Massachusetts Institute of Technology, JEFFREY C. GROSSMAN, Dept. of Materials Science and
DAVID A. STRUBBE, ERIC C. JOHLIN, Dept. of Materials Science and Engineering, Massachusetts Institute of Technology, TIMOTHY R. KIRKPATRICK,

11:15AM B15.00001 Dynamical and anharmonic effects on the electron-phonon coupling and the zero-point renormalization of the band structure, GABRIEL ANTONIUS, University of Montreal, SAMUEL PONCÉ, Université Catholique de Louvain, ÉTIENNE LANTAGNE-HURTUBISE, GABRIEL AUCLAIR, MICHEL CÔTÉ, University of Montreal, XAVIER GONZE, Université Catholique de Louvain — The electron-phonon coupling in solids renormalizes the band structure, reducing the band gap by several tenths of an eV in light-atoms semiconductors. Using the Allen-Heine-Cardona theory (AHC), we compute the zero-point renormalization (ZPR) as well as the quasiparticle lifetimes of the full band structure in diamond, BN, LiP and MgO. We show how dynamical effects can be included in the AHC theory, and still allow for the use of a Sternheimer equation to avoid the summation over unoccupied bands. The convergence properties of the electron-phonon coupling self-energy with respect to the Brillouin zone sampling prove to be strongly affected by dynamical effects. We complement our study with a frozen-phonon approach, which reproduces the static AHC theory, but also allows to probe the phonon wavefunctions at finite displacements and include anharmonic effects in the self-energy. We show that these high-order components tend to reduce the strongest electron-phonon coupling elements, which affects significantly the band gap ZPR.

11:27AM B15.00002 Raman spectra calculations for nanostructures using ab initio real-space methods, N. SCOTT BOBBITT, JAMES R. CHELIKOWSKY, University of Texas at Austin — We use a real-space pseudopotential method within density functional theory to calculate Raman spectra for Si nanocrystals. We examine the effects of quantum confinement and the presence of impurities, including dopant concentration and location of dopant within the nanocrystal. The ability to predict the effects of dopant concentration and location on a Raman spectrum from first principles suggests that this calculation technique could be coupled with spectroscopic experiments to identify the size and nature of doped nanocrystals.

1This work is supported by the DOE under grant number DE-FG02-06ER46286. Computations were performed on machines at TACC and NERSC.

11:39AM B15.00003 The atomistic limit of envelope function theory, CRAIG PRYOR, Dept. of Physics and Astronomy, University of Iowa, Iowa City, IA 52242, MATS-ERIC PISTOL, Lund University, Solid State Physics and the Nanometer structure consortium, Box 118, SE-221 00, Lund, Sweden — Electronic properties of semiconductor nanostructures and impurity states are typically calculated using one of three different methods: tight-binding models, pseudopotentials, or envelope function theory. The first two are well suited to modeling atomistic scale structures, however their parameters must be fit to bulk properties which can be a complicated procedure. In contrast, envelope function theory is best at describing larger scales in which the placement of individual atoms is not important and the parameters are directly related to experimentally determined quantities. As usually implemented, envelope function theory is insensitive to atomic scale structure. We show that this does not need to be the case, and construct an atomistic envelope function theory. This is advantageous for nanostructure modeling because it provides an atomistic model parameterized in terms of physical matrix elements rather than by complicated fitting procedures.

11:51AM B15.00004 Quantum Mechanics of Chemisorption on GaAs Clusters, FRANK NARANJO, AJIT HIRA, RUBEN RIVERA, OLIVER OVIEDO, Northern New Mexico College — This research focuses on the theoretical study of molecular clusters to examine the chemical properties of small Ga₅₅As₅₅ clusters (n = 2 - 10). We study the chemisorption of different atomic and molecular species on small clusters of metallic elements, by examining the interactions of H, H₂, Li and Be adsorbates with the GaAs clusters. Semiconductor clusters are of interest for the study of quantum size effects and for metallization phenomena. Hybrid ab initio methods of quantum chemistry (particularly the DFT-B3LYP model) are used to derive optimal geometries for the clusters of interest. We compare calculated binding energies, bond-lengths, ionization potentials, electron affinities and HOMO-LUMO gaps for these clusters. Mapping of the singlet, triplet, and quintet, potential energy surfaces is performed. Implications for fundamental mechanisms of atomistic assembly on the GaAs surfaces are examined.

1Research funded by NSF

12:03PM B15.00005 Stress effects on Raman spectroscopy of aSi:H — theory and experiment, DAVID A. STRUBBE, ERIC C. JOHLIN, Dept. of Materials Science and Engineering, Massachusetts Institute of Technology, TIMOTHY R. KIRKPATRICK, TONIO BUONASSISI, Dept. of Mechanical Engineering, Massachusetts Institute of Technology, JEFFREY C. GROSSMAN, Dept. of Materials Science and Engineering, Massachusetts Institute of Technology — Raman microscopy has proven to be a very useful technique for inferring stress distributions in materials, since the positions of vibrational peaks are sensitive to local stress. This method has been applied extensively for crystalline silicon, and would be useful for amorphous silicon as well, particularly for studying local stress and composition of nanostructured amorphous/crystalline devices. Toward that goal, we have simulated the Raman spectrum of hydrogenated amorphous silicon with density-functional perturbation theory, using atomistic structures from the WWWW algorithm with different stress states. We obtain a spectrum in good agreement with experimental results, and calculate a coefficient for the change in the TO peak position proportional to stress. We then performed Raman experiments on an a-Si:H film deposited on a c-Si wafer, in which stress was applied with a 4-point bending setup, and found a stress coefficient consistent with the simulations, in contrast to inconsistent previous results in the literature. These results can be used to map out local stress distributions, and also relate to thermal expansion and vibrational anharmonicity via the Gruneisen parameter.
12:15PM B15.00006 Angle resolved photoemission studies of the Rashba states in ferroelectric GeTe, BEOMYOUNG KIM, WONSEOK KYUNG, GARAM HAN, Institute of Physics and Applied physics, Yonsei University, 134 Shinchon-Dong, Seodaemun-Gu, Seoul 120-749, Republic of Korea, YEONGKWAN KIM, JONATHAN DENLINGER, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA., IN CHUNG, Graduate School of Nanoscience and Technology, KAIST, 291 Daehak-ro, Yuseong-gu, Daejeon 305-701, Republic of Korea, CHANGYOUNG KIM, Institute of Physics and Applied physics, Yonsei University, 134 Shinchon-Dong, Seodaemun-Gu, Seoul 120-749, Republic of Korea — There has been significant increase in the research of spin orbit coupling (SOC) induced exotic phenomena. The Rashba effect, theoretically predicted to exist, is one of the SOC related phenomena. The phenomenon was later experimentally observed in the surface states of metals and topological insulators as well as interfaces of hetero structures that have inversion symmetry breaking (IBS). Even bulk states with intrinsic IBS such as BiTe is found to have Rashba split bands. It was very recently proposed that ferroelectric GeTe has Rashba effect in the bulk. This is a unique situation where IBS is provided not by the structure IBS but by an electrical polarization. We have performed angle-resolved photoemission spectroscopy (ARPES) on GeTe single crystals to investigate the unique bulk Rashba state. Our results indeed show the existence of a Rashba-type band splitting as theoretically predicted. We discuss various aspect of the Rashba state in GeTe.

12:27PM B15.00007 Electronic structure of parabolically confined quantum wire with Rashba and Dresselhaus spin-orbit interactions under the influence of perpendicular magnetic field 1. SEVIL SARIKURT, Department of Materials Science and Engineering, Texas A&M University, College Station, TX 77843-3003, SERPIL SAKIROGLU, KADIR AKGUNOR, ISMAIL SOKMEN, Department of Physics, Faculty of Science, Dokuz Eylul University, Izmir, 35390, TURKEY — We have investigated the effect of spin-orbit (SO) coupling on the energy level spectrum and spin texturing of parabolically confined quantum wire that is subjected to an externally applied perpendicular magnetic field. Additionally we have also taken into account exchange-correlation contribution. Highly accurate numerical calculations have been carried out by finite element method. Our results have revealed that the interplay of the SO coupling with effective magnetic field significantly modifies the band structure, producing additional subband extrema and energy gaps. Energy subband structure varies depending on which type of SO coupling strength is considered and also the magnitude of SO coupling. We also obtain that spatial modulation of spin density along the wire width can be considerably modified by SO coupling strength, magnetic field and charge carrier concentration. Besides, we have observed that the presence of exchange-correlation contribution leads to a softening behavior in the local maxima at subbands and shifts all energy subbands to lower energy values. Numerical results point out that the combined effect of exchange-correlation and SO coupling produces asymmetry in the dispersion relations.

1Supported by Scientific and Technological Research Council of Turkey.

12:39PM B15.00008 Strongly Anisotropic Ballistic Magnetoresistance in Compact Three-Dimensional Semiconducting Nanodevices 1. CARMINE ORTIX, CHING-HAO CHANG, JEROEN VAN DEN BRINK, Institute for Theoretical Solid State Physics - IFW Dresden — In this talk, I will show that in non-magnetic semiconducting bilayer or multilayer thin film systems rolled-up into compact quasi-one-dimensional nanodevices, the ballistic magnetoresistance is very anisotropic: conductances depend strongly on the direction of an externally applied magnetic field. This phenomenon originates from the curved open geometry of rolled-up nanotubes, which leads to a tunability of the number of one-dimensional magnetic subbands crossing the Fermi energy. The experimental significance of this phenomenon is illustrated by a sizable anisotropy that scales with the inverse of the number of windings, and persists up to a critical temperature that can be strongly enhanced by increasing the strength of the external magnetic field or the characteristic radius of curvature, and can reach room temperature.

1The financial support of the Future and Emerging Technologies (FET) programme within the Seventh Framework Programme for Research of the European Commission, under FET-Open grant number: 618083 (CNTQC), is gratefully acknowledged.

12:51PM B15.00009 Electronic Structure Evolution of Fullerene on CH3NH3PbI3 1. CHENGGONG WANG, CONGCONG WANG, university of rochester, XIAOLIANG LIU, Hunan Key Laboratory for Super-microstructure and Ultrafast Process, College of Physics and Electronics, Central South University, Changsha, 410083, P. CHENGBI, YUCHUANSHAO, ZHENGGUOXIAO, JINSONGHUANG, University of Nebraska, Lincoln, YONGLI GAO, university of rochester — The thickness dependence of fullerene on CH3NH3PbI3 perovskite film surface has been investigated by using ultraviolet photoemission spectroscopy (UPS). X-ray photoemission spectroscopy (XPS) and inverse photoemission spectroscopy (IPES). The lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO) can be observed directly with UPS and IPES. It is observed that the HOMO level in fullerene shifts to lower binding energy. The XPS results show an initial shift of core levels to lower binding energy in the perovskite, which indicates that electrons transfer from the perovskite film to fullerene molecules. We observed that the WF of the perovskite is 5.0 eV and the VBM is 0.6 eV. The band gap of the perovskite is 1.66 eV, which is in accordance with previous reports. We also observed the HOMO level of C60 shifts to lower binding energy, indicating a band bending in the C60 region. The perovskite core levels show a strong initial shift to lower binding energy, indicating electron transfer from the perovskite film to fullerene molecules. The strongest electron transfer happened at 1/4 monolayer of fullerene, and further deposition reduced the transfer as forms fullerene forms C60 solid film.

1NSF CBET-1437656

1:03PM B15.00010 Auger recombination in scintillator materials from first principles 1. ANDREW MCALLISTER, EMMANOULI KIOUPAKIS, University of Michigan, DANIEL ÅBERG, Lawrence Livermore National Laboratory, ANDRÉ SCHLEIFE, University of Illinois at Urbana-Champaign — Scintillators convert high energy radiation into lower energy photons which are easier to detect and analyze. One of the uses of these devices is identifying radioactive materials being transported across national borders. However, scintillating materials have a non-proportional light yield in response to incident radiation, which makes them less useful. One possible cause of the non-proportional light yield is non-radiative Auger recombination. Auger recombination can occur in two ways - direct and phonon-assisted. We have studied both types of Auger recombination from first principles in the common scintillating material sodium iodide. Our results indicate that the phonon-assisted process, assisted primarily by short-range optical phonons, dominates the direct process. The corresponding Auger coefficients are $5.6 \pm 0.3 \times 10^{-32} \text{cm}^6 \text{s}^{-1}$ for the phonon-assisted process versus $1.17 \pm 0.01 \times 10^{-32} \text{cm}^6 \text{s}^{-1}$ for the direct process. At higher electronic temperatures the direct Auger recombination rate increases but remains lower than the phonon-assisted rate.

1This research was supported by the National Science Foundation CAREER award through Grant No. DMR-1254314 and NA-22. Computational Resources provide by LLNL and DOE NERSC Facility.
1:15PM B15.00011 Pressure Dependent Electronic Properties of Organic Semiconductors from First Principles, FRANZ KNUTH, CHRISTIAN CARBONOGHI, Fritz-Haber-Institut der MPG, Berlin, DE; VOLKER BLUM, Fritz-Haber-Institut der MPG, Berlin, DE; DUKE UNIVERSITY, Durham, NC, USA; MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, DE. — The electronic properties of organic semiconductors typically exhibit a significant dependence on the strain, stress, and pressure [1]. In this contribution, we present the theoretical background, assessment of approximations, and results of electronic and transport properties in the framework of density-functional theory. Our implementation considers the analytical strain derivatives (stress tensor) including the contributions that stem from (a) van-der-Waals interactions [2] and (b) the Fock-exchange in hybrid functionals. We validate our approach by investigating the geometric and electronic changes that occur in polyacetylene and anthracene under hydrostatic pressure. We show that the fraction of exact exchange included in the calculations is critical — and non-trivial to choose — for a correct description of these systems. Furthermore, we point out trends for the electrical conductivity under pressure and identify the dominant charge carriers and transport directions.


1:27PM B15.00012 Investigation of Observing the role of orbital angular momentum with in Rashba and Dresselhaus effects system, SOOHYUN CHO, WONSIG JUNG, BEOMYOUNG KIM, GARAM HAN, Yonsei University, MATS LEANDERSSON, BALASUBRAMANIAN THIAGARAJAN, MAX Laboratory, CHANGYOUNG KIM, Yonsei University, MAX LABORATORY COLLABORATION — In our previous studies of Au(111) surface states with circular dichroism angle-resolved photoemission spectroscopy (CD-ARPES), we found strong CD signal, indicating probable existence and role of orbital angular momentum (OAM) in the Rashba effect. We proposed that OAM plays a key role in the electronic structures of such systems in the presence of inversion symmetry breaking and spin-orbit coupling (SOC). Semiconductors with the zinc blende structure with an inversion symmetry breaking have band splitting near the \( \Gamma \) point as predicted by the band calculation. In addition, the overall spin structure can be understood within in the Dresselhaus effect. While the net OAM in the bulk should be normally zero for semiconductors with an inversion symmetry, non-zero OAM can appear in the bulk of zinc-blende structures due to the inversion symmetry breaking. Moreover, as for ARPES experiments, the sample surface provide an additional inversion symmetry breaking. To investigate the OAM structure, we have performed CD-ARPES experiments on InSb, CdTe and GaAs. Our results show CD signal in the \( J_{3/2} \) states (heavy and light hole band). We attribute the CD modulations of the three bands (heavy hole, light hole and split-off bands) to the existence of OAM. The OAM structure deduced from the CD-ARPES results is explained if we assume both the Rashba (from surface) and Dresselhaus (from bulk) effects are present. These results suggest that OAM also plays a role in the Dresselhaus effect through SOC.

1:39PM B15.00113 Towards simple orbital-dependent density functionals for molecular dissociation, IGOR YING ZHANG, Fritz-Haber-Institut der MPG, Berlin, DE; PATRICK RICHTER, Aalto University, Helsinki, FI, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, DE. — Density functional theory (DFT) is one of the leading first-principles electronic-structure theories. However, molecular dissociation remains a challenge, because it requires a well-balanced description of the drastically different electronic structure at different bond lengths. One typical and well-documented case is the dissociation of both \( \text{H}_2^+ \) and \( \text{H}_2 \), for which all popular DFT functionals fail [1,2]. We start from the Bethe-Goldstone equation to propose a simple orbital-dependent correlation functional which generalizes the linear adiabatic connection approach. The resulting scheme is based on second-order perturbation theory (PT2), but includes the self-consistent coupling of electron-hole pairs, which ensures the correct \( \text{H}_2 \) dissociation limit and gives a finite correlation energy for systems with a (near)-degenerate energy gap. This coupling PT2-like (CPT2) approximation delivers a significant improvement over all existing functionals for both \( \text{H}_2 \) and \( \text{H}_2^+ \) dissociation. We will demonstrate the reason for this improvement analytically for \( \text{H}_2 \) in a minimal basis. [1] A. J. Cohen et al., Chem. Rev. 112 289 (2012), [2] F. Caruso et al., Phys. Rev. Lett. 110 146403 (2013).

1:51PM B15.00014 DFT Predictions of Electronic, Transport, and Bulk Properties of Li_2S, YURI MALOZOVSKY, LASHOUNDA FRANKLIN, Southern Univ & A&M Coll, CHINEDU EKUMA, Louisiana State University and A&M College, DIOLA BAGAYOKO, Southern Univ & A&M Coll, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, DE. — Density functional theory (DFT) is one of the leading first-principles electronic-structure theories. However, molecular dissociation remains a challenge, because it requires a well-balanced description of the drastically different electronic structure at different bond lengths. One typical and well-documented case is the dissociation of both \( \text{H}_2^+ \) and \( \text{H}_2 \), for which all popular DFT functionals fail [1,2]. We start from the Bethe-Goldstone equation to propose a simple orbital-dependent correlation functional which generalizes the linear adiabatic connection approach. The resulting scheme is based on second-order perturbation theory (PT2), but includes the self-consistent coupling of electron-hole pairs, which ensures the correct \( \text{H}_2 \) dissociation limit and gives a finite correlation energy for systems with a (near)-degenerate energy gap. This coupling PT2-like (CPT2) approximation delivers a significant improvement over all existing functionals for both \( \text{H}_2 \) and \( \text{H}_2^+ \) dissociation. We will demonstrate the reason for this improvement analytically for \( \text{H}_2 \) in a minimal basis. [1] A. J. Cohen et al., Chem. Rev. 112 289 (2012), [2] F. Caruso et al., Phys. Rev. Lett. 110 146403 (2013).

2:03PM B15.00015 Metallic 2D Surface State of Silicon by Ionic Liquid gating and observation of Reentrant Insulating behavior, J.J. NELSON, A.M. GOLDMAN, Univ of Minn - Minneapolis — Metal insulator transitions are usually observed in high mobility and low carrier density 2D electron systems. There are several open questions regarding the metallic state including its existence in the limit of zero temperature. The current experimental focus is on the production of higher mobility samples to push the critical carrier density to even lower values, which will increase the effects of the Coulomb interaction. Here we report an unexpected result, the observation of the onset of a metallic state at high carrier densities in silicon gated with the ionic liquid DEME-TFSI. In addition we have observed a return to the insulating state as the carrier density was further increased. This reentrant insulating behavior is an effect that was recently predicted [Das Sarma, S. and Hwang, E. H., PRB 89 121413, 2014].

1Supported in part by NSF/DMR-1263316. Part of this work was carried out at the Minnesota Nanocenter.

11:15AM B16.00001 Computational Discovery of Metal-Organic Frameworks for CO$_2$ Capture and Energy Storage, DONALD SIEGEL, Univ of Michigan - Ann Arbor — Because of their high surface areas, crystallinity, and tunable properties, metal–organic frameworks (MOFs) have attracted intense interest as materials for gas capture and energy storage. An often-cited benefit of MOFs is their large number of possible structures and compositions. Nevertheless, this design flexibility also has drawbacks, as pinpointing optimal compounds from thousands of candidates can be time consuming and costly using experimental approaches. Consequently, computational approaches are garnering increasing importance as a means to accelerate the discovery of high-performing MOFs. Here we combine several computational techniques to identify promising MOFs for CO$_2$ capture and the storage of gaseous fuels (methane and hydrogen). The techniques include: (i) high-throughput screening based on data-mining and empirical correlations [1]; (ii) Monte Carlo simulations based on quantum-mechanically-informed forcefields [2,3]; and (iii) first-principles calculations of thermodynamics and electronic structure [4,5]. For CO$_2$ capture and CH$_4$ storage, these techniques are used to explore metal-substituted variants of M-DODBC and M-HKUST-1. In the case of H$_2$, we identify trends and promising adsorbents amongst 4,000 compounds mined from the Cambridge Structure Database.

1. Goldsmith et al., Chem. Mater. 25, 3373 (2013);
2. Rana et al., J. Phys. Chem. C 118, 2929 (2014);
3. Koh et al., submitted;

11:27AM B16.00002 Computational screening and design of new materials for energy storage and conversion: batteries and thermoelectrics, BORIS KOZINSKY, Bosch Research, Cambridge MA — Understanding the atomic-level origins of thermoelectricity is necessary for the design of higher-performing materials, and we demonstrate that ab-initio computation is a valuable tool. By developing and using advanced methods to compute intrinsic contribution to electron lifetimes from electron-phonon coupling, we are able to predict temperature and doping dependence of electronic transport properties in doped semiconductors. We combine these tools to perform rapid screening of new thermoelectric compositions. In energy storage, a promising path to enabling safe high-energy-density batteries is the introduction of inorganic solid electrolytes that can protect the Li-metal anode. We have achieved a detailed understanding of a promising class of garnet compounds by developing a set of efficient atomistic computational techniques to analyze structure ordering and ionic transport mechanisms. These methods allow us to map the transport phase diagram of a broad range of compositions and to predict new phases and phase transitions. The computational techniques are coupled with a novel software platform AiiDA that combines high-throughput automation with data analysis capabilities.

11:39AM B16.00003 Discovery of optimal zeolites for challenging separations and chemical conversions through predictive materials modeling, J. ILJA SIEPMANN, PENG BAI, MICHAEL TSAPATSIS, University of Minnesota, CHRIS KNIGHT, Argonne National Laboratory, MICHAEL W. DEEM, Rice University — Zeolites play numerous important roles in modern petroleum refineries and have the potential to advance the production of fuels and chemical feedstocks from renewable resources. The performance of a zeolite as separation medium and catalyst depends on its framework structure and the type or location of active sites. To date, 213 framework types have been synthesized and ~330,000 thermodynamically accessible zeolite structures have been predicted. Hence, identification of optimal zeolites for a given application from the large pool of candidate structures is attractive for accelerating the pace of materials discovery. Here we identify, through a large-scale, multi-step computational screening process, promising zeolite structures for two energy-related applications: the purification of ethanol beyond the ethanol/water azeotropic concentration in a single separation step from fermentation broths and the hydroisomerization of alkanes with 18-30 carbon atoms encountered in petroleum refining. These results demonstrate that predictive modeling and data-driven science can now be applied to solve some of the most challenging separation problems involving highly non-ideal mixtures and highly articulated compounds.

1Financial support from the Department of Energy Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences under Award DE-FG02-12ER16362 is gratefully acknowledged.

11:51AM B16.00004 Novel tools for accelerated materials discovery in the AFLOWLIB.ORG repository: breakthroughs and challenges in the mapping of the materials genome, MARCO BUONGIANNI, NARASIMHULU, Univ of North Texas — High-Throughput Quantum-Mechanics computation of materials properties by ab initio methods has become the foundation of an effective approach to materials design, discovery and characterization. This data driven approach to materials science currently presents the most promising path to the development of advanced technological materials that could solve or mitigate important social and economic challenges of the 21st century. In particular, the rapid proliferation of computational data on materials properties presents the possibility to complement and extend materials property databases where the experimental data is lacking and difficult to obtain. Enhanced repositories such as AFLOWLIB, open novel opportunities for structure discovery and optimization, including uncovering of unsuspected compounds, metastable structures and correlations between various properties. The practical realization of these opportunities depends on the development of algorithms for electronic structure simulations of realistic material systems, the systematic compilation and classification of the generated data, and its presentation in easily accessed form to the materials science community, the primary mission of the AFLOW consortium.

1This work was supported by ONR-MURI under contract N00014-13-1-0635 and the Duke University Center for Materials Genomics.

12:27PM B16.00005 Computational search for rare-earth free hard-magnetic materials, JOSÉ A. FLORES LIVAS, SANGEETA SHARMA, JOHN KAY DEWHURST, EBERHARD GROSS, Max Planck Inst Microstructure, MAGMAT TEAM — It is difficult to overstate the importance of hard magnets for human life in modern times; they enter every walk of our life from medical equipments (NMR) to transport (trains, planes, cars, etc) to electronic appliances (for house hold use to computers). All the known hard magnets in use today contain rare-earth elements, to over state the importance of hard magnets for human life in modern times; they enter every walk of our life from medical equipments (NMR) to transport (trains, planes, cars, etc) to electronic appliances (for house hold use to computers). An often-cited benefit of MOFs is their large number of possible structures and compositions. Nevertheless, this design flexibility also has drawbacks, as pinpointing optimal compounds from thousands of candidates can be time consuming and costly using experimental approaches. Consequently, computational approaches are garnering increasing importance as a means to accelerate the discovery of high-performing MOFs. Here we combine several computational techniques to identify promising MOFs for CO$_2$ capture and the storage of gaseous fuels (methane and hydrogen). The techniques include: (i) high-throughput screening based on data-mining and empirical correlations [1]; (ii) Monte Carlo simulations based on quantum-mechanically-informed forcefields [2,3]; and (iii) first-principles calculations of thermodynamics and electronic structure [4,5]. For CO$_2$ capture and CH$_4$ storage, these techniques are used to explore metal-substituted variants of M-DODBC and M-HKUST-1. In the case of H$_2$, we identify trends and promising adsorbents amongst 4,000 compounds mined from the Cambridge Structure Database.

1J.A.F.L. acknowledge financial support from EU’s 7th Framework Marie-Curie scholarship program within the “ExMaMa” Project (329386).
12:39PM B16.00006 Combinatorial Libraries of Transition Metal Oxides Using an Ab Initio High Throughput Approach¹

GUO LI, QIMIN YAN, Lawrence Berkeley Natl Lab, PAUL NEWHOUSE, LAN ZHOU, JOHN GREGOIRE, California Institute of Technology, JEFFREY NEATON, Lawrence Berkeley Natl Lab, UC-Berkeley, KAVLI Energy NanoSciences Institute at Berkeley — Using the results of first-principles calculations and data from the Materials Project (materialsproject.org), we have developed a simple but efficient scheme to theoretically simulate phase coexistence in experimental combinatorial libraries as a function of composition and temperature. In our approach, each experimental sample in a combinatorial library at a fixed composition is considered as a mixture of all the known compounds; and the compound concentrations are determined from calculations of their compositions and relevant thermodynamic potentials. Consequently, multiple compounds can be identified in every sample. To test our approach, we studied the pseudobinary library MnxV(1-x)Oy, and found that, together with those stable compounds predicted in a phase diagram, some of the above-convex-hull compounds, which are viewed unstable, also play a significant role in the combinatorial library. We validated our approach via comparison of calculated X-ray diffraction spectra for multiple phases and recent measurements.

¹This work supported by DOE (the JCAP under Award number DE-SC000499 and the Molecular Foundry of LBNL), and computational resources provided by NERSC.

12:51PM B16.00007 Combinatorial Search of Hydrogen Catalysts Based on Transition Metal Embedded Graphitic Carbons

WOON IH CHOI, BRANDON WOOD, ERIC SCHWEGLER, TADASHI OGITSU, Lawrence Livermore National Laboratory, QUANTUM SIMULATION GROUP TEAM — To find right d-orbital configuration for hydrogen catalyst among embedded transition metal (TM) atoms into the lattice of graphene, we performed high-throughput computational search out of 300 combinatorial material pools. Theoretical criteria, so called descriptors regarding material stability and catalytic activity are considered and we were able to narrow down to ten materials for hydrogen evolution, two for hydrogen oxidation reaction. Since catalytically active sites are related to single TM atom, Volmer-Kasuya type of new reaction pathway is expected for hydrogen evolution. Earth-abundant element Mo, bulk form of which doesn’t show good catalytic activity at all, turns into catalytically active site as it is dispersed atomically and its d-orbitals splits by the symmetry of local coordination at the binding sites.

1:03PM B16.00008 A Computational Method for Materials Design of New Interfaces

JAKUB KAMINSKI, CHRISTIAN RATSCH, University of California Los Angeles, JUSTIN WEBER, MICHAEL HAVERTY, Intel Corporation, SADASIVAN SHANKAR, formerly Intel Corporation — We propose a novel computational approach to explore the broad configurational space of possible interfaces formed from known crystal structures to find new heterostructure materials with potentially interesting properties. In a series of steps with increasing complexity and accuracy, the vast number of possible combinations is narrowed down to a limited set of the most promising and chemically compatible candidates. This systematic screening encompasses (i) establishing the geometrical compatibility along multiple crystallographic orientations of two materials, (ii) simple functions eliminating configurations with unfavorable interatomic steric conflicts, (iii) application of empirical and semi-empirical potentials estimating approximate energetics and structures, (iv) use of DFT based quantum-chemical methods to ascertain the final optimal geometry and stability of the interface in question. For efficient high-throughput screening we have developed a new method to calculate surface energies, which allows for fast and systematic treatment of materials terminated with non-polar surfaces. We show that our approach leads to a maximum error around 3% from the exact reference. The representative results from our search protocol will be presented for selected materials including semiconductors and oxides.

1:15PM B16.00009 Property-based cascade genetic algorithms for tailored searches of metal-oxide nano-structures

SASWATA BHATTACHARYA, LUCA M. GHIRINGHELLI, Fritz-Haber-Institut der MPG, Berlin, DE, NOA MAROM, Physics and Engineering Physics, Tulane University, New Orleans, LA, USA — There is considerable interest in the computational determination of structures of atomic clusters that are detected in spectroscopy experiments. It has been suggested that in photo-emission experiments performed on anions, isomers of small (TiO)n clusters with high electron affinity (EA) are selectively observed rather than those with the lowest energy [1]. For the theoretical modelling of these situations, searching for the energy global minimum of the potential energy surface (PES) is inefficient. By using such an approach, in fact, it is unlikely to find meta-stable isomers that have high EA or low ionization potential (IP), but energy significantly above the ground state. We present an extension to our recently developed ab initio cascade genetic algorithm [2], here tailored to conduct property-based (e.g., high EA, low IP) searches over the PES. The term cascade refers to a multi-stepped algorithm where successive steps employ a higher level of theory, and each step of the next level takes information obtained at the immediate lower level. The new algorithms are benchmarked and validated for (TiO)n clusters (n = 3 − 10, 15, 20). — [1] N. Marom et al. PRL 108, 106801 (2012) [2] S. Bhattacharya et al., NJP, in press (2014).

1:27PM B16.00010 First principles characterization of novel single-layer materials predicted with an evolutionary algorithm¹

BENJAMIN REVARD, WILL TIPTON, Department of Materials Science and Engineering, Cornell University, RICHARD HENNIG, Department of Materials Science and Engineering, University of Florida — Single-layer materials represent a new materials class with potentially transformative properties for applications in nanoelectronics and solar-energy harvesting. With the goal to discover novel 2D materials with unexpected compositions and structures, we have developed a grand-canonical evolutionary algorithm for two-dimensional materials. Here we present the results of applying the algorithm, coupled with first principles total energy methods, to several technologically relevant binary 2D systems, including C-Si, Sn-S and Pbo. We currently use computational techniques to characterize the vibrational and electronic properties of the low energy 2D materials predicted by the algorithm and will report the findings.

¹This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1144153.

1:39PM B16.00011 High-throughput thermodynamics of vibrational degrees of freedom with AFLOW

PINKU NATH, JOSE J. PLATA, CORMAC TOHER, STEFANO CURTAROLO, Duke University, MEMS Department — Phonons are responsible for many thermodynamic properties of the materials. Quasiharmonic approximations have been used successfully as a strong theory in order to incorporate phonon contributions to material properties [1]. We have implemented this method to calculate Gruneisen parameter (GP) which captures the properties related to thermal variations and connects two important thermodynamic variables such as isobaric and isochoric specific heat. This method has been implemented in AFLOW framework for high-throughput computational materials science to accelerate the discovery of new materials and properties interesting for industries. GP has been calculated with the derivative of the frequency and the Feynman-Hellman technique, and the results for both techniques are consistent. We have also calculated coefficient of thermal expansion and bulk modulus using a quadratic fit followed by Birch Murnaghan fit of volume-energy data. For a large set of the materials tested, our results are in agreement with the experimental data.

11:51AM B17.00002 Measurement of the resistance induced by a single atomic impurity on a (7,6) semiconducting carbon nanotube: scattering strength of individual potassium atoms as a function of gate voltage. SHU-JEN HAN, IBM T. J. Watson Research Center — In the last four decades, we have witnessed a tremendous information technology revolution originated from the relentless scaling of Si complementary metal-oxide semiconductor (CMOS) devices. CMOS scaling provides ever-improved transistor performance, density, power and cost, and will continue to bring new applications and functions to our daily life. However, the conventional homogeneous scaling of silicon devices has become very difficult, firstly due to the unsatisfactory electrostatic control from the gate dielectric. In addition, as we look forward to the technology nodes with sub-10 nm channel length, non-Si based channel materials will be required to provide continuous carrier velocity enhancement when the conventional strained-Si techniques run out of steam. Single-walled carbon nanotubes are promising to replace silicon as the channel material for high-performance electronics near the end of silicon scaling roadmap, with their superb electrical properties, intrinsic ultrathin body, and nearly transparent contact with certain metals. This talk discusses recent advances in modeling and experimental works that reveal the properties and potential of ultra-scaled nanotube transistors, separation and assembly techniques for forming nanotube arrays with high semiconducting nanotube purity and tight pitch separation, and engineering aspects of their implementation in integrated circuits and functional systems. A concluding discussion highlights most significant challenges from technology points of view, and provides perspectives on the future of carbon nanotube based nanoelectronics.

1This work is based upon research supported by the National Science Foundation under Grant No. 0955625 and 1006230.

12:03PM B17.00003 Unusual conductance suppression in metallic carbon nanotubes. AMIN AHMADI, RYUICHI TSUCHIKAWA, DANIEL HELIGMAN, University of Central Florida, ZHENGYI ZHANG, Columbia University, EDUARDO MUCCIOLI, University of Central Florida, JAMES HONE, Columbia University, MASA ISHIGAMI, University of Central Florida — Despite many years of research, no measurements have been performed to determine resistance induced by impurities in carbon nanotubes. Over the last few years, we have developed a capability to measure the resistance induced by a single impurity atom on nanotubes with known chirality. Using this capability, we measured the resistance induced by an individual potassium atom on a (7,6) semiconducting carbon nanotube. The “atomic” resistance of potassium is found to be in the kohm range and has a strong dependence on the applied gate voltage. The scattering strength of the p-type (valence band) channel is approximately 20 times greater than that of the n-type (conduction band) channel. We integrate our atomically-controlled experimental result to a numerical recursive Green’s function technique, which can precisely model the experiment, to understand the measured “atomic” resistance and the asymmetry.

2This work is based upon research supported by the National Science Foundation under Grant No. 0955625 and 1006230.

12:15PM B17.00004 Electrical contact to carbon nanotubes encapsulated in hexagonal boron nitride. JHAO-WUN HUANG, CHENG PAN, SON TRAN, Department of Physics and Astronomy, University of California, Riverside, CA, USA, TAKASHI TANIGUCHI, National Institute for Materials Science, Namiki 1-1, Tsukuba, Ibaraki 305-0044, Japan, MARC BOCKRATH, JEANIE LAU, Department of Physics and Astronomy, University of California, Riverside, CA, USA — Hexagonal boron nitride has been an excellent platform for low dimensional materials. We have fabricated ultra clean single-walled carbon nanotube (SWNT) devices encapsulated in hexagonal boron nitride by a dry transfer technique. Contacts to the SWNTs were made by reactive ion etching to expose the ends of SWNTs, followed by metal deposition. Ohmic contacts to SWNTs were achieved. We will discuss the quality of the contacts using different combinations of metals and present latest transport data.

12:27PM B17.00005 One-dimensional Poole-Frenkel conduction in the single defect limit. ELLIOT J. FULLER, DENG PAN, BRAD L. CORSO, O. TOLGA GUL, PHILIP G. COLLINS, Dept. of Physics and Astronomy, University of California Irvine — Theory predicts a range of phenomena in disordered one-dimensional (1D) conductors, but few physical systems exist for direct comparison with experimental observation. Recently, we demonstrated an electrochemical technique for adding a single, isolated point defect to a single-walled carbon nanotube (SWNT) in a field effect transistor device. A point defect, surrounded on either side by quasi-ballistic, semi-metallic SWNT is an ideal system for investigating disorder in 1D. Here, transport and Kelvin probe force microscopy independently demonstrate high-resistance depletion regions that can extend from 0.3 - 2.0 µm wide surrounding the defect site. The defect assists tunneling through this depletion region via a modified, 1D version of Poole-Frenkel conduction. The width of the depletion region is found to depend sensitively on SWNT diameter and carrier density, as expected for a molecular scale wire. Surprisingly, conduction is well described by the 1D Poole-Frenkel model over a wide range of temperature from 77 - 300 K and over a wide range of source-drain bias from 0.1 - 2.0 V.

This work is based upon research supported by the National Science Foundation under Grant No. 0955625 and 1006230.
12:39PM B17.00006 Electronic Properties of Graphene and Single Wall Carbon Nanotubes in the Presence of Hexagonal BN Islands, MOHAMMED ALABBOODI, JAIME BOHORQUEZ, ERIKA PUTZ, HANSIKA SIRIKUMARA, THUSHARI JAYASEKERA, Southern Illinois University, Carbondale — Silicon Carbide (SiC) is a semiconductor material with wide band gap and high thermal conductivity. One of the most promising uses of single walled carbon nanotubes is in a two-level system near the nanotube or noncovalently attached to the nanotube perturbs the current electrostatically. In a second case, a sidewall defect or other covalent modification sensitizes one site along the conductor. Comparative research has helped reveal differences in the transduction mechanism of the two cases and provides design rules for maximizing reliable signals for sensing applications. The covalent modifications are not mere perturbations and they are far more sensitive than noncovalent attachments, for example. However, the new degrees of freedom that accompany covalent disorder often have similar energy scales, leading to multiple independent fluctuations that degrade the overall signal-to-noise. Noncovalent sensitization generally produces a smaller signal amplitude in a background of other low-energy fluctuators, but a well-designed noncovalent linker can result in a highly predictable signal amplitudes. Furthermore, noncovalent fabrication methods are scalable, so that wafer-scale arrays of molecular sensors are most likely to follow this path.

12:51PM B17.00007 Ambipolar Transistors with Heterostructures of Single-Walled Carbon Nanotubes and Zinc Tin Oxide, BONGJUN KIM, SEONPIL JANG, Microelectronics Research Center, The University of Texas at Austin — The unique operation of ambipolar thin-film transistors (TFTs), in which both electrons and holes can be injected and transported in a single device, have attracted significant attention since it was first demonstrated in mid-1990s. In addition to their unique operation, these devices have great potential in complementary-like circuits and novel light emitting transistors. Single-walled carbon nanotubes (SWCNTs) exhibit ambipolar behavior intrinsically; however, SWCNTs under ambient conditions show strong p-type behavior due to adsorption of oxygen and moisture from air. In this work, we will discuss the performance characteristics of ambipolar TFTs with heterostructures of a network of SWCNTs and amorphous zinc tin oxide. These TFTs exhibit well-balanced electron and hole mobilities under ambient conditions, and both carriers are injected through Ti/Au contacts without large injection barriers. Charge transport in this material system will be described. In addition, complementary-like inverters which are composed of two ambipolar TFTs will be demonstrated.

1:03PM B17.00008 Zero-Dimensional Electrical Contact to a One-Dimensional Material, CHENG PAN, JHAO-WUN HUANG, SON TRAN, BIN CHENG, CHUN NING LAU, MARC BOCKRATH, University of California - Riverside — Recent work has shown that one-dimensional contacts can be made to two-dimensional graphene using boron nitride encapsulated graphene structures along with an etch process[1]. Here we report the encapsulation of carbon nanotubes, a one-dimensional material, between layers of boron nitride. By etching the edges we are able to use only the zero-dimensional ends of the carbon nanotube to yield high-quality electrical contacts. This end-contact geometry along with an encapsulated nanotube provides possibilities for the realization of more complex nanotube heterostructure devices. [1] L. Wang et al., Science 342, 614-617 (2013).

1:15PM B17.00009 Sensitizing Carbon Nanotube Transistors for Single Molecule Sensor Applications, PHILIP G. COLLINS, MAXIM AKHTEROV, PATRICK C. SIMS, ELLIOT J. FULLER, O. TOLGA GUL, DENG PAN, Department of Physics and Astronomy, University of California Irvine, Irvine, California 92697, USA — Recent work has demonstrated single-charge sensitivity in two types of carbon nanotube transistors. In one case, a two-level system near the nanotube or noncovalently attached to the nanotube perturbs the current electrostatically. In a second case, a sidewall defect or other covalent modification sensitizes one site along the conductor. Comparative research has helped reveal differences in the transduction mechanism of the two cases and provides design rules for maximizing reliable signals for sensing applications. The covalent modifications are not mere perturbations and they are far more sensitive than noncovalent attachments, for example. However, the new degrees of freedom that accompany covalent disorder often have similar energy scales, leading to multiple independent fluctuations that degrade the overall signal-to-noise. Noncovalent sensitization generally produces a smaller signal amplitude in a background of other lower-energy fluctuators, but a well-designed noncovalent linker can result in a highly predictable signal amplitudes. Furthermore, noncovalent fabrication methods are scalable, so that wafer-scale arrays of molecular sensors are most likely to follow this path.

1:27PM B17.00010 Defect Screening Effects of Fluoropolymer Capping in Single Walled Carbon Nanotube Transistors, SEONPIL JANG, BONGJUN KIM, The University of Texas at Austin, MICHAEL GEIER, MARK HERSAM, Northwestern University, ANANTH DODABALAPUR, The University of Texas at Austin — One of the most promising uses of single walled carbon nanotubes (SWCNTs) is as active channel semiconductor materials in field-effect transistors (FETs). Recent advances in the availability of highly sorted semiconducting SWCNT source material and in printing such nanotubes to realize high-performance thin-film transistors make them very promising candidates for printed electronics. In this presentation, we report on the substantial improvements in the characteristics of SWCNT FET devices and circuits comprised of these devices by the use of coatings of the fluoropolymer containing copolymer, PVDF-TrFE. The origins of these improvements may be attributed to the polar nature of C-F bonds and the local organization of the fluoropolymer at the interfaces with the SWCNTs so as to partially neutralize charged defects. This hypothesis was tested by the experiments using a number of vapor phase polar molecules which produce similar effects on the FET characteristics. The polar vapor experiments show that dipoles can partially neutralize residual charges arising from defects/impurities. The dipole present in polar molecules adopts an orientation that tends to cancel the effects of the charged defect/impurity from the perspective of mobile charges in the SWCNTs.

1:39PM B17.00011 Low Energy Dissipation Nano Device Research, JENNY YU, Cal Poly - Pomona — The development of research on energy dissipation is rapid in energy efficient area. Nano-material power FET is operated as an RF power amplifiers, the transport is ballistic, noise is limited and power dissipation is minimized. The goal is Green-save energy by developing the Graphene and carbon nanotube microwave and high performance devices. Higher performing RF amplifiers can have multiple impacts on widely for broad field, for example communication equipment, (such as mobile phone and RADAR); higher power density and lower power dissipation will improve spectral efficiency which translates into higher system level bandwidth and capacity for communications devices. Thus, fundamental studies of power handling capabilities of new RF (nano)technologies can have broad, sweeping impact. Because it is critical to maximizing the power handling ability of graphene and carbon nanotube FET, the initial task focuses on measuring and understanding the mechanism of electrical breakdown. We aim specifically to determine how the breakdown voltage in graphene and nanotubes is related to the source-drain spacing, electrode material and thickness, and substrate, and thus develop reliable statistics on the breakdown mechanism and probability.

1:51PM B17.00012 ABSTRACT MOVED TO W22.00012 —

2:03PM B17.00013 ABSTRACT WITHDRAWN —

Monday, March 2, 2015 11:15AM - 2:15PM
Session B18 GQI DAMOP: Invited Session: Optimal Control of Quantum Systems
Mission Room 103A - Adolfo del Campo, University of Massachusetts Boston
11:51AM B18.00002 Optimizing control for implementing error correction in superconducting quantum circuits. RAMI BARENDS, Google, Santa Barbara — Fault-tolerant quantum computing hinges on implementing gates and measurement with fidelities above the threshold for error correction schemes. We have constructed a nine qubit device with integrated control and readout to implement the repetition code error correction scheme, a one-dimensional version of the surface code. We show how rapid scans, randomized benchmarking, and the error correction code itself can be used to optimize gates in this complex quantum device to fidelities which allow for protecting states from environmentally-induced bit errors.

12:27PM B18.00003 Controlling open quantum systems: Tools, achievements, limitations. CHRISTIANE KOCH, Universität Kassel — Quantum control is an important prerequisite for quantum devices. A major obstacle is the fact that a quantum system can never completely be isolated from its environment. The interaction with the environment causes decoherence. Optimal control theory is a tool that can be used to identify control strategies in the presence of decoherence. I will show how to adapt optimal control theory to quantum information tasks for open quantum systems and present examples for cold atoms and superconducting qubits. In particular, I will discuss how non-Markovianity of the open system time evolution can be exploited for control. The perspective on decoherence only as the adversary of quantum control is nevertheless too narrow. There exist a number of control tasks, such as cooling and measurement, that can only be achieved by an interplay of control and dissipation. I will show how to utilize optimal control theory to derive efficient cooling strategies when the timescales of coherent dynamics and dissipation are very different. Our approach can be generalized to quantum reservoir engineering, opening up new avenues for control.

1:03PM B18.00004 Quantum Control Engineering with Trapped Ions. MICHAEL BIERCUK, University of Sydney — Technologies fundamentally enabled by quantum mechanics are poised to transform a broad range of applications from computation to precision metrology over the coming decades. This talk will introduce a new field of research which is seeing concepts from control engineering translated to the domain of quantum mechanics in an effort to realize the full potential of engineered quantum technologies. We focus on understanding the physics underlying controlled quantum dynamics in the presence of rapidly fluctuating time-dependent Hamiltonians, leveraging the unique capabilities provided by trapped ions as a model quantum system. Our results introduce and experimentally validate generalized filter-transfer functions which cast arbitrary quantum control operations on qubits as noise spectral filters. We demonstrate the utility of these constructs for directly predicting the evolution of a quantum state in a realistic noisy environment, for developing novel robust control and sensing protocols, and for improving the stability of atomic clocks. This work demonstrates how quantum control can be leveraged to overcome some of the most challenging problems in quantum engineering, and even provide totally new functionality to quantum systems.

1:39PM B18.00005 A general transfer-function approach to noise filtering in open-loop quantum control1. LORENZA VIOLA, Dartmouth College — Hamiltonian engineering via unitary open-loop quantum control provides a versatile and experimentally validated framework for manipulating a broad class of non-Markovian open quantum systems of interest, with applications ranging from dynamical decoupling and dynamically corrected quantum gates, to noise spectroscopy and quantum simulation. In this context, transfer-function techniques directly motivated by control engineering have proved invaluable for obtaining a transparent picture of the controlled dynamics in the frequency domain and for quantitatively analyzing performance. In this talk, I will show how to identify a computationally tractable set of “fundamental filter functions,” out of which arbitrary filter functions may be assembled up to arbitrary high order in principle. Besides avoiding the infinite recursive hierarchy of filter functions that arises in general control scenarios, this fundamental set suffices to characterize the error suppression capabilities of the control protocol in both the time and frequency domain. I will show, in particular, how the resulting notion of “filtering order” reveals conceptually distinct, albeit complementary, features of the controlled dynamics as compared to the “cancellation order,” traditionally defined in the Magnus sense. Implications for current quantum control experiments will be discussed.

1Work supported by the U.S. Army Research Office under contract No. W911NF-14-1-0682.


11:15AM B19.00001 The Use of Theater and the Performing Arts in Science Education and the Teaching of History1. BRIAN SCHWARTZ, Brooklyn College and the Graduate Center of the City University of New York — Over the past 15 years there has been a surge in the general field of the interaction of STEM and the arts including theatre, music dance and the visual arts leading to STEAM. There seems to be no limits to the amount of creativity and diversity of subject matter especially in areas of biography; major science events, scientific and technical innovation, the benefits and dangers of modern science, and science as metaphor. For the past 15 years, I and my colleagues have been running a science outreach series under the title Science & the Performing Arts at the Graduate Center of the City University of New York. The objective is to bring science to students and the public in ways that are engaging, instructive, and artistic and always, content-driven: the medium is the arts; the message is the joy of science. This has resulted in over 120 science and performing arts programs which have been documented on the website http://sciart.commons.gc.cuny.edu/staging-science/outline-of-the-course-staging-science/ with Marvin Carlson, Professor of Theatre at CUNY. An excellent book, Science on Stage: From Doctor Faustus to Copenhagen by Kirsten Shepherd-Barr, can be used. The author co-taught a course titled Staging Science, http://sciart.commons.gc.cuny.edu/staging-science/outline-of-the-course-staging-science/ with Marvin Carlson, Professor of Theatre at CUNY. An excellent book, Science on Stage: From Doctor Faustus to Copenhagen by Kirsten Shepherd-Barr, can be used.

1Supported in part by the National Science Foundation

11:51AM B19.00002 Bruno, Galileo, Einstein: The Value of Myths in Physics. ALBERTO MARTINEZ, University of Texas at Austin — Usually, historical myths are portrayed as something to be avoided in a physics classroom. Instead, I will discuss the positive function of myths and how they can be used to improve physics education. First, on the basis of historical research from primary sources and significant new findings about the Catholic Inquisition, I will discuss how to use the inspirational story of Giordano Bruno when discussing cosmology. Next, I will discuss the recurring story about Galileo and the Leaning Tower of Pisa. Finally, I will discuss how neglected stories about the young Albert Einstein can help to inspire students.
This paper will argue that incorporation of nanoscopic fluctuations is a necessary component for post-yield stress softening and its dependence on annealing time, (ii) the inversion of the strain dependence of nonlinear stress relaxation with the loading rate, (e.g. local stress and local entropy) vs. traditional viscoelastic/viscoelastic models where macroscopic mobility depends upon the macroscopic state. The SCM behavior of polymeric glasses, where (i) temporal fluctuations are explicitly included and (ii) the postulate. In order to acknowledge dynamic heterogeneity, a Stochastic Constitutive Model (SCM) has been developed to describe the nonlinear viscoelastic a critical challenge to the traditional nonlinear continuum models, where both temporal and spatial fluctuations are averaged as a result of the continuum.
1:03PM B20.00004 Atomic motion and physical aging in structural glasses revealed by coherent X-rays, BEATRICE RUTA, ESRF- The European Synchrotron, Grenoble. — Glasses are essential materials in present day science and technology. Nevertheless, many of their properties remain the subject of numerous studies, since their intrinsic non-equilibrium nature poses formidable problems both at the technological and fundamental level. Although their physical aging has practical implication for material science, a microscopic understanding is still missing since experiments that study the dynamics at the microscopic level are extremely challenging [1]. Here, we will report on the first experiments that follow the evolution of the structural relaxation process in glasses at the atomic length scale. Measurements on metallic glasses have revealed the existence of microscopic structural rearrangements, contrary to the common expectation of a completely arrested state [2,3]. In these systems, the dynamics evolves from a diffusive atomic motion in the supercooled liquid phase to a stress-dominated dynamics in the glass, characterized by a complex hierarchy of aging regimes. These finding present many similarities with the dynamics of various complex soft materials, like emulsions, gels and glassy colloidal suspensions [4] suggesting the existence of a common physical mechanism. Albeit this apparent universal out-of-equilibrium dynamics, an even more complex scenario emerges when the investigation is enlarged to other glasses. Measurements on sodium-silicate glasses show a surprising fast atomic motion, even hundreds degrees below the glass transition temperature [5]. In addition, aging of glassy materials is observed on experimental time scales of several hours, not even in the glass transition regions, in marked disagreement with macroscopic studies. This surprising stationary dynamics has been observed also in the case of metallic glasses but only for very large annealing times [2,3] and suggests the existence of a very peculiar relaxation dynamics at the atomic level, unaccounted for in previous experimental and theoretical works [1]. [1] L. Berthier and G. Biroli, Rev. Mod. Phys. 83, 587 (2011). [2] B. Ruta et al. Phys. Rev. Lett. 109, 165701 (2012). [3] B. Ruta et al. J. Chem. Phys. 138, 054508 (2013). [4] L. Cipelletti et al. Faraday Discuss. 123, 237, (2003). [5] B. Ruta et al. Nature Commun. 5, 3939 (2014).

1:39PM B20.00005 Inelastic Neutron Scattering Studies of the Dynamics of Glass-Forming Materials in Confineoment, REINER ZORN, JCSN-1, Forschungszentrum Juelich, D-52425 Juelich, Germany — The study of the dynamics of glass-forming liquids in nanoscopic confinement may contribute to the understanding of the glass transition. Especially, the question of a cooperativity length scale may be addressed. In this presentation, results obtained by inelastic neutron scattering are presented. The first experiments were done to study the α relaxation of glass-forming liquids and polymers in nanoroporous silica. Neutron scattering is a suitable method to study such composite materials because the scattering of the liquid component can be emphasized by the choice of isotopes. By combining time-of-flight spectroscopy and backsctattering spectroscopy it is possible to cover the large dynamical range spanned by the dynamics of glass-forming materials. The experiments demonstrated a broadening of the spectrum of relaxation times with faster as well as slower components compared to the bulk. In later experiments 'soft' confinement in a microemulsion was used to reduce surface effects. In this system a definite acceleration of the dynamics was observed. In all cases the glass-specific fast vibrational dynamics (boson peak) was also studied revealing a characteristic confinement dependence which allows conclusions on its nature. Finally, studies were carried out on polymers by neutron spin echo spectroscopy with the aim of observing the confinement effect on polymer specific dynamics (Rouse motion). These studies showed that a comparatively simple model is able to explain the deviation from bulk behavior.

Monday, March 2, 2015 11:15AM - 2:03PM –
Session B21 GIMS: Detectors, Sensors, & Transducers 201 - Charles Mielke, Los Alamos National Laboratory

11:15AM B21.00001 Neutron detection using far ultraviolet radiation from noble-gas excimers, MICHAEL A. COPLAN, JACOB C. MCCOMB, MOHAMAD I. AL-SHEIKHLY, University of Maryland, ERIC MILLER, CHRISTOPHER M. LAVELLE, Johns Hopkins University Applied Physics Laboratory, ALAN K. THOMPSON, ROBERT E. VEST, National Institute of Standards and Technology, CHARLES W. CLARK, Joint Quantum Institute, NEUTRON OBSERVATORY COLLABORATION — When triggered in a noble gas medium at around atmospheric pressure, low-energy neutron-absorption reactions such as \(^{4}\text{He}(n,\alpha)\text{He}^+\) and \(^{10}\text{B}(n,\alpha)\text{Li}^+\) can generate tens of thousands of far ultraviolet photons per neutron absorbed. In some cases, up to 30% of the \(\sim\) MeV nuclear reaction energy is channeled into far ultraviolet emission. The far ultraviolet photons are produced by noble-gas excimer radiation, to which the noble gas medium is transparent, facilitating efficient optical detection. We report progress in the development of the Neutron Observatory, http://j.mp/N3utr0n, an absolute neutron detector stationed at the fundamental physics beamline at the NIST Center for Neutron Research. Our reaction initiators consist of arrays of thin films of \(^{10}\text{B}\) and boron-coated vitreous carbon foams.


11:27AM B21.00002 Shunt-Enhanced, Lead-Driven Bifurcation of Epilayer GaAs based EEC Sensor Responsivity, STUART SOLIN1, FLETCHER WERNER2, Washington Univ — The results reported here explore the geometric optimization of room-temperature EEC sensor [1] responsivity to applied bias by exploring contact geometry and location. The EEC sensor structure resembles that of a MESFET, but the measurement technique and operation distinguish the EEC sensor significantly; the EEC sensor employs a four-point resistance measurement as opposed to a two-point source-drain measurement and is operated under both forward and reverse bias. Under direct forward bias, the sensor distinguishes itself from a traditional FET by allowing current to be admitted from the gate, referred to as a shunt, into the active layer. We show that the observed bifurcation in EEC sensor response to direct reverse bias depends critically on measurement lead location. A dramatic enhancement in responsivity is achieved via a rotation of the four-point measurement leads. [1] A.K.M. Newaz, et al, Phys Rev B. 79, 195308 (2009).

1S.A.S. is a co-founder of and has a financial interest in PixelLEX, a start-up company whose mission is to market imaging arrays.
2Current Address: Cutting Edge Optronics

11:39AM B21.00003 The GlueX Start Counter, ERIC POOSER, Florida Intl Univ, GLUEX COLLABORATION — The GlueX experiment will study meson photoproduction with unprecedented precision. This experiment will use the coherent bremsstrahlung technique to produce a 9 GeV linearly polarized photon beam incident on an liquid H\(_2\) target. A Start Counter detector has been fabricated to identify the accelerator electron beam, approximately 2 ns apart, and to provide accurate timing information which is used in the level-1 trigger of the experiment. This detector is designed to operate at photon intensities of up to \(10^{7}\gamma/s\) in the coherent peak and provide a timing resolution < 350 ps so as to provide successful identification of the electron beam buckets to within 99\% accuracy. Furthermore, the Start Counter detector will provide excellent solid angle coverage, \(\sim 90\%\) of \(4\pi\) hemericty, and a high degree of segmentation for background rejection. It consists of a cylindrical array of 30 scintillators with pointed ends that bend towards the beam at the downstream end. Silicon PhotoMultiplier (SIPM) detectors have been selected as the readout system. The physical properties of the Start Counter have been studied extensively. The results of these studies are discussed.

1This material is based upon work supported by the U.S. Department of Energy, Office of Science, and Office of Nuclear Physics under contracts DE-AC05-06OR23177 & DE-FG02-99ER41065.
12:03PM B21.00005 Ranged Isotope Detection and Identification Using Gas Ionization, BENJAMIN GRABER, DONG HO WU, US. Naval Research Laboratory — Radioactive isotopes produce gamma rays, and the gamma rays ionize gases. Since an isotope has a characteristic gamma energy spectrum, and also gas molecules have characteristic ionization energies, we speculated that the gas ionization rate would uniquely depend on not only the type of isotope but also the type of gas. Our experiments have confirmed these concepts — the experiments clearly exhibit that different isotopes produce different ion densities in different gases. Utilizing a set of four gas cells with embedded ion counters, it is then possible to construct a standoff nuclear-isotope detection system. This system has demonstrated a standoff detection and identification of isotopes at a substantial distance (more than 5 m) while testing Am, Ba, Co, Cs and Na isotopes of less than 75 uCi activity. Our prototype is cheaper, faster and easier to operate than commercial gamma-ray spectrometers. In this talk our experimental results and theoretical models for gas ionization will be presented.

12:15PM B21.00006 Broadband Coupling of Microwave Signals to Thin Conductors in Cryogenic Systems1, SCOTT DIETRICH, WILLIAM MAYER, JESSE KANTER, Graduate Center, City University of New York, New York 10016, USA, SERGEY VITKALOV, CUNY-CCNY — Three techniques are used to determine the microwave (MW) coupling through semi-rigid coaxial lines to samples installed on stages at the bottom of long probes (≈1m or longer) placed in a liquid helium cryostat. Samples are mounted between the MW delivery line and ground and are placed in parallel with a 50Ω impedance-matching terminal resistor. One method to determine the delivery of MW signal uses bolometric measurements of the MW power dissipated at the terminal resistor. Another method employs reflection measurements to obtain the reflection coefficient Γ of the sample stage, which is sensitive to variations in sample resistance. A third method initially uses the sample itself as a detector of a small, amplitude-modulated MW signal; the resulting variations of sample resistance are then applied as a calibration factor. Each method appears to reliably measure the actual MW signal delivered to the sample. The presented studies focus on two different electronic systems: GaAs quantum wells and La(2–x)Sr,xCuO superconducting films.

1Work supported by National Science Foundation (ECCS 1128459) and (DMR 1104503).

12:27PM B21.00007 ABSTRACT WITHDRAWN —

12:39PM B21.00008 ABSTRACT WITHDRAWN —

12:51PM B21.00009 SAW devices based on novel surface wave excitations, JOEL THERRIEN, LIAN DAI, ECE Dept, U Mass Lowell — Surface Acoustic Wave (SAW) devices have applications in radio frequency and microwave filtering as well as highly sensitive sensors. Current SAW design employs the use of an array of electrode pairs, referred to as Inter-Digitated Transducers (IDTs) for creating and receiving surface waves on piezoelectric substrates. The pitch of the electrode pairs along with the properties of the substrate determine the operating frequency. The number of electrode pairs determines the bandwidth of the emitted waves. We will present a novel configuration that eliminates the need for the IDTs and replaces with a single circular electrode located inside a larger ground ring. This configuration induces drumhead modes. We will show that the resonant frequencies follow the zeros of Bessel functions of the first kind. Applications in RF filtering and mass sensing will be presented.

1:03PM B21.00110 Multifunctional sensors operating at 300 K based on quasi-ballistic InSb quantum well nanostructures, ADAM GILBERTSON, DOMINIC MOSELEY, MIKHAIL KUSTOV, STUART SOLIN1, LESLEY COHEN, Imperial College London, SIMON BENDING, University of Bath — The high mobility (μ) of InSb quantum well (QW) heterostructures at 300 K makes them ideally suited for both magnetic and optical sensing. While macroscopic InSb Hall sensors offer the best magnetic sensitivity at 300 K of any material, the operation of sub-micron InSb QW Hall probes have not been reported. Ballistic transport at 300 K in nano-InSb devices was recently described [1]. Here we report the 300 K sensing properties of InSb QW structures fabricated into scanning probe geometries operating in the photoconductive (PC), Hall, and magnetocductive modes. Sub-micron InSb QW probes exhibit excellent magnetic sensitivity <1μT/Hz and are demonstrated in a scanning Hall probe measurement. InSb QWxs exhibit long lived negative photoconductivity in the visible to near-IR for cw excitation, however, significant improvements in dynamic response are found with ac modulated techniques. From spatially resolved PC measurements we determine μT ~ 3.5 x 10^−3 cm²/V. These results provide a benchmark for developing novel InSb QW-metal hybrid nanosensors [2].


1On sabattical from Washington University in St. Louis.

1:15PM B21.00011 A Simple Instrument for Measuring Surface Forces in Liquids, JAMES HANNON, RUDOLF TROMP, RICHARD HAIGHT, ARTHUR ELLIS, IBM Research Division — We have constructed a simple instrument to measure the interaction force between two surfaces in solution, or in vacuum. Specifically, we measure the interaction between a lens and a thin silicon cantilever. Either the lens, or the cantilever (or both) can be coated with the species of interest. When the lens is brought close to the cantilever surface, the force of interaction causes the cantilever to bend. By measuring the deflection as a function of the distance between the lens and cantilever, the long-range interactions between the two surfaces can be determined. Our approach includes three important innovations. First, a commercial lens with a radius of ≈1 cm is used for one surface. The relatively large radius of curvature enhances force sensitivity of the method. Second, we use optical interference (Newton’s Rings) to determine the distance between lens and cantilever with ~ 1 nm accuracy. Third, we make use of thin crystalline cantilevers (100 μm thick) whose elastic properties can be easily measured. We have achieved a force sensitivity F/R better than 0.001 mN/m. I will discuss the theory of operation of the new instrument and describe measurements made on SiO2 and metal oxide surfaces in water.

11:51AM B21.00004 Alpha-particle emissivity screening of materials used for semiconductor manufacturing, MICHAEL GORDON, KENNETH RODBELL, IBM TJ Watson Research Center — Single-Event Upsets (SEU’s) in semiconductor memory and logic devices continue to be a reliability issue in modern CMOS devices. SEU’s result from deposited charge in the Si devices caused by the passage of ionizing radiation. With technology scaling, the device area decreases, but the critical charge required to flip bits decreases as well. The interplay between both determines how the SEU rate scales with shrinking device geometries and dimensions. In order to minimize the alpha-particle component of SEU, the radiation in the device environment has to be at the Ultra-Low Alpha (ULA) activity levels, e.g. less than 2nCi/khr-cm². Most detectors have background levels that are significantly larger than that level which makes making these measurements difficult and time consuming. A new class of alpha particle detector, utilizing pulse shape discrimination, is now available which allows one to make measurements quickly with ultra-low detector background. This talk will discuss what is involved in making alpha particle measurements of materials in the ULA activity levels, in terms of calibration, radon adsorption mitigation, the time required for obtaining reasonable statistics and comparisons to other detectors.
1:27PM B21.00012 Particle Imaging, Characterization and Extinction Measurement with Digital Holography. NAVA SUBEDI, MATTHEW BERG, Mississippi State University — This work extends the concept of application of digital holographic microscopy (DHM) from particle imaging to the measurement of photothermally induced particle expansion and energy flow that gives rises to extinction cross section. In this work, a particle is illuminated by a pulsed laser and the interference pattern produced by superposition of particle’s forward-scattered wave with the incident wave is recorded by a digital camera. This recorded pattern constitutes a digital hologram which can be numerically processed to get image, photo-thermally induced expansion and extinction cross-section of the particle. These information of the particle are the basic requirements for the characterization of respirable-sized (1-10 μm) aerosol particles.

1:39PM B21.00013 Highly sensitive direct conversion ultrasound interferometer. OLEKSY SVITELSKY, Gordon College, MA 01942, JOHN GROSSMANN, Colgate University, NY 13436, ALEXEY SUSLOV, National High Magnetic Field Laboratory, FL 32310 — Being invented more than fifty years ago, the ultrasonic pulse-echo technique has proven itself as a valuable and indispensable non-destructive tool to explore elastic properties of materials in engineering and scientific tasks. We propose a new design for the instrument based on mass-produced integral microchips. In our design the radiofrequency echo-pulse signal is processed by AD8302 RF gain and phase detector (www.analog.com). Its phase output is linearly proportional to the phase difference between the exciting and response signals. The gain output is proportional to the log of the ratio of amplitudes of the received to the exciting signals. To exclude the non-linear fragments and to enable exploring large phase changes, we employ parallel connection of two detectors, fed by in-phase and quadrature signals respectively. The instrument allowed us exploring phase transitions with precision of Δϕ<10^-7 (ϕ is the ultrasound speed). The high sensitivity of the logarithmic amplifiers embedded into AD8302 requires good grounding and screening of the receiving circuitry.

1:51PM B21.00014 Resonance Splitting in RF Cylindrical Cavities with Circular Apertures. LUIS MARTINEZ, University of California, Merced — Coupling of two RF cylindrical cavities is achieved with the use of a single, thin, circular aperture (iris) located between the two cavities in the transverse plane. A tunable splitting, in which the single resonance splits into a closely spaced doublet for the TE011 mode is experimentally observed. It is found that the frequency spacing of the doublet is related to the circular aperture size. A model based on the analogy of a multi-mirror optical Fabry-Perot cavity, in which the frequency spacing of the doublet is related to the reflection coefficient, is found to be in excellent agreement with the experimental results. Calculation of the reflection coefficient for the circular aperture is performed using the closed form solutions derived from scattering amplitude and circular aperture theory.

Monday, March 2, 2015 11:15AM - 2:03PM — Session B22 DCMP: Optical Studies of Strongly Correlated Systems 202A.

11:15AM B22.00001 Spatially ordered transit through a canonical Mott transition revealed by cryogenic nano-imaging. A.S. MCLEOD, University of California San Diego, 9500 Gilman Dr, La Jolla, CA 92093, E. VAN HEUMEN, University of Amsterdam, Sciepark 904, 1098 XH Amsterdam, Netherlands, J.G. RAMIREZ, S. WANG, T. SAERBECK, S. GUENON, M. GOLDFLAM, L. ANDEREGG, P. KELLY, A. MUELLER, M.K. LIU, I.K. SCHULLER, D.N. BASOV, University of California San Diego, 9500 Gilman Dr, La Jolla, CA 92093 — We report on temperature-dependent (24K-300K) near-field infrared (IR) imaging of the canonical Mott insulator VO2 across its temperature-driven metal-insulator transition. This was accomplished using a home-built s-SNOM (scattering-type scanning near-field optical microscope) affording unprecedented spatial resolution (~20 nm) to surface optical properties with simultaneously acquired AFM topography at cryogenic temperatures. Our VO2 thin film is found to exhibit extreme nano-scale electronic heterogeneity near the Mott transition (170K) from paramagnetic metal to antiferromagnetic insulator. A sequence of nano-IR images acquired across the transition provides a direct probe of the metal/insulator fill fraction in accord with an observed percolation-driven resistive transition. We resolve dynamic evolution of electronic phases and a crossover from long- to short-range spatial correlations. Identification of the attendant VO2 structural transition by X-ray diffraction reveals an unexpected decoupling of Mott and structural transitions. Supported by nano-IR imaging of remnant metallic puddles below the Mott transition, these observation point towards a novel low-temperature metallic phase.

11:27AM B22.00002 New Insights into the Diverse Electronic Phases of a Novel Vanadium Dioxide Polymorph: A Terahertz Spectroscopy Study. JAMES LOUREMBAM, Nanyang Technological University, AMAR SRIVASTAVA, National University Singapore, CHAN LA-O-VORAKIAT, Nanyang Technological University, HELENE ROTELLA, THIRUMALAI VENKATESAN, National University Singapore, ELBERT CHIA, Nanyang Technological University — A remarkable feature of vanadium dioxide is that it can be synthesized in two polymorphs. The electronic phase diagram is constructed, revealing that the width and onset of the metal-insulator transition in the B phase develop differently from the two polymorphs. The conductivity mechanism in the metastable layered polymorph VO2(B) thin films has been investigated by terahertz time-domain spectroscopy (THz-TDS). In VO2(B), a critical temperature of 240 K marks the appearance of a non-zero Drude term in the observed complex conductivity, indicating the evolution from a pure insulating state towards a metallic state. In contrast, the THz conductivity of the well-known VO2(M) is well fitted only by a modification of the Drude model to include backscattering. We also identified two different THz conductivity regimes separated by temperature in these two polymorphs. The electronic phase diagram is constructed, revealing that the width and onset of the metal-insulator transition in the B phase develop differently from the M1 phase.

11:39AM B22.00003 On the Repeatability of Domain Formation and Growth During the Metal-Insulator Transition in Vanadium Dioxide Films. T.J. HUFFMAN, PENG XU, M.M. QAZILBASH, Department of Physics, College of William and Mary, BONG-JUN KIM, HYUN-TAK KIM, Electronics and Telecommunications Institute (ETRI) — Nanoscale phase coexistence between insulating and metallic domains has been observed in films of vanadium dioxide (VO2) using scattering-type scanning near-field infrared microscopy (s-SNIM). When insulating VO2 transitions to the metallic phase, small regions of the metallic phase first nucleate, and then grow as the metal-insulator transition (MIT) progresses. It is an open question if the patterns of insulating and metallic VO2 in a given scan area are reproducible upon repeated thermal cycling across the MIT. To investigate this matter, we image the same area of a VO2 film with s-SNIM over multiple thermal cycles through the MIT. In this way, we uncover the relative contributions of deterministic and random events occurring at the nanoscale during the progress of the MIT. Our experiments reveal the nature of phase coexistence in VO2 films and the real-space dynamics of the MIT.

1This work was supported by the National Science Foundation.
12:03PM B22.00005 Closing of the pseudogap in Fe$_{1.03}$Te$^1$. C.C. HOMES, Y.M. DAI, J. SCHNEELOCH, R.D. ZHONG, Q. LI, G.D. GU, Condensed Matter Physics and Materials Science Dept., Brookhaven National Laboratory, Upton, New York, A. AKRAP, Ecole de Physique, Université de Genève, CH-1211 Genève 4, Switzerland — The optical properties of strongly-correlated Fe$_{1.03}$Te have been measured over a wide frequency range for light polarized in the a-b planes at temperatures above and below the structural and magnetic transition, $T_N \approx 68$ K. For $T > T_N$, in the paramagnetic state, the resistivity is increasing with decreasing temperature, and the optical conductivity is flat over much of the infrared region, except for a weak Drude-like response at low frequency. Below $T_N$, in the antiferromagnetic state, there is dramatic increase in the low-frequency conductivity with a commensurate transfer of spectral weight (area under the conductivity curve) from low to high energy. The roughly constant value of the scattering rate indicates that it is the plasma frequency ($\omega_p$) that is increasing. This increase in $\omega_p \propto n/m^* \propto 1/T$ is associated with the closing of the pseudogap on the electron pocket resulting in an increase in the number of carriers (n). In addition, below $T_N$ the effective mass ($m^*$) is also thought to decrease. Both effects lead to an increase in $\omega_p$ on the electron pocket.$^{[1]}$

1Supported by the DOE under Contract No. DE-AC02-98CH10886.


12:15PM B22.00006 Optical spectroscopy of the metallic Nd$_{1-x}$TiO$_3$ system. NATHAN ARMSTRONG, McMaster University, ATHENA SEFAT, Materials Science and Technology Division, Oak Ridge National Laboratory, JING YANG, Tianjin University, JOHN GREEDAN, THOMAS TIMUSK, McMaster University — The neodymium titanate system, Nd$_{1-x}$TiO$_3$, exhibits two metal-to-insulator transitions at $x = 0.08$ and $x = 0.24$. The n-type metallic regime between the two transitions exhibits the Fermi liquid $T^2$ DC resistivity over a large range of temperatures. We have measured the reflectivity of the $x = 0.15$ and $x = 0.2$ samples from 4 meV to 5.5 eV at temperature from 15 K to 300 K. Previous optical work by Yang et al. measured an insulating, a semiconducting, and a metallic sample. The metallic sample was found to have the Fermi liquid $\omega^2$ dependence in the scattering rate. We reevaluate the Yang et al. data for the $x = 0.095$ metallic sample, just inside the MIT, and compare it to our samples deeper in the metallic regime that have $T^2$ coefficients an order of magnitude smaller.

12:27PM B22.00007 Resilient quasiparticles in Ruthenates: transport properties within LDA+DMFT method. XIAOYU DENG, KRISTIAN HAULE, GABRIEL KOTLIBAR, Rutgers Univ — Many Rutheniums are strongly correlated metals with Fermi Liquid behavior found only a small temperature scale. Non-Fermi signatures appear in both their resistivity and optical conductivity. We study the transport properties of a set of Ruthenates within first principle methods in combination with dynamical mean field theory and find reasonable agreement with experimental findings. The non-Fermi-liquid features are attributed to the temperature dependence of resilient quasiparticles, which survives above the Fermi liquid temperature scale and exhibits a strong temperature dependence in their effective mass enhancement and scattering rate.

12:39PM B22.00008 Abrupt changes in electronic relaxation and lattice dynamics across the structural phase transition in lightly doped Ca$_3$RuO$_4$ observed via time-resolved optical reflectivity. HAO CHU, DARIUS TORCHINSKY, LIUJIAN ZHAO, PATRICK RALL, Institute for Quantum Information and Matter, California Institute of Technology, JASMINKA TERRACE, GANG CAO, Department of Physics and Astronomy, University of Kentucky, DAVID HSIEH, Institute for Quantum Information and Matter, California Institute of Technology, INSTITUTE FOR QUANTUM INFORMATION AND MATTER, CALIFORNIA INSTITUTE OF TECHNOLOGY COLLABORATION, DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF KENTUCKY COLLABORATION — Ca$_3$RuO$_4$ is a multiband strongly correlated electron system that undergoes a structural phase transition at $T_s$ 360K that is concomitant with an insulator-to-metal transition and a rearrangement of orbital occupancy. Understanding its structural and electronic response to ultrafast optical excitation can provide insight about the microscopic mechanism of this phase transition. We report temperature and fluence dependent time resolved optical reflectivity measurements from lightly doped Ca$_3$RuO$_4$ single crystals. Abrupt changes in both the electronic relaxation dynamics and multiple lattice vibrational modes are observed, including the softening of two optical phonon modes as $T_s$ is approached. We will discuss the relevance of our results to existing theories of the mechanism underlying the structural phase transition in Ca$_3$RuO$_4$ as well as the possibility of photo-inducing this phase transition on ultrafast time scales.

12:51PM B22.00009 THz investigation of non-Drude transport in the ferromagnetic metal SrRuO$_3$. GRACE BOSE, Y. LUBASHEVSKY, The Institute for Quantum Matter, Department of Physics and Astronomy, Johns Hopkins University, D. E. SHAI, Department of Physics, Laboratory of Atomic and Solid State Physics, Cornell University, C. ADAMO, Department of Materials Science and Engineering, Cornell University, D. G. SCHLOM, K. M. SHEN, Kavli Institute at Cornell for Nanoscale Science, N. P. ARMITAGE, The Institute for Quantum Matter, Department of Physics and Astronomy, Johns Hopkins University — While the highly correlated complex oxide perovskite ferromagnet SrRuO$_3$ has been studied for decades, interest remains in its unusual transport properties. In view of this, we present time-domain terahertz conductivity measurements taken from room temperature to 5K on a low disorder film of SrRuO$_3$. Previous optical measurements have shown a deviation from Fermi liquid transport predictions in this material. We investigate these deviations in the context of both an extended Drude model analysis and the previously used fractional power law form. The high quality of our film, reflected in its large residual resistivity ratio, allows us to better isolate the inelastic scattering channels, which were masked by disorder in earlier studies. We also comment on the possible ferromagnetic resonance present in our optical data.


Observation of a third, previously unknown charge-density-wave order in RTe$_3$ by optical spectroscopy

Antiferromagnetic fluctuations in the metallic state of organic superconductor κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br observed by Raman scattering

Optical Conductivity in the Cuprates and Gauge/Gravity duality

Optical Conductivity in the Cuprates from Unparticle

Why a quantum wire can act as an optical amplifier

Applications of the explicitly correlated Gaussian approach to cold few-atom systems

With infinitely large interspecies s-wave scattering length consisting of up to ten particles. As a second example, we investigate the behavior of weakly-bound as aspects of ultracold gaseous and liquid few-atom systems using explicitly correlated Gaussians. In the ultracold regime, where the de Broglie wave length is setting are capable of yielding power law optical conductivities observed in the cuprates is examined critically. We first show that charge density in the Q-lattice conducor simply expanding a four-point correlation function using Wick's theorem is not sufficient to obtain the power law. We investigate the role played by non-Wick power law behavior. We apply unparticle-gauge couplings and linear response theory at finite temperature to calculate the optical conductivity. We find that scale-invariant matter with an algebraic propagator, is a candidate to explain this phenomenon. We explore the possibility of using unparticle to produce such processes in determining the power law.

We would like to thank NSF Contract No. DMR-1104909 for partially funding of this project. K. L. is supported by the Department of Physics at the University of Illinois and by the Ministry of Science and Technology, Royal Thai Government.

We present results of a recent study of the magnetic field induced second and third charge-density-wave (CDW) orders in the organic superconductor R$_x$Cu[N(CN)$_2$]Cl. The occurrence of the second CDW order with the wave vector $q_2$ has been observed in many R$_x$Cu[N(CN)$_2$]Cl compounds, while the third CDW order has only been observed in a few R$_x$Cu[N(CN)$_2$]Cl compounds. In this talk, we will discuss the observation of the third CDW order in the series by optical spectroscopy probe. This third CDW order also evolves systematically with the size of R element. With increased chemical pressure, the first and third CDW orders are both substantially suppressed and compete with the second one by depleting the low energy spectral weight. A complete phase diagram for the multiple CDW orders in this series is established. We acknowledge B. Cheng and R. H. Yuan for their help in the experiments.

Donald and Shirley Jones Graduate Research Fellowship

We discuss the fundamental issues associated with the magnetoplasmon excitations in a semiconducting quantum wire characterized by a harmonic confining potential and subjected to an applied (perpendicular) magnetic field. Essentially, we focus on the device aspects of the intersubband collective (magnetoroton) excitation, which observes a negative group velocity (NGV) between maxon and roton. Consequently, it leads to tachyon-like (superluminal) behavior without one's having to introduce the negative energies. Existence of the NGV is a clear manifestation of a medium with population inversion brought about due to a metastable state caused by the magnetic field that satisfies the condition $B > B_c$. $B_c$ being the threshold value below which the magnetoroton does not exist. The interest in NGV is based on anomalous dispersion in a medium with inverted population, so that gain instead of absorption occurs at the frequencies of interest. A medium with an inverted population has the remarkable ability of amplifying a small optical signal of definite wavelength, and serves as an optical amplifier. Examining the life-time of magnetorotons leads us to infer that relatively smaller magnetic fields are optimal.


Applications of the explicitly correlated Gaussian approach to cold few-atom systems

Supported by the NSF.
11:51 AM B23.00002 Very accurate variational non-relativistic non-Born-Oppenheimer atomic & molecular spectra predictions employing explicitly correlated Gaussian basis functions\(^1\), KEEPER SHARKEY, University of Arizona — Due to the fast increasing capabilities of modern computers it now becomes feasible to calculate spectra of small atom and molecules with accuracy which matches the accuracy of high-resolution measurements. The algorithms for the calculations are directly derived from the first principles of quantum mechanics. The Hamiltonian operator used in the approach is called the internal Hamiltonian and is obtained by rigorously separating out the center-of-mass motion from the laboratory-frame Hamiltonian. Algorithms for determining the isotopic energy shifts of L=0 and M=0 states of atoms were implemented and tested in the calculations of the ground \(^5S\) state of the nitrogen atom. Bound states of diatomic molecules corresponding to the total angular momentum quantum number equal to one (\(N=1\)) was derived and implemented and was tested in the calculations of the \(N=–1, v=0, \ldots, 22\) states of the HD\(^+\) ion and in the calculations of the ortho-para spin isomerization of the hydrogen molecule in its all bound vibrational states. This has lead to the development of a new studying of muonic molecules (\(dp, tp\) and \(td\)). The algorithms for calculating rovibrational states of small molecules is currently being extended to H\(_2^+\) using \(\sin\) and \(\cos\) ECGs.

\(^1\)National Science Foundation

12:03 PM B23.00003 Challenges and advances in calculations of highly non-adiabatic systems employing the explicitly correlated Gaussian functions, NIKITA KIRNOSOV, The University of Arizona — Accurate calculations of the highly non-adiabatic systems have been drawing attention for several decades. While most accurate modern methods allow outstanding accuracy, they are limited to only three or four particles. In the current work we have developed a highly accurate method which is not limited by the number of particles in the system but is only limited by the computer resource available. Examples of calculations of exotic systems with and without rotational excitation and of conventional electronic molecule are presented and the future development of the method is discussed.


12:15 PM B23.00004 High precision variational calculations of five-electron systems: S-states of boron, SERGIY BUBIN, Nazarbayev University, LUDWIK ADAMOWICZ, University of Arizona — We have performed benchmark variational calculations of the lowest two S-states of the boron atom. The spatial part of the wave function has been expanded in terms of all-particle explicitly correlated Gaussians, whose nonlinear variational parameters were extensively optimized. We have also computed leading relativistic corrections and various expectation values for both states. This work demonstrates that the level of accuracy achievable in calculations of five-electron atoms is now approaching the one previously seen only in three- or four-electron systems.

12:27 PM B23.00005 Calculation of energies of three-electron systems in a strong magnetic field using Explicitly Correlated Gaussian Basis, JORGE SALAS, KALMAN VARGA, Vanderbilt University — Strong magnetic fields can significantly alter the properties of atoms and allow the formation of stable negative ions such as He\(^–\). We have calculated the energies of systems comprised of three electrons in the presence of strong magnetic fields by using the Stochastic Variational Method with deformed Explicitly Correlated Gaussian basis. This approach yields accurate values for three-electron systems and predicts that the He\(^–\) ion in a strong magnetic field has stable states, within the non-relativistic framework, in the infinite nuclear mass approximation. The energy spectrum and the properties of three-electron systems as a function of the strength of the magnetic field show the effect of the rivalry between the Coulomb interaction and the magnetic confinement.


12:39 PM B23.00006 High-order Path Integral Monte Carlo methods for solving strongly correlated fermion problems, SIU A. CHIN, Texas A&M Univ — In solving for the ground state of a strongly correlated many-fermion system, the conventional second-order Path Integral Monte Carlo method is plagued with the sign problem. This is due to the large number of anti-symmetric free fermion propagators that are needed to extract the squared of the ground state wave function at large imaginary time. In this work, I show that optimized fourth-order Path Integral Monte Carlo methods, which uses no more than 5 free-fermion propagators, in conjunction with the use of the Hamiltonian energy estimator, can yield accurate ground state energies for quantum dots with up to 20 polarized electrons. The correlations are directly built-in and no explicit wave functions are needed.

This work is supported by the Qatar National Research Fund NPRP GRANT #5-674-1-114

12:51 PM B23.00007 Beyond the Born-Oppenheimer approximation with quantum Monte Carlo, NORM TUBMAN, University of Illinois - Urbana Champaign, ILKKA KYLANPAA, Tampere University of Technology, SHARON HAMMES-SCHIFFER, DAVID CEPERLEY, University of Illinois - Urbana Champaign — We develop tools that enable the study of non-adiabatic effects with variational and diffusion Monte Carlo methods. We introduce a highly accurate wave function ansatz for electron-ion systems that can involve a combination of both clamped ions and quantum nuclei. We explicitly calculate the ground state energies of H\(_2\), LiH, H\(_2\)O and FHF\(^–\) using fixed-node quantum Monte Carlo with wave function nodes that explicitly depend on the ion positions. The obtained energies implicitly include the effects arising from quantum nuclei and electron-nucleus coupling. We compare our results to the best theoretical and experimental results available and find excellent agreement.

1 This work is supported by the Qatar National Research Fund NPRP GRANT #5-674-1-114

1:03 PM B23.00008 Physical Sputtering vs. Gas Assisted Etching of Silicon Dioxide with a Gallium Focused Ion Beam: Elucidating Experiments via Monte Carlo Simulations, RAJENDRA TIMILSINA, University of Tennessee Knoxville, SHIDA TAN, RICHARD LIVENGROOT, Intel Corporation, PHILIP RACK, University of Tennessee Knoxville and CNMS, Oak Ridge National Laboratory — In order to increase ion beam nanomachining precision and improve imaging resolution, fine tuning of the ion beam profile is absolutely necessary. To understand the effects of ion beam tails, experiments and Monte Carlo simulations were conducted with a 40 keV gallium beam with and without gas assisted chemical etching. A gallium ion beam was scanned in an area of 25x25 nm\(^2\) on a silicon dioxide film with and without a localized XeF\(_2\) gas at 1pA current. Four different ion doses (0.23, 0.9, 1.8 and 3.6 nC/\(\mu\)m\(^2\)) were experimentally considered to study the sputtered and etched via profiles. Monte Carlo simulations using EnvisiON program was performed to elucidate the sputtered and gas-assisted etch process. New features including gas-assisted etching by secondary electrons and a binary collision model to dissociate the precursor molecules were introduced. Sputtered via and gas assisted etching (XeF\(_2\) precursor gas) via profiles with various gas-assist pressures were studied to understand the experimental temporal behavior. Various contributions including sputtering from primary, forward scattered, backscattered ions as well as etching by recoiled atoms and secondary electrons will be discussed.
unbiased way. First we consider a multiband model for graphene, where we integrate out the resulting effective interactions to the cRPA. The employed wick-ordered fRG scheme generalizes the cRPA approach by including all interaction channels in an interactions. Here we present applications of a constrained functional renormalization group (cfRG) scheme to two simple multi-band systems and compare the solids targeting the bands near the Fermi level, the constrained random phase approximation (cRPA) has become an appreciated tool to compute the effective, MICHAEL KINZA, CARSTEN HONERKAMP, RWTH Aachen University — In the derivation of low-energy effective models for

1:15PM B23.00009 Fully Exponentially Correlated Wave Functions for Few-Body Systems . FRANK E. HARRIS, University of Utah and University of Florida — Analytical methods now make practical the study of three- and four-body problems using wave functions in which all the interparticle distances (and not just their squares) occur as exponentials. This type of basis yields wave functions that exhibit superior initial convergence toward exact results and that facilitate the accurate treatment of systems in which no one of the particles is far more massive than the others. Progress in the practical use of this formulation is reviewed.

1:27PM B23.00010 Calculating Properties of Finite Mass Atoms . STEVEN ALEXANDER, Southwestern University, R.L. COLDWELL, Retired — Most atomic calculations assume that the mass of the nucleus is finite. If one is interested in evaluating atomic properties to high precision then this approximation cannot be made. We have developed a simple method that includes the kinetic energy of the nucleus into atomic calculations and does not increase the time or the complexity of these calculations. Our results for a variety of properties for several different atoms will illustrate some of the advantages of this method.

1:39PM B23.00011 ABSTRACT WITHDRAWN –

1:51PM B23.00012 Electron shake-off and recoil following 6He beta decay\(^1\) . GORDON W.F. DRAKE, EVA SCHULHOFF, University of Windsor — When the helium isotope \(^6\)He undergoes beta decay in the process \(^6\)He \rightarrow \(^6\)Li \(e^- + \nu\), the atomic electrons suddenly find themselves in a \(^6\)Li\(^+\) environment. The electrons subsequently redistribute themselves over all possible states of the \(^6\)Li\(^+\) ion, including the continuum leading to \(^6\)Li\(^{3+}\) and \(^6\)Li\(^{4+}\). There is currently considerable interest in studying the recoil ions in connection with experiments to look for evidence of new physics as revealed by angular correlations between the electron and the antineutrino \([1]\). We will present calculations employing Stieltjes imaging techniques in Hylleas coordinates to study the probabilities for the shake-up and shake-off mechanisms, and especially the additional recoil accompanying the emission of the shake-off electrons.

\(^1\)Research supported by the Natural Sciences and Engineering Research Council for Canada

2:03PM B23.00013 Coulombic few-body systems in the adiabatic hyperspherical representation\(^1\) . KEVIN DAILY, Purdue Univ, JAVIER VON STECHER, Seagate Technology, CHRIS GREENE, Purdue Univ — We study few-body systems consisting of charged particles in free space using the adiabatic hyperspherical representation. We use a correlated Gaussian basis at a fixed hyperradius with efficiently calculated matrix elements \([1]\) to generate the adiabatic potentials and non-adiabatic couplings as a function of the hyperradius. \([1]\) K. M. Daily and Chris H. Greene, Phys. Rev. A 89, 012503 (2014).

\(^1\)We gratefully acknowledge support by the NSF.

2:15PM B23.00014 Low-energy effective interactions beyond cRPA by the functional renormalization group , MICHAEL KINZA, CARSTEN HONERKAMP, RWTH Aachen University — In the derivation of low-energy effective models for solids targeting the bands near the Fermi level, the constrained random phase approximation (cRPA) has become an appreciated tool to compute the effective interactions. Here we present applications of a constrained functional renormalization group (cfRG) scheme to two simple multi-band systems and compare the resulting effective interactions to the cRPA. The employed wick-ordered fRG scheme generalizes the cRPA approach by including all interaction channels in an unbiased way. First we consider a multiband model for graphene, where we integrate out the \(\sigma\)-bands to get an effective theory for \(\sigma\)-bands. It turns out that terms beyond cRPA are strongly suppressed by \(xy\)-plane reflection-symmetry of the bands and that in our model, the cRPA stays qualitatively correct even if one breaks this symmetry slightly. The second example is a model for a Cu-O-chain, where we consider an effective theory for the Cu 3d-orbital. Here the RG data points to relevant corrections compared to the cRPA results.


11:15AM B24.00001 Electron localization in exact time-dependent density-functional potentials , MATTHEW HODGSON, JAMES RAMSDEN, University of York, Department of Physics, THOMAS DURRANT, JACOB CHAPMAN, University College London, Department of Physics and Astronomy, PIERS LILLYSTONE, University of Waterloo, Department of Physics and Astronomy, REX GODBY, University of York, Department of Physics — By propagation of the exact many-electron wavefunction, we determine exact Kohn-Sham (KS) potentials for 1D systems with strong correlation \([1]\). From this we have developed a density functional which incorporates several features, present in the exact KS potential, that are entirely missing from the usual approximations made in time-dependent density-functional theory (TDDFT) \([2]\). We find a strong and time-dependent self-interaction correction, owing to electron localization, as well as large static and dynamic spatial steps in the KS potential. Our new functional, suited to simulating ground-state and time-dependent electronic systems, combines an expression for the exact KS potential in the limit of complete electron localization with a measure of the actual localization. Self-consistent application of the functional provides accurate densities for a range of systems, even where the KS potential requires non-local dependence on the charge density, such as potential steps; the self-interaction correction is accurately described. We explore the relationship between features in the KS potential and the “derivativeness of discontinuity.”

\([1]\) M. J. P. Hodgson et al. Phys. Rev. B 88, 241102(R)

\([2]\) M. J. P. Hodgson et al. arXiv:1409.5666

11:27AM B24.00002 Constructing Multi-Slater-Jastrow Wavefunctions via Reduced Density Matrix Covariance . KIEL WILLIAMS, LUCAS WAGNER, Univ of Illinois - Urbana — The multi-determinant Slater-Jastrow ansatz wavefunction is a powerful tool for conducting ab initio electronic structure calculations in strongly correlated systems. We illustrate a new method of systematically constructing multi-determinant expansions by analyzing the covariance of elements of the two-body reduced density matrix (2RDM) with respect to the local energy distribution for a Slater-Jastrow wave function. By ordering the elements of the 2RDM with respect to their computed mean and associating each matrix element with a new determinant, we construct new multi-determinant expansions. We show that the energies of an H\(_2\) and stretched N\(_2\) molecule converge more rapidly with respect to the number of included determinants using this technique than in conventional configuration interaction calculations. This suggests that our analysis of the 2RDM captures qualitative differences between the single Slater determinant and the Slater-Jastrow wave function. This method provides a new way of diagnosing and correcting the deficiencies of certain trial wavefunction types in quantum Monte Carlo calculations. This work was supported by NSF DMR 12-06242.
11:39 AM B24.00003 Unitarily Invariant Self-Interaction Corrections to the Uniform Electron Gas, MARK PEDERSON, Department of Energy - US, JIANWEI SUN, Department of Physics, Temple University — A new formulation of the self-interaction correction (SIC) to density functional theory (DFT) based upon symmetrically orthogonalized “Fermi-Löwdin orbitals” (FLO) is reviewed [1]. This method leads to an energy that is explicitly unitarily invariant and size extensive and allows for implementation of SIC with the same efficient scaling offered by DFT. Initial applications to small molecules [1] provided orbitals that are similar to past results but yielded SIC-LDA cohesive energies that are competitive with GGA results. Investigations on a uniform electron gas (UEG) provide an additional challenging limit to consider. Results from FLO-based SIC calculations on the UEG, enclosed in a finite box, are presented. In accord with Ref. [2], the FLO-based formulation of SIC finds that localized Wannier orbitals lead to lower energies than plane waves in the exchange-only limit. We compare total energies of the uniform electron gas, calculated within DFT, FLO-SIC-DFT, and HF, as a function of functional (including MGGA[3]), electron number, volume, and Fermi-surface shape.


11:51 AM B24.00004 Using Dielectric Properties to Design Nonempirical Hybrid Functionals for Accurate Electronic Structure, JONATHAN SKONE, Institute for Molecular Engineering, The University of Chicago; Materials Science Division, Argonne National Laboratory, MARCO GOVONI, Institute for Molecular Engineering, The University of Chicago, GIULIA GALLI, Institute for Molecular Engineering, The University of Chicago — Building upon a recently proposed self-consistent hybrid (sc-hybrid) functional [1], where the optimal dielectric screening is included self-consistently, we propose an improved form by incorporating range-separation of the exchange part. We discuss the choice of the non-empirical parameters defining range separation, and we present results for condensed media including semiconductors, amorphous insulators, and molecular crystals. We find that the range-separated sc-hybrid functional further improves upon the electronic gaps obtained with full-range sc-hybrids, thus providing an accurate functional for high throughput band gap engineering.


12:03PM B24.00005 Range optimized theory of electron liquids with application to jellium, JAMES DONLEY, Valence Technologies, CRAIG PRYOR, University of Iowa — A simple optimization scheme is used to compute the density-density response function of the 3-D homogeneous electron gas at zero temperature. Higher order terms in the perturbation expansion beyond the random phase approximation are summed approximately by enforcing the constraint that the spin density radial distribution functions be positive. Quantitative comparison is made with previous theory and data from quantum Monte Carlo simulation. Agreement with the available simulation data is good for the entire paramagnetic region. Generalization of the theory to inhomogeneous electron liquids such as in semiconductors will be discussed.

12:15PM B24.00006 Inaccurate prediction of metal properties by hybrid functionals, WEIWEI GAO, TESFYAYE ABTEW, PEIHONG ZHANG, Department of Physics, University at Buffalo, SUNY, Buffalo, New York 14260 — Although computationally demanding, hybrid functionals have been widely used in electronic structure calculations and have demonstrated certain advantages in predicting the band gap of semiconductors and insulators. The applications of hybrid functionals to metals, however, results in several serious issues. In this talk, we will discuss the applicability and limitations of hybrid functionals when it comes to predicting several important properties of metals such as electron-photon coupling, lattice stability, and magnetism.

1The work is supported by the US Department of Energy under Grant No. DE-SC0002623 and by the National Science Foundation under Grant N0. DMR-0946401.

12:27PM B24.00007 Density matrix perturbation theory for magneto-optical response of periodic insulators, IRINA LEBEDEVA, ILYA TOTKATLY, ANGEL RUBIO, Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Universidad del Pais Vasco, Spain — Density matrix perturbation theory offers an ideal theoretical framework for the description of response of solids to arbitrary electromagnetic fields. In particular, it allows to consider perturbations introduced by uniform electric and magnetic fields under periodic boundary conditions, though the corresponding potentials break the translational invariance of the Hamiltonian. We have implemented the density matrix perturbation theory in the open-source Octopus code on the basis of the efficient Sternheimer approach. The procedures for responses of different order to electromagnetic fields, including electric polarizability, orbital magnetic susceptibility and magneto-optical response, have been developed and tested by comparison with the results for finite systems and for wavefunction-based perturbation theory, which is already available in the code. Additional analysis of the orbital magneto-optical response is performed on the basis of analytical models. Symmetry limitations to observation of the magneto-optical response are discussed.

The financial support from the Marie Curie Fellowship PIIF-GA-2012- 326435 (RespSpatDisp) is gratefully acknowledged.

12:39PM B24.00008 Theoretical and experimental electronic structure of quinacridone, SIVAN REFAELY-ABRAMSON, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth, Israel, DANIEL LUEFTNER, Institute of Physics, University of Graz, Graz, Austria, MICHAEL PACHLER, Institute of Physics, University of Graz, Graz, Austria; Institute of Solid State Physics, Graz University of Technology, Graz, Austria, ROLAND RESEL, Institute of Solid State Physics, Graz University of Technology, Graz, Austria, MICHAEL G. RAMSEY, Institute of Physics, University of Graz, Graz, Austria, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth, Israel, PETER PUSCHNIG, Institute of Physics, University of Graz, Graz, Austria — Although density functional theory is often used to study the frontier energy levels of organic electronic materials, standard functionals tend to predict too small fundamental gaps, may lead to wrong orbital energy ordering, and do not capture polarization-induced gap renormalization. We examine a strategy for overcoming these issues by studying the gas phase and bulk electronic structure of the organic molecule quinacridone, a promising material for organic devices. We employ the recently developed optimally tuned screened range-separated hybrid (OT-SRSH) functional [PRB 88, 081204(R) (2013)], where the electronic screening is taken into account, and compare with angle-resolved photoemission spectroscopy on multi-layers of quinacridone. Our method leads to the desired band gap renormalization and results in a valence band spectrum in excellent agreement with experimental data and with full-frequency G0W0 results based on a hybrid functional starting point. [PRB 90, 075204 (2014)]
**12:51PM B24.00009** Helmholtz Fermi surface harmonics: an efficient approach for treating anisotropic problems involving Fermi surface integrals, ASIER EIGUREN, IDOIA G. GURTUBAY, Condensed Matter Physics. University of the Basque Country & Donostia International Physics Center (DIPC). — We present a new efficient numerical approach for representing anisotropic physical quantities and/or matrix elements defined on the Fermi surface (FS) of metallic materials. The method introduces a set of numerically calculated generalized orthonormal functions, which are the solutions of the Helmholtz equation defined on the FS, where the periodicity of the reciprocal space is treated as a boundary condition. In essence, what we introduce is a generalization of the Spherical Harmonics for any periodic Fermi Surface and regardless of its topology. The main motivation of the approach is to handle an-isotropic many-body problems very efficiently. In this context we demonstrate how our theory reduces, by several orders of magnitude, the computational effort when applied to several well known many-body theoretical models such as the electron-phonon. Moreover, the method is demonstrated to be very robust in handling problems with any crystal structure or topology of the FS. We illustrate the method showing applications on several relevant surface and bulk systems.

**1:03PM B24.00010** Efficient mixing scheme for self-consistent all-electron charge density, TATSUYA SHISHIDOU, Hiroshima University, MICHAEL WEINERT, University of Wisconsin, Milwaukee — In standard ab initio density-functional theory calculations, the charge density $\rho$ is gradually updated using the “input” and “output” densities of the current and previous iteration steps. To accelerate the convergence, Pulay mixing has been widely used with great success. It expresses an “optimal” input density $\rho^{\text{opt}}$ and its “residual” $R^{\text{res}}$ by a linear combination of the densities of the iteration sequences. In large-scale metallic systems, however, the long range nature of Coulomb interaction often causes the “charge sloshing” phenomenon and significantly impacts the convergence. Two treatments, represented in reciprocal space, are known to suppress the sloshing: (i) the inverse Kerker metric for Pulay optimization and (ii) Kerker-type preconditioning in mixing $R^{\text{res}}$. In all-electron methods, where the charge density does not have a converging Fourier representation, treatments equivalent or similar to (i) and (ii) have not been described so far. In this work, we show that, by going through the calculation of Hartree potential, one can accomplish the procedures (i) and (ii) without entering the reciprocal space. Test calculations are done with a FLAPW method.

**1:15PM B24.00011** Quest for a workhorse MGGA functional, BERNARD DELLEY, Paul Scherrer Institut — A semi-empirical, numerically robust, parametrization of the exchange functional has been obtained by optimization of bond energies in a database of 500 species. The variables, density, gradient and kinetic energy density, can differentiate efficiently among the wide variety of bonds in the database. The resulting MGGA rivals the thermochmistry accuracy of composite quantum chemistry approaches when applied to a wider data set. But, not only, it also provides noticeable improvements over GGA’s for solid state properties, including properties not obviously related to bonding energies. As an MGGA is not significantly more demanding computationally than a GGA, this MGGA may become the workhorse density functional for a wide range of applications.

**1:27PM B24.00012** First-Principles Investigation of Electronic Excitation Dynamics in Water under Proton Irradiation, KYLE REEVES, YOSUKE KANAI, Univ of NC - Chapel Hill — A predictive and quantitative understanding of electronic excitation dynamics in water under proton irradiation is of great importance in many technological areas ranging from utilizing proton beam therapy to preventing nuclear reactor damages. Despite its importance, an atomistic description of the excitation mechanism has yet to be fully understood. Identifying how a high-energy proton dissipates its kinetic energy into the electronic excitation is crucial for predicting atomistic damages, later resulting in the formation of different chemical species. In this work, we use our new, large-scale first-principles Ehrenfest dynamics method [1,2] based on real-time time-dependent density functional theory to simulate the electronic response of bulk water to a fast-moving proton. In particular, we will discuss the topological nature of the electronic excitation as a function of the proton velocity. We will employ maximally-localized functions to bridge our quantitative findings from first-principles simulations to a conceptual understanding in the field of water radiolysis. [1] “Plane-wave Pseudopotential Implementation of Explicit Integrators for Time-Dependent Kohn-Sham Equations in Large Scale Simulations” A. Schleife, E. W. Draeger, Y. Kanai, A. A. Correa, J. Chem. Phys., 137, 22A546 (2012) [2] “Quantum Dynamics Simulation of Electrons in Materials on High-Performance Computers” A. Schleife, E. W. Draeger, V. Anisimov, A. A. Correa, Y. Kanai, Computing in Science and Engineering, 16 (5), 54 (2014).

**1:39PM B24.00013** Strongly Constrained and Appropriately Normed (SCAN) Meta-Generalized Gradient Approximation for Exchange and Correlation1, JIANWEI SUN, ADRIENN RUZSINSZKY, JOHN PERDEW, Department of Physics, Temple University — Meta-generalized gradient approximations (meta-GGAs) construct the exchange-correlation (xc) energy density from the local electron density, its gradient, and the orbital kinetic energy density. They are the most accurate of the computationally-efficient semilocal density functionals. We construct a SCAN meta-GGA which satisfies all the known exact constraints that a meta-GGA can, including a new tight lower bound on the exchange energy [1]. SCAN is constructed as an interpolation/extrapolation on $\alpha$, the dimensionless variable that can recognize covalent single ($\alpha \approx 0$), metallic ($\alpha \approx 1$), and weak ($\alpha >> 1$) bonds [2]. A few parameters are included for appropriate norming on systems where a meta-GGA should be especially accurate due to xc hole localization.

1Supported by NSF (DMR).


**1:51PM B24.00014** A Generalized Slave-Particle Method1, ALEXANDRU BOGDAN GEORGESCU, Department of Physics and Center for Research on Interface Structures and Phenomena, Yale University, SOHRAB ISMAIL-BEIJI, Department of Physics, Department of Applied Physics and Center for Research on Interface Structures and Phenomena, Yale University — Two slave-particle methods, namely the slave-rotor and the slave-spin approaches, have been of recent interest in the computational correlated electron community. Both methods solve Hubbard-type models and go beyond the single-particle approximations by describing aspects of correlated electron behavior in a computationally efficient manner. We present a generalized slave-particle formalism that connects the the two while reproducing the results of each method in the appropriate limit. The framework automatically corrects the problematic small U behavior of the slave-rotor approach while reproducing its behavior in situations where it has been found physically relevant (e.g., for nickelate heterostructures).

1This work is supported by the National Science Foundation through grant MRSEC NSF DMR-1119826

**2:03PM B24.00015** Selectively localized Wannier functions, RUNZHI WANG, Columbia University, EMANUEL LAZAR, University of Pennsylvania, HYOWON PARK, University of Illinois at Chicago, ANDREW MILLIS, CHRIS MARIANETTI, Columbia University — Since the seminal work of Marzari and Vanderbilt, maximally localized Wannier functions have become widely used as real-space representations of electronic structure in periodic systems. In this talk we discuss selectively localized Wannier functions (SLWF) which allow localization of a particular subset of orbitals of interest, and also enable the fixing of orbital centers and ensuring the preservation of point-group symmetries. Applications of our method to GaAs, SmMnO$_3$, and Co demonstrate that SLWF can offer improvements over standard techniques, especially in beyond DFT methods.
11:15AM B26.00001 Multistate trajectory and statistical theories of spin-forbidden kinetics. AHREN JASPER, Sandia National Laboratory — Rate coefficients for several spin-forbidden reactions relevant to combustion are calculated using multistate trajectory and statistical theories. The two approaches are compared, and the appropriateness of treating singlet/triplet crossing seams as “nonadiabatic transition state” for spin-forbidden reactions is discussed. We show that the spin-forbidden reaction coordinate is coupled to the remaining nuclear degrees of freedom, leading to multidimensional effects not typically included in statistical treatments. We identify: static multidimensional effects due to the geometry-dependence of the shape of the crossing seam and spin-orbit coupling, dynamical multidimensional effects where the electronic transition probability depends on the distribution of the total internal energy of the system, and nonlocal multidimensional effects due to the instantaneous value of the electronic phase at multiple seam crossings. A semiclassical model based on short-time full-dimensional trajectories that includes all three multidimensional effects as well as a model for electronic decoherence is presented. The results of this new multidimensional nonadiabatic statistical theory are compared with the results of one-dimensional Landau-Zener and weak coupling models for several reactions.

11:51AM B26.00002 Evidence for quantum effects in laser driven photodissociation of methyamines. ILANA BAR, MICHAEL EPSHTEIN, ALEXANDER PORTNOV, Ben-Gurion University of the Negev — Non-adiabatic dynamics at conical intersections (CI) extensively affects the photostability of biomolecules by efficiently photoinducing decay routes that dissipate harmful excess ultraviolet energy. Here the photodissociation of the model test molecules, methylamine (CH₃NH₂) and its partially deuterated isotopeologue (CD₃ND₂), excited to different specific vibrational modes in the electronically excited state has been investigated by H(D) photofragments detection with two-color reduced-Doppler ion imaging [1]. The H products, resulting from N-H bond cleavage via two dissociation pathways, showed anomalous distributions for some of the vibronic states, as indicated by dynamic resonances in the product branching ratio and in the anisotropy parameters. This vibronic-specific control is attributed to distinctive dynamical interferences of the initially prepared wavepackets, affecting the passage efficiency through the S₁/S₀ CIs. It is suggested that the H product distributions are extremely sensitive to the positions and energies of the CIs in the two molecules, rather than to the unique initial nuclear motion that promotes the coupling between the two electronic states. These observations reveal uniquely detailed insights into the dynamics of state-specific control of internal conversion.


12:03PM B26.00003 ABSTRACT MOVED TO Q48.00005 —

12:15PM B26.00004 Real-Time Subsystem TD-DFT and its Ehrenfest Dynamics: Applications to solvation and exciton transfer. MICHELE PAVANELLO, Rutgers Univ - Newark — The subsystem formulation of DFT known as Frozen Density Embedding (FDE) provides a divide-and-conquer approach to Kohn-Sham DFT for a collection of weakly bound subsystems. We present theory and computer code development of the time-dependent extension of FDE. The code is now part of the Quantum–ESPRESSO suite of softwares. We also present the associated Ehrenfest dynamics, in which nuclei and electrons of selected subsystems are propagated simultaneously. Application of the code to exciton transfer phenomena as well as to solvatochromic shifts are discussed.

1 M.P. acknowledges funding by the ACS Petroleum Research Fund

12:27PM B26.00005 Ultrafast dynamics in DNA base pairs following ultraviolet excitation. ANDREW ORR-EWING, University of Bristol — Photo-protective mechanisms in DNA are essential to maintain the integrity of the genetic code by preventing damage from absorption of solar ultraviolet (UV) radiation. We have used time-resolved infra-red (TRIR) spectroscopy to observe the dynamics of Watson-Crick nucleobase pairs following absorption of femtosecond UV laser pulses. The base pairs are prepared as nucleosides in solution, and photo-induced dynamics are probed in the carbonyl and N-H bond stretching regions using broadband IR pulses with picosecond time resolution. Results will be presented for the guanine- and cytosine (G-C) base pair, contrasting the rapid recovery of ground-state products (the photo-protection pathway) with formation of other photoproducts which are probed in the carbonyl and N-H bond stretching regions using broadband IR pulses with picosecond time resolution. Results will be presented for the guanine- and cytosine (G-C) base pair, contrasting the rapid recovery of ground-state products (the photo-protection pathway) with formation of other photoproducts which might represent photo-damage mechanisms. This work is a collaboration with the group of Prof F. Temps (Christian-Albrechts-Universität zu Kiel).

3 This research is supported by ERC Advanced Grant 290966 CAPRI

1:03PM B26.00006 Femtosecond Heterodyne Transient Grating Studies of Nonradiative Decay in β-Carotene and Peridinin: Contributions of Dark Intermediates and Double Quantum Coherences. SOUMEN GHOSH, JEROME ROSCIOLI, Michigan State Univ, HARRY FRANK, University of Connecticut, WARREN BECK, Michigan State Univ — Femtosecond transient grating spectroscopy with optical heterodyne detection was employed to characterize the ultrafast events in the nonradiative decay of β-carotene and peridinin in solution from the S₂ state. The contribution of double-quantum coherences to the time evolution of the third order signal was probed by scanning the interpulse delay between the first two pulses in the transient grating or stimulated photon-echo sequence. The results show that the double-quantum coherence pathways contribute significantly to the transient grating signal only at negative population delays, which is consistent with the requirements determined from double-sided Feynman diagrams when the third order signal is detected in the −k₁ + k₂ + k₃ direction. Response function calculations support the conclusion that the ultrafast (<20 fs) decay that contributes to the third order signal at positive population delays arises from an intermediate, which has been previously assigned to the S₄ state. We suggest that this intermediate arises not from a discrete electronic state but rather from a twisted conformation of the conjugated polyene. This proposal has significant implications with respect to the energy transfer function of carotenoids in photosynthesis.

1:15PM B26.00007 Vibrational Conical Intersections: Implications for Ultrafast Vibrational Dynamics. MAHESH DAWADI, BISHNU PRASAD THAPALIYA, Department of Chemistry, The University of Akron, RAM BHATTA, Department of Polymer Science, The University of Akron, DAVID PERRY, Department of Chemistry, The University of Akron — The presence of conical intersections (CIs) between electronic potential energy surfaces is known to play a key role in ultrafast electronic relaxation in diverse circumstances. Recent reports have documented the existence of vibrational CIs connecting vibrationally adiabatic surfaces. Just as electronic CIs are now appreciated to be ubiquitous, controlling the rates of many photochemical processes, the present work on methanol and methyl mercaptan suggests that vibrational CIs may also be widespread, possibly controlling the outcome of some high-energy processes where vibrationally excited species are present. Other examples of vibrational CIs include the vibrationally Jahn-Teller effect in C₂O₂ organic molecules and transition metal complexes. While the present work addresses only the couplings within bound molecules, the concept of vibrational CIs providing pathways for ultrafast relaxation also applies to molecular collisions.

3 This work is supported by DOE (DEFG02- 90ER14151).
11:15AM B27.00001 Tracking the charge and spin dynamics of electronic excited states in inorganic complexes\(^1\), KELLY GAFFNEY, Stanford Synchrotron Radiation Lightsource and PULSE Institute at SLAC National Accelerator Laboratory and Stanford University — Inorganic complexes have many advantageous properties for solar energy applications, including strong visible absorption and photocatalytic activity. Whether used as a photocatalyst or a photosensitizer, the lifetime of electronic excited states is a key property for solar energy applications. This work demonstrates the usefulness of many coordination compounds. Isoelectronic iron and ruthenium based complexes represent a clear example. Ru-porphyril based molecules have been the workhorse of solar energy related research and dye sensitized solar cells for decades, but the replacement of low abundance Ru with Fe leads to million-fold reductions in metal to ligand charge transfer (MLCT) excited state lifetimes. Understanding the origin of this million-fold reduction in lifetime and how to control excited state relaxation in 3d-metal complexes motivates the work I will discuss. We have used the spin sensitivity of hard x-ray fluorescence spectroscopy and the intense femtosecond duration pulses generated by the LCLS x-ray laser to probe the spin dynamics in a series of electronically excited \([\text{Fe} (\text{CN})_6]^{-2N} [2,2’-\text{bipyridine}]_N^{2N-4}\) complexes, with \(N = 1-3\). These femtosecond resolution measurements demonstrate that modification of the solvent and ligand environment can lengthen the MLCT excited state lifetime by more than two orders of magnitude. They also verify the role of triplet ligand field excited states in the spin crossover dynamics from singlet to quintet spin configurations.\(^1\)

1 Work supported by the AMOS program within the Chemical Sciences, Geosciences, and Biosciences Division of the Office of Basic Energy Sciences, Office of Science, U. S. Department of Energy.

11:51AM B27.00002 Time-resolved X-Ray Absorption Spectroscopy of a Cobalt-Based Hydrogen Evolution System for Artificial Photosynthesis, DOOSHAYE MOonsoHiram, Argonne National Laboratory, CAROLINA GIMBERT, Institut Català d’Investigació Química, CARL LEHMANN, STEPHEN SOUTHWORTH, Argonne National Laboratory, ANTONI LLORET, Institut Català d’Investigació Química, ARGONNE NATIONAL LABORATORY TEAM, INSTITUT CATALÁ D’INVESTIGACIÓ QUÍMICA COLLABORATION — Production of cost-effective hydrogen gas through solar power is an important challenge of the Department of Energy among other global industry initiatives. In natural photosynthesis, the oxygen evolving complex (OEC) can carry out four-electron water splitting with an efficiency of around 60\%. Although much progress has been carried out in determining mechanistic pathways of the OEC, biophysical approaches have not duplicated Nature’s efficiency in function. Over the past years, we have witnessed progress in developments of light harvesting modules, such as chromatophore/catalytic assemblies. In spite of reportedly high catalytic activity of these systems, quantum yields of hydrogen production are below 40\% when using monochromatic light. Proper understanding of kinetics and bond making/breaking steps has to be achieved to improve efficiency of hydrogen evolution systems. This project shows the timing implementation of ultrafast x-ray absorption spectroscopy to visualize in “real time” the photo-induced kinetics accompanying a sequence of redox reactions in a cobalt-based molecular photocatalytic system. Formation of a Co(I) species followed by a Co(III) hydride species all the way towards hydrogen evolution is shown through time-resolved XANES.

12:03PM B27.00003 Spatiotemporal Imaging of Chemical Reactions: Making Molecular Movies with Femtosecond X-Ray Scattering, J.M. BUDARZ, Brown Univ., SLAC National Accelerator Laboratory, M.P. MINITTI, SLAC National Accelerator Laboratory, A. KIRRANDER, Univ. of Edinburgh, J.B. HASTINGS, SLAC National Accelerator Laboratory, P.M. WEBER, Brown Univ. — The study of ultrafast reaction dynamics of molecular systems has benefited from the rapid development of spectroscopic and imaging techniques that follow their temporal evolution on a sub-picosecond time scale. More complete understanding of molecular behavior, however, is expected to arise from a full observation of electronic and nuclear motions during reactions. Our recent experiments at the Linc Coherent Light Source (LCLS) have allowed us to develop and implement a method wherein the ultrafast reaction dynamics of molecules in dilute gases (4 Torr) are captured by time-resolved x-ray scattering. Using a pump-probe scheme with 267 nm excitation laser and 8.3 keV x-ray probe pulses, we performed a series of measurements on the interatomic positions at variable delay relative to a 'molecular movie.' In our experiment, 1,3-cyclohexadiene (CHD) is excited on an excited state surface, causing the molecule to accelerate down several potential energy surfaces coupled by conical intersections, to open into 1,3,5-hexatriene within 80 fs. The resulting 'movie' has been supplemented with molecular trajectory calculations to separate the multiple pathways the excited molecule takes toward the open ring. In this talk, the experimental methods and designs that made these experiments possible will be presented together with the first results describing the photochemical reaction dynamics of CHD.

12:15PM B27.00004 The orbital-based view on reaction dynamics: ligand exchange of \(\text{Fe}(\text{CO})_5\) in solution, ALEXANDER FÖHLSICH, Helmholtz-Zentrum Berlin für Materialien und Energie, Potsdam University — Time resolved soft x-ray spectroscopy has proven recently, that it can be applied to the complex dynamics occurring in materials and chemical processes by its high selectivity towards elemental, chemical, and magnetic properties. Changes in chemical bonding, in particular bond breaking and bond formation seem conceptually simple, but as a result of coherent wave packet motion it is difficult to access the dynamic pathways in a multidimensional potential energy landscape. In this contribution we exploit the unique approach of femtosecond time resolved resonant inelastic x-ray scattering at LCLS to derive information about excited state configurations and electronic excited states. As an outlook, it will be discussed, how non-linear X-ray processes can push time resolved soft X-ray spectroscopy to a new phase. In particular, stimulated Raman scattering and amplified spontaneous emission can overcome the weak scattering cross-sections of spontaneous processes, help to suppress sample damage and increase spectral resolution and excited state selectivity through the exploitation of Anti-Stokes Raman Scattering.

12:51PM B27.00005 Tracking picosecond molecular dynamics in solution using a suite of synchrotron-x-ray spectroscopic tools\(^1\), ANNE MARIE MARCH, GILLES DOUMY, ELLIOT P. KANTER, STEFAN LEHMANN, DOOSHAYE MOonsoHiram, STEPHEN H. SOUTHWORTH, LINDA YOUNG, Argonne National Lab, TADESSE A. ASSEFA, CHRISTIAN BRESSLER, WOJCIECH GWALEDA, European XFEL, ZOLTÁN NEMETH, GYÖRGY VANKÓ, Hungarian Academy of Sciences — Laser-pump, X-ray-probe techniques are powerful tools for exploring molecular structures and electronic states in complex environments such as solutions, during a photo-initiated reaction. We are developing such methods using hard x-rays from the Advanced Photon Source, combining x-ray emission spectroscopy and x-ray absorption spectroscopy as probes of electronic and geometric structure and using high-power, MHz lasers as pumps. The high-duty-cycle pump-probe measurements efficiently utilize the synchrotron-x-ray source and enable high-fidelity measurement of intermediates. We present measurements of two model systems, \([\text{Fe}(\text{II})(\text{CN})_6]^{4-}\) (ferrocyanide) in an aqueous solution after excitation with 355 nm and 266 nm laser light. The system undergoes two wavelength dependent reactions: photooxidation and photoaquation. Iron K-edge absorption spectra were obtained along with iron emission spectra. Our data support the presence of a previously unobserved pentacoordinated intermediate species in the photoaquation reaction. Its lifetime has been measured to be 4.6 ns and details of its structure will be discussed.\(^1\)

1 The work was supported by the U.S. Department of Energy, Office of Science, Chemical Sciences, Geosciences, and Biosciences Division.
1:03PM B27.00006 Ultrafast Coherent Photoelectron Spectroscopy of Electronic States on a Cu (111) Surface, ADRA CARR, CONG CHEN, ZHENSHENG TAO, MARGARET MURNANE, HENRY KAPTEYN, PIOTR MATYBA, JILA/NIST, SEBASTIAN EMMERICH, MARTIN AESCHLIMANN, University of Kaiserslautern, Germany, ULRICH HOFEPER, University of Marburg, Germany — We use laser-assisted high-harmonic time- and angle-resolved photoemission to directly observe coherent photoemission from a Cu(111) metal surface and the interferences between the emitted photoelectron wavepackets. A comb of high harmonics in combination with interferometrically timed infrared pulses enable a powerful combination of attosecond time resolution and high energy resolution, making it possible to extract phase information about the emitted photoelectron wavepackets and the distinct electronic states from which they emerge. By comparing photoemission from the well-known Shockley surface state to the sp and d bulk bands of Cu(111), we can observe non-negligible phase shifts in the emitted wavepackets, which cannot be attributed to time delays resulting from classical electron transport to the surface. Rather, we interpret these phase shifts as due to an intrinsic photoemission phase that is different for the sp and d band wavefunctions, thus providing a physical interpretation of temporal delays observed in photoemission from surfaces.

1:15PM B27.00007 Circularly polarized attosecond pulses for molecular atto-magnetism, ANDRE D. BANDRAUK1, University of Sherbrooke — Circularly polarized molecular high order harmonic generation, MHOHG, is modelled from numerical solutions of the time-dependent Schrödinger equation, TDSE, for the one-electron H2+ in the nonlinear nonperturbative regime of laser-molecule interaction. It is shown that molecules due to their nonspherical symmetry are the preferred medium for producing circularly polarized harmonics by few cycle intense IR (800,400nm) circularly polarized laser pulses. An intense Terahertz (4um) pulse is combined to force recollision of the ionized electron with the parent ion thus enhancing the efficiency of the circularly polarized MHOHG process through single recollision [1]. Superposition of these harmonics allows for the synthesis of single circularly polarized attosecond (10-18s) pulses. Such new ultrashort pulses allow for controlling electrons on their natural time scale [2]. In particular the TDSE simulations illustrate the generation with such new pulses coherent quantum electronic currents inside molecules for the creation of attosecond magnetic field pulses of intensity >10 Teslas [3].

1:27PM B27.00008 Coherent Chemistry with THz Pulses: TDDFT-Ehrenfest Simulations of Field-Induced LiNC Isomerization1, LENSON PELLOUCHOUD, EVAN REED, Stanford Univ — The ability to coherently rearrange molecular structures is among the grand challenges of physical chemistry. Some of the primary obstacles are non-adiabatic increases in energy, such as intramolecular vibrational relaxation (IVR) and electronic excitations. Motivated by recent advances in the generation and control of strong terahertz (THz) pulses, we have investigated their potential to circumvent these obstacles. THz pulses are promising because their spectral content is well separated from electronic excitation frequencies, yet they may be fast enough to add and remove energy from the electronic system without allowing IVR to take place. In this work, we utilize simulations to discover that LiNC can be isomerized to two distinct metastable conformations with very low residual heating and ionization rates, pointing out a new route towards THz coherent control of chemical bonds and materials. We use time-dependent DFT (TDDFT)-based Ehrenfest molecular dynamics simulations to test a variety of strong time-varying THz pulses applied to the molecule. We find the limits of how quickly an activation barrier can be surmounted before the driving pulse becomes strong enough to ionize the molecule, and how well the target must be aligned in order for the final configuration to be stable.

1:39PM B27.00009 Ultrafast high harmonics for probing the fastest spin and charge dynamics in magnetic materials, PATRICK GRYCHTOL, JILA, University of Colorado, Boulder, CO 80309, USA — Ultrafast light based on the high-harmonic up-conversion of femtosecond laser pulses have been successfully employed to access resonantly enhanced magnetic contrast at the μ-absorption edges of the 3d ferromagnets Fe, Co and Ni in a table-top setup. Thus, it has been possible to study element-specific dynamics in magnetic materials at femtosecond time scales in a laboratory environment, providing a wealth of opportunities for a greater fundamental understanding of correlated phenomena in solid-state matter. However, these investigations have so far been limited to linear polarized harmonics, since most techniques by which circular soft x-rays can be generated are highly inefficient reducing the photon flux to a level unfit for scientific applications. Besides presenting key findings of our ultrafast studies on charge and matter, we interpret these phase shifts as due to an intrinsic photoemission phase that is different for the sp and d bands, thus providing a physical interpretation of temporal delays observed in photoemission from surfaces.


205 - Mathias Weiler, Walther Meissner Institute

11:15AM B28.00001 Investigation on spin-orbit torque induced perpendicular switching through voltage controlled magnetism1, CHONG BI, MENG XU, MARCUS ROSALES, TY NEWHOUSE-ILLIGE, HAMID ALMASI, WEIGANG WANG, Department of Physics, University of Arizona, Tucson, Arizona 85721, USA — Spin-orbit torques are shown to induce perpendicular magnetic switching in ultrathin ferromagnets (FM)s adjacent to heavy metals (HMs). Here, we demonstrated that the critical current density (Jc) for such perpendicular switching in HM/FM/oxide structures can be dramatically modulated by gate voltage induced reversible oxidation at FM/oxide interfaces [1]. Through controlling perpendicular anisotropy and saturation magnetization (M_s) of FM layer, respectively, we show M_s, rather than anisotropy field as suggested in macrospin model [2], dominates Jc. Moreover, the measured external field dependent Jc results indicate that the spin-orbit torques have either a bulk or interface origin under different magnetization states. These results not only provide a promising means toward energy-efficient switching, but also offer further insights in understanding the reversal mechanism of the ferromagnetic layer. This work was supported in part by NSF (ECCS-1310338) and by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA.[1] C. Bi et al, submitted, [2] L. Liu et al. Phys. Rev. Lett. 109, 096602 (2012).

1This work was supported in part by NSF (ECCS-1310338) and by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA.
11:27AM B28.00002 Magnon-phonon interactions and spin transport in insulators1. STEPHEN R. BOONA, HYUNGYU JIN, Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH, JOSEPH P. HEREMANS, Department of Mechanical and Aerospace Engineering, Department of Physics, The Ohio State University, Columbus, OH — The spin Seebeck effect (SSE) is now a well-established phenomenon whereby a spin current can be thermally pumped from a ferromagnetic (FM) material into a normal metal (NM), where the spin current is then converted into a transverse charge current through the inverse spin Hall effect. The most interesting feature of SSE is that it occurs even if the FM is an insulator, e.g., yttrium iron garnet (YIG). Although the existence of the effect is well established, its microscopic origins are still not completely understood; the detailed nature of interactions between the elementary excitations (electrons, phonons, and magnons) that give rise to SSE are complex and strongly dependent on factors like materials selection and temperature. One particularly important issue that remains unclear is the role that magnon-phonon interactions play in generating spin currents, especially within the context of diffusive vs drag currents. This talk will address this question by discussing some of our recent experiments aimed at exploring the temperature and length dependence of thermal and spin transport phenomena in magnetoically ordered insulators.

1Work partially supported by ARO-MURI W911NF-14-1-0016 and NSF MRSEC program, Grant No. DMR 1420451

11:39AM B28.00003 Temperature-dependent spin Hall magnetoresistance in ferromagnetic insulator/normal metal hybrids1, MATTHIAS ALTHAMMER, SIBYLLE MEYER, STEFAN GEPRÄGS, MATTHIAS OPEL, RUDOLF GROSS, SEBASTIAN T.B. GOENNENWEIN, Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meissner-Strasse 8, 85748 Garching, Germany — Pure spin currents, i.e. the net flow of spin angular momentum without an accompanying charge current, represent a new paradigm for spin transport and spintronics. We have experimentally studied a new type of magnetoresistance effect, which arises from the interaction of charge and spin current flows in ferromagnetic insulator/normal metal hybrid structures. The resistance changes observed can be quantitatively traced back to the combined action of spin Hall and inverse spin Hall effect in the normal metal layer, and are thus termed spin Hall magnetoresistance (SMR) [1,2]. In more detail, we studied the temperature dependence of the SMR in yttrium iron garnet / platinum hybrid structures via magnetization orientation dependent magnetoresistance measurements. Our experiments show that the SMR amplitude decreases with decreasing temperature, which can be quantitatively modeled in terms of a spin Hall angle in platinum decreasing from 0.11 at 300K to 0.075 at 10K [3], while the spin diffusion length and the spin mixing conductance of the ferrimagnetic insulator / normal metal interface remain almost constant.


1Financial support by the DFG via SPP 1538 (project no. GO 944/4) and the Nanoinitiative Munich (NIM) is gratefully acknowledged.

11:51AM B28.00004 Spin Seebeck effect in YIG-based systems, GENE SIEGEL, MEGAN PRESTGARD, SHIANG TENG, ASHUTOSH TIWARI, University of Utah, Department of Materials Science & Engineering — Recently, the use of magnetic insulators (yttrium iron garnet, YIG) in conjunction with platinum has sparked interest in spintronics research. This is due to the existence of the spin Seebeck effect which could potentially be a source of pure spin current for spintronic devices. Furthermore, these coatings could potentially show the versatility of spintronics by acting as a spin-based thermoelectric generator, thereby providing a new method of transforming heat into power. However, there remain questions regarding the origins and legitimacy of the spin Seebeck effect. Moreover, recent publications claim that the observed effects are a manifestation of magnetic proximity effects in platinum and not a true SSE signal. Because of these concerns, we are providing supporting evidence that the voltages observed in the YIG/Pt films are truly SSE voltages. We are reaffirming claims that magnon transport theory provides an accurate basis for explaining SSE behavior. Finally, we illustrate the advantages of pulsed laser deposition, as these YIG films possess a large SSE voltage compared to those films grown using liquid phase deposition techniques.

12:03PM B28.00005 Subthermal-magnon-driven longitudinal spin Seebeck effect in yttrium iron garnets (YIG)1, STEPHEN BOONA, Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH, ZHIAO YANG, ROBERTO MYERS, Department of Materials Science and Engineering, The Ohio State University, Columbus, OH. — Since its discovery in 2008, the spin Seebeck effect (SSE) has intrigued many interesting research all around the world, which has led to the birth of a new field of research, called “spin caloritronics”. Of the two different experimental configurations used for detecting SSE, the longitudinal geometry (LSSE) seems to be generally accepted [1]. The yttrium iron garnet (YIG) / Pt bilayer structure has been most commonly used for LSSE experiments because absence of electrons in YIG excludes contaminations from other thermomagnetic effects. The dependence of the LSSE on YIG film thickness [2] and on temperature [3] have been reported, but not yet both together. Here we present experimental data on the temperature dependence of LSSE in Pt/YIG below room temperature in systems in which the thickness of YIG varies. Detailed discussion is given on the experimental results, with emphasis on the role of subthermal-magnons in the temperature dependence of LSSE in the YIG/Pt system.


1Work supported by the AFOSR-MURI #FA9550-10-1-0533 and the ARO-MURI #W911NF-14-1-0016.

12:15PM B28.00006 Spin Seebeck Effect in a Compensated Ferrimagnet, SEBASTIAN T.B. GOENNENWEIN, S. GEPRÄGS, Walther-Meissner-Institut, Garching, Germany, A. KEHLBERGER, T. SCHULZ, C. MIX, University of Mainz, Mainz, Germany, F. DELLA COLETTA, S. MEYER, Walther-Meissner-Institut, Garching, Germany, A. KAMRA, Kavli Institute of Nanoscience, Delft, The Netherlands, G. JAKOB, University of Mainz, Mainz, Germany, M. ALTHAMMER, H. HUEBL, R. GROSS, Walther-Meissner-Institut, Garching, Germany, M. KLÄUI, University of Mainz, Mainz, Germany — Thermal gradients allow for driving pure spin currents in electrically insulating magnetic materials. In magnetic insulator/normal metal heterostructures, such thermally driven spin currents can be electrically detected via the inverse spin Hall effect in the normal metal, in so-called spin Seebeck effect (SSE) experiments. We have fabricated Gadolinium Iron Garnet/Platinum (GdIG/Pt) thin film heterostructures, and measured the spin Seebeck effect in these samples as a function of temperature. We observe two sign changes as a function of T in the SSE signal. The first sign change occurs around the GdIG magnetic compensation temperature, and can be straightforwardly understood in terms of the reorientation of the iron sublattice magnetizations at this temperature. The second, more gradual SSE sign change takes place around the ordering temperature of the Gd magnetic sublattice, suggesting that the thermally driven spin current is mainly determined by the Gd sublattice at low T. Our results thus show that the SSE spin currents do not simply replicate the effective magnetization of the magnetic insulator, but rather reflect a complex interplay of magnetic sublattice properties.
12:27PM B28.00007 Transverse Spin Seebeck Effect on YIG/Pt

HYUNGYU JIN, JOSEPH HEREMANS, The Ohio State University — The existence of the longitudinal spin-Seebeck effect (LSSE) is well established and supported by theory. Much more controversial is the nature of the signals observed in the transverse spin-Seebeck (TSSE) geometry, where the heat current (x) is orthogonal to the direction of spin current propagation (y). TSSE has been described as simply non-local thermal spin-injection [1], but questions remain about the fact that the effect is observed at macroscopic length scales. To explore possible explanations for the observed TSSE signals, we report data from new TSSE measurements on the YIG/Pt system. The system studied has multiple Pt strips deposited in series upon bulk single crystals of YIG. We investigate the TSSE coefficient as a function of four variables: (1) sample temperature; (2) magnitude of the temperature gradient; (3) position of Pt strips along x; and (4) width of Pt strips along x. We consider nonlinear effects and the role of magnon density in the interpretation of our results. [1] Boona et al., Energy and Environ. Sci. 7 885 (2014)

1Work supported by the ARO- MURI grant W911NF-14-1-0016 and NSF MRSEC program, Grant No. DMR 1420451

12:39PM B28.00008 DC Rectification of Microwaves in YIG/Pt/Pt Trilayers 1, JOSEPH SKLENAR, JOHN KETTERSON, Northwestern University, MATTHIAS JUNGFLEISCH, WANJUN JIANG, WEI ZHANG, JOHN PEARSON, AXEL HOFFMANN, Argonne National Laboratory, ONGHUI YANG, QIYE WEN, HUAIWU ZHANG, State Key Laboratory of Electronic Films and Integrated Devices, University of Electronic Science and Technology, Chengdu, Sichuan, China, 610054 — The DC voltage arising from the rectification of microwaves passing through a ferromagnet/spin Hall bilayer structure at ferromagnetic resonance is a powerful tool in understanding spin-orbit torques from spin Hall effects. Rectification mechanisms such as anisotropic magnetoresistance of the ferromagnetic or spin Hall magnetoresistance of the spin Hall metal can contribute depending on whether the ferromagnet is conductive or insulating. For both types of ferromagnets, spin pumping acting in concert with the inverse spin Hall effect can also generate additional DC voltages. We have studied rectification in a trilayer system of YIG/Pt/Pt under conditions where both ferromagnets are simultaneously excited. By tipping the DC magnetic field out of the sample plane we can make the resonances of both ferromagnet materials degenerate. In this simultaneous resonance regime we observe an enhancement in the voltage of the YIG lineshape coming at the expense of the Py signal. Furthermore, at arbitrarily tipped out-of-plane tipping angles we observe asymmetries of the Py signal under field reversal. We compare this observation with the DOE, Office of Science, Materials Science and Engineering Division.

1This work was supported by DOE, Office of Science, Materials Science and Engineering Division.

12:51PM B28.00009 Surface sensitivity of the spin Seebeck effect in the Pt/YIG system 1, AISHA AQEEQ, IVAN J. VERA-MARUN, BART J. VAN WEES, THOMAS T.M. PALSTRA, Zernike Institute for Advanced Materials, University of Groningen — It is well-known that the surface plays an important role in the spin Seebeck effect (SSE) [1]. However the effect of mechanical treatment on the SSE has not been systematically studied yet. Here, we have investigated the influence of the interface quality on the SSE in a bilayer system of platinum and yttrium iron garnet (Pt/YIG). The surfaces of the YIG crystals are modified by different types of mechanical polishing before Pt deposition for different samples. We observed that the magnitude and magnetic field dependence of the SSE is strongly influenced by mechanical treatment of the YIG surface. No definite relation has been found between the SSE response and the sample roughness. However, we observe a direct correlation between the saturation magnetic field (Hsat) of the SSE and the roughness of sample, as the former increases by moving from soft toward coarse particle polishing. The change in the magnitude of Hsat can be attributed to the presence of a perpendicular magnetic anisotropy due to the treatment induced surface strain or shape anisotropy in the Pt/YIG system [2].

1:03PM B28.00010 Magnons and Phonons Driven out of Equilibrium in a Magnetic Insulator 1, KYONGMO AN, KEVIN OLSSON, NIKITA KLIMOVICH, Department of Physics, The University of Texas at Austin, SEAN SULLIVAN, ANNIE WEATHERS, LUKE MARSHALL, XI CHEN, JIANSHI ZHOU, LI SHI, Department of Mechanical Engineering, The University of Texas at Austin, XIAOQIN LI, Department of Physics, The University of Texas at Austin — We investigate magnons and phonons in a bulk YFeO3 (YIG) under a large temperature gradient created by laser radiation. YIG is a good playground to study the interaction between phonons and magnons. Because of its absence of itinerant electrons, energy transport is only carried by magnons and phonons. Understanding the coupling between them is a key to the thermally driven spin transport such as Spin Seebeck Effect. We use Brillouin light scattering technique to measure phonon and magnon temperature. We found that they can be driven out of equilibrium under a large temperature gradient. We numerically simulate the phonon and magnon temperatures using two-temperature model. Our results suggest a lower bound of magnon phonon relaxation time in YIG.

1We acknowledge support from DOE, AOR under contract W911NF-14-1-0016 and NSF via grant CBET-1336968.

1:15PM B28.00011 Engineering damping in insulating magnet-metal bilayers using ultrathin spacer layers 1, SRIHARSHA V. ARADHYA, COLIN L. JERMAIN, HANJONG PAIK, JOHN T. HERON, DARRELL G. SCHLOM, DANIEL C. RALPH, ROBERT A. BUHRMAN, Cornell University — Insulating magnetic materials, particularly yttrium iron garnet (YIG), are of significant interest for fundamental research as well as technological applications. Thus far copper spacer layers of ~10 nm - 1 µm thickness sandwiched between YIG and heavy metal films have been shown to modulate the damping of the magnetic layer either higher or lower. We report on the effect of ultrathin nonmagnetic spacer layers on the damping of YIG with different heavy metal overlayers. We start with YIG films grown by oxide molecular beam epitaxy with thicknesses below 20 nm and Gilbert damping as low as 0.0005. We observe that a spacer layer can increase the damping by 50% in YIG/spacer/Ta samples compared to YIG/Ta, and the increase can be as large 500% for YIG/spacer/Pt compared to YIG/Pt. These observations suggest a significant increase in the effective spin mixing conductance at the YIG-heavy metal interface that might be used to improve the efficiency of the spin torque produced by the spin Hall effect.

1:27PM B28.00012 Low-temperature magnetization dynamic properties of yttrium iron garnet films 1, YUE ZHAO, QI SONG, WEI YUAN, TANG SU, International Center for Quantum Materials, Peking University, Beijing, YONG WU, YONG JIANG, School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing, WEI HAN, International Center for Quantum Materials, Peking University, Beijing, JING SHI, Department of Physics and Astronomy, University of California, Riverside, California 92521, USA — The long lifetime of collective spin excitations in yttrium iron garnet (YIG) has spurred intense interest in spintronics. Ferromagnetic resonance (FMR) is a sensitive tool for investigating the magnetization dynamics in YIG films as well as YIG-based heterostructure devices. Previous studies have been mainly focused on the room temperature magnetization dynamics of YIG thin films. In this talk, I will first describe a low-temperature broad-band FMR setup with a wide frequency range from 1 to 18 GHz incorporated in Quantum Design’s Physical Properties Measurement System. Using this setup, we study the magnetization dynamic properties of the YIG thin films. In YIG films we observe an intriguing non-monotonic behavior in the temperature dependence of the FMR linewidth from which the Gilbert damping parameter can be extracted. Furthermore, various thicknesses of YIG films are studied to probe the underlying mechanisms that dominate the low-temperature magnetization dynamic behavior. Our temperature-dependence FMR results are very important for the understanding of the relaxation processes of YIG thin films.
1:39PM B28.00013 Growth of high-quality nanometre-thick yttrium iron garnet by sputtering and their magnetic properties , ARPITA MITRA, OSCAR CESPEDES, MANNAN ALI, B.J. HICKEY, Univ of Leeds, UNIVERSITY OF REGENSBURG COLLABORATION — Observation of Spin Seebeck effect (SSE) in magnetic insulators has led to dramatic advances in spin currents research and its applications for thermo-spintronics devices. Here we report deposition of high quality nm-thick yttrium iron garnet(YIG) film on gadolinium gallium garnet(GGG) by RF magnetron sputtering. The morphology and magnetic properties of the films were studied by using AFM and SQUID VSM respectively. 10-60 nm thick films have surface roughness of 1.3Å and (111) orientation. Our results show that magnetic properties of YIG depend strongly on thickness: magnetic moment has linear dependence at room temperature. The saturation magnetization and coercive field observed in thick films are 136 emu/cc and 0.50 Oe, respectively. Temperature dependence of magnetization of nm-thick YIG films has revealed an interesting result, which can be attributed to an additional magnetic phase at the YIG/GGG interface. The reduction in magnetization at low temperatures up to now has not been reported, but has significant relevance for the spin hall magnetoresistance(SMR) at low temperature. Our results on the temperature dependence of Gilbert damping factor of YIG and YIG/Pt films will lead to new physics, to understand its effect on spin mixing conductance and SMR in magnetic insulators.

1:51PM B28.00014 Modeling the Interface of a Heavy Metal/Ferromagnetic Bilayer Using the Boltzmann and Drift-Diffusion Equations , VIVEK AMIN, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA, KYOUNG-WHAN KIM, Basic Science Research Institute, Pohang University of Science and Technology, Pohang 790-784, Korea, KYUNG-JIN LEE, Department of Materials Science and Engineering, Korea University, Seoul 136-701, Korea, HYUN-WOO LEE, PCTP and Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea, M.D. STILES, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA — Accurate models for spin torques due to electrical currents in heavy metal/ferromagnetic bilayers allow for the meaningful extraction of parameters from measurements and optimization of devices. Descriptions of coherent spin transport across magnetic interfaces used to date typically take the form of resistor-like components that neglect the spin-orbit interaction. Using the Boltzmann equation, we develop new boundary conditions for the drift-diffusion equations to include both interfacial spin-orbit coupling and the exchange interaction due to the magnetization. These boundary conditions capture interfacial spin-flip scattering, coupling between longitudinal and transverse spin components, and significant modifications to the interfacial torques on the magnetization. They address the spin-orbit interaction at the interfaces of heavy metal/ferromagnetic bilayers, and allow for the calculation of interfacial spin-orbit torques within the drift-diffusion approach.


11:15AM B29.00001 Thermalization, Charge Ordering, and other Recent Developments in Artificial Spin Ice1,2 , PETER SCHIFFER2, Department of Physics, University of Illinois at Urbana-Champaign — Artificial spin ice consists of arrays of lithographically fabricated single-domain ferromagnetic elements, arranged in different geometries such that the magnetostatic interactions between the moments are frustrated. Magnetic force microscopy imaging of these arrays allows us to study the accommodation of frustration through the local correlations between the moments as a function of both the strength of the interactions and the geometry of the frustration. The interactions can be closely mapped onto those of the “spin ice” materials, and allow a detailed analysis of the local correlations and monopole-like excitations. We have probed a number of different lattice geometries and find both local ordering and disordered states that match classic models for frustrated spin systems. Our recent work has focused on thermalization of these arrays as well as investigation of lattice geometries that are unavailable in natural systems and are specifically designed to exhibit unusual behavior associated with frustration, e.g., the shakti lattice. Thermalization reveals ordering both of the moments and of the effective magnetic charges that characterize correlated many-body dynamics in these systems. Other recent work has involved studies of return point memory as well as measurements of electrical transport in these systems.

1This work was primarily funded by the US Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division under grant no. DE-SC0010778.
2Work performed in collaboration with Ian Gilbert, Sheng Zhang, Brian Le, Gia-Wei Chern, Bryce Fore, Yuyang Lao, Jungskil Park, Michael J. Erickson, Liam O’Brien, Chris Leighton, Paul E. Lammert, Vincent H. Crespi, Nitin Samarth, and Cristiano Nisoli.

11:51AM B29.00002 ABSTRACT WITHDRAWN —

12:03PM B29.00003 Dynamics of artificial square spin ice during a non-equilibrium field ramp and quench1,2 , JUAN CARLOS ANDRESEN, Department of Theoretical Physics, KTH Stockholm, SHRAWAN MISHRA, Advanced Light Source, Lawrence Berkeley National Laboratory, JAMES LEE, XIAOWEN SHI, Advanced Light Source, Lawrence Berkeley National Laboratory & Department of Physics, University of Oregon, BARRY FARMER, LANCE DE LONG, University of Kentucky, PATRIK HENELIUS, Department of Theoretical Physics, KTH Stockholm, STEVE KEVAN, SUJOY ROY, Advanced Light Source, Lawrence Berkeley National Laboratory — Recent advances in nanotechnology make it possible to create arrays of single-domain ferromagnetic nanowires that can be fabricated to mimic a variety of Ising-like model systems. This has opened up new ways of studying frustrated systems, such as artificial square spin ice. One of the main advantages of studying these nanomagnet systems is that the Ising-like moments can be directly visualized; but a persistent drawback has been the inaccessibility of the ground state, due to the highly athermal nature of these systems. We present the magnetic autocorrelation function of artificial square spin ice, as measured by XPCS following a non-equilibrium field quench. Our large-scale Monte Carlo simulations agree qualitatively with the experimental relaxation measurements. Furthermore, our simulation results indicate that a simple field ramp demagnetization protocol can be a viable way of reaching a low-energy state.

1US DoE Grant No. DE-FG02-97ER45653 (U. KENTUCKY)

12:15PM B29.00004 Exchange Bias and Magnetotransport in Permalloy Connected Kagome Artificial Spin Ice , BRIAN LE, University of Illinois at Urbana-Champaign, DAVID RENCH, RAJIV MISRA, Pennsylvania State University, LIAM O’BRIEN, CHRIS LEIGHTON, University of Minnesota, NITIN SAMARTH, Pennsylvania State University, PETER SCHIFFER, University of Illinois at Urbana-Champaign — Artificial spin ice consists of nanoscale ferromagnets arranged in a periodic lattice, with the resultant magnetostatic interactions emulating the local magnetic behavior of spin ice. Kagome artificial spin ice consists of elongated ferromagnetic islands or nanowires arranged in a honeycomb lattice. We present magnetotransport results in connected kagome artificial spin ice composed of permalloy (Ni81Fe19) nanowires. Magnetoresistance was measured as a function of applied field strength at different temperatures. At temperatures below 20 K, the field reversal symmetry of the magnetoresistance is broken. This asymmetry appears to be associated with exchange bias due to the surface oxidation of permalloy and is suppressed in aluminum-capped samples. These results signify that exchange bias can play a substantial role in the physics of artificial spin ice that has potential as a new mode of controlling its behavior. Supported by the US Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division under grant number DE-SC0010778. Work at the University of Minnesota was supported by the NSF MRSEC under award DMR-0819885 and a Marie Curie International Outgoing Fellowship within the 7th European Community Framework Programme (project no. 299376).
12:27PM B29.00005 Return Point Memory in Artificial Spin Ice1. JAN GILBERT, University of Illinois at Urbana-Champaign, GIA-WEI CHERN, Los Alamos National Laboratory, BRYCE FORE, YUYANG LAO, University of Illinois at Urbana-Champaign, CRISTIANO NISOLI, Los Alamos National Laboratory, PETER SCHIFFER, University of Illinois at Urbana-Champaign — Return point memory, in which the spins of a magnet return to their original configuration after the magnet is driven through a hysteresis loop, has been studied extensively with theory, simulations, and bulk experimental probes. However, due to the difficulties associated with directly imaging single spins, microscopic experimental examination of return point memory has proven to be elusive. Here we describe a study of return point memory in arrays of single-domain nanomagnets known as artificial spin ice. In this system, the individual moments can be experimentally resolved by magnetic force microscopy (MFM), so we can both verify the existence of return point memory and explore the mechanism by which it develops. We find that, in artificial spin ice, magnetic monopole excitations drive the development of return point memory through a ratchet-like interaction with the local field produced by the surrounding nanoislands. The number of hysteresis loops required to produce return point memory can be adjusted by tuning the applied magnetic field and array geometry.

1This work was primarily funded by the US Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division under grant no. DE-SC0010778.

12:39PM B29.00006 Charge-ordering in FePd3 artificial kagome ice . JASPER DRISKO, STEPHEN DAUNHEIMER, JOHN CUMINGS, University of Maryland, College Park — Artificial spin ices (ASIs) are arrays of lithographically-patterned, Ising-like nanomagnets built-by-design to be geometrically frustrated. ASIs have proven to be a novel and powerful tool for studying the effects of frustration due to its success in modeling real frustrated materials like spin ice, its highly tunable nature, and its amenability to a variety of techniques to directly characterize exact spin configurations. A fundamental question for frustrated systems is how they find long-range ordered states or whether this is even possible at all in the presence of frustration. In this work we investigate theoretical predictions of charge-ordering in the kagome ice-II state [1]. We employ ASI fabricated from FePd3, which has a relatively low Curie temperature and thus easily allows for thermally activated reversal of individual spins. We have fabricated samples with magnets of varying lengths and investigate them using Lorentz Transmission Electron Microscopy. Samples are heated above their Curie temperature and cooled slowly back to room temperature, allowing the macro-spins to interact, flip, and relax during the cooling process. We find that shorter lattice constant samples tend to exhibit better ordering of magnetic charges after cooling. We have also performed simulations of our samples using a kinetic Monte Carlo technique. We find very good agreement between the simulations and experiment when we incorporate a disordered spread of magnet widths into the simulations, representative of our real samples due to lithography artifacts.

12:51PM B29.00007 Nanoscale SEMPA imaging of an artificial quasicrystal spin ice at remanence , ANDREW BALK, Center for Nanoscale Science and Technology, National Institute of Standards and Technology. Maryland Nanocenter, University of Maryland, VINAYAK BHAT, BARRY FARMER, LANCE DELONG, University of Kentucky, Department of Physics and Astronomy, JOHN UNGURIS, Center for Nanoscale Science and Technology, National Institute of Standards and Technology., ELECTRON PHYSICS GROUP, CNST TEAM — Artificial spin ice has emerged in the past decade as a model metamaterial for studying frustrated magnetic ordering at length scales large enough to be experimentally probed in real space. Recently, complex designs have been engineered to explore exotic behavior in non-square lattices. However, direct measurements of the actual moment directions have not been very common, and interpretation from techniques such as magnetic force microscopy and magneto-optical Kerr effect magnetometry can be complicated by the more complex geometries. Here we demonstrate using SEMPA (scanning electron microscopy with polarization analysis) as a method to robustly measure the ordering direction of elements in a connected artificial quasicrystal. We discuss the applicability of SEMPA to this system, details of the imaging and potential artifacts, and conclusions that can be drawn from the nanoscale two dimensional maps of the moment direction.

1This work is partially funded by DoE grant #DE-FG02-97ER45653. ALB acknowledges support of this research under the Cooperative Research Agreement between the University of Maryland and NIST.

1:03PM B29.00008 First observation of ferromagnetic order in an artificial 2D quasicrystal1. BARRY FARMER, VINAYAK BHAT, University of Kentucky, Department of Physics and Astronomy, ANDREW BALK, JOHN UNGURIS, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, LANCE DE LONG, University of Kentucky, Department of Physics and Astronomy — Magnetic order in bulk quasicrystals is not well understood and known materials exhibit short-range, spin-glass order. We patterned ferromagnetic (FM) thin films into artificial quasicrystals, a new class of metamaterials that exhibits complex magnetic reversal and dynamics that can be controlled via tiling design. We analyzed two-dimensional SEMPA images of magnetization textures of Penrose P2 tilings (P2T) patterned into Permalloy. Samples are heated above their Curie temperature and cooled slowly back to room temperature, allowing the macro-spins to interact, flip, and relax during the cooling process. We find that shorter lattice constant samples tend to exhibit better ordering of magnetic charges after cooling. We have also performed simulations of our samples using a kinetic Monte Carlo technique. We find very good agreement between the simulations and experiment when we incorporate a disordered spread of magnet widths into the simulations, representative of our real samples due to lithography artifacts.

1Kentucky research supported by U.S. DoE Grant DE-FG02-97ER45653 and NSF Grant EPS-0814194. ALB acknowledges support under the Cooperative Research Agreement between the University of Maryland and NIST.

1:15PM B29.00009 ABSTRACT WITHDRAWN –

1:27PM B29.00010 Honeycomb artificial spin ice at low temperatures1. KATHARINA ZEISSLER, MEGHA CHADHA, LESLEY COHEN, WILL BRANDFORD, Imperial College London — Artificial spin ice is a macroscopic playground for magnetically frustrated systems. It consists of a geometrically ordered but magnetically frustrated arrangement of ferromagnetic macroscopic spins, e.g. an arrangement of single domain ferromagnetic nanowires on a honeycomb lattice. Permalloy and cobalt which have critical temperature scales far above 290 K, are commonly used in the construction of such systems. Previous measurements have shown unusual features in the magnetotransport signature of cobalt honeycomb artificial spin ice at temperatures below 50 K which are due to changes in the artificial spin ice’s magnetic reversal. In that case, the artificial spin ice bars were 1 micron long, 100 nm wide and 20 nm thick. Here we explore the low temperature magnetic behavior of honeycomb artificial spin ice structures with a variety of bar dimensions, indirectly via electrical transport, as well as, directly using low temperature magnetic imaging techniques. We discuss the extent to which this change in the magnetic reversal at low temperatures is generic to the honeycomb artificial spin ice geometry and whether the bar dimensions have an influence on its onset temperature.

1The EPSRC (grant no. EP/G004765/1; grant no. EP/L504786/1) and the Leverhulme Trust (grant no. RPG 2012-692) funded this scientific work.

1:39PM B29.00011 ABSTRACT WITHDRAWN –
Magneto-optical and magneto-transport studies of hexagonal artificial spin ice nano-structures.

**Monday, March 2, 2015 11:15AM - 2:15PM**

**Session B30 GMAG DMP: Focus Session: Nanomagnetic Devices II**

11:15AM B30.00001 Micromagnetic Architectures for On-chip Microparticle Transport

**11:27AM B30.00002 Parallel Dipole Line System: A Novel Magnetic Trap and High Sensitivity Hall system**

**11:39AM B30.00003 Geometric Constraints on Planar Manipulation of Microparticles via Magnetic Traps**
11:51 AM B30.00004 (001) Oriented \( L_10 \) FeCuPt for Heat-Assisted Magnetic Recording, Kai Liu, University of California - Davis — High magnetic anisotropy materials are critical to key technologies such as ultrahigh density magnetic recording and permanent magnets. Among them, ordered FePt alloys in the \( L_10 \) phase are particularly sought after, for the emerging heat-assisted magnetic recording (HAMR) media. However, the highly desirable properties are associated with the tetragonal \( L_10 \) phase. Key challenges exist in the high annealing temperature necessary to transform the as-deposited disordered cubic \( L_1 \) phase into the ordered tetragonal \( L_10 \) phase and the ability to maintain the magnetic easy axis perpendicular to the film. We have achieved (001) oriented \( L_10 \) FeCuPt thin films, with magnetic anisotropy up to \( 3.6 \times 10^7 \) erg/cm\(^2\), using atomic-scale multilayer sputtering and rapid thermal annealing (RTA) at 400 °C for 10 seconds, which is much more benign compared to earlier studies [1]. The artificial ordering in the multilayer structure and a significant tensile stress exerted by the underlying Si/SiO\(_2\) during RTA facilitate the formation of (001) oriented \( L_10 \) phase. The \( L_1 \) to \( L_10 \) phase transformation has been investigated by x-ray diffraction and the first-order reverse curvature (FORC) method [2]. The \( L_10 \) ordering takes place via a nucleation-and-growth mode. Traditional x-ray diffraction is not always reliable in generating a true order parameter, due to non-ideal crystallinity of the \( L_1 \) phase in some of the samples. A magnetization-based \( L_10 \) phase fraction is extracted, providing a quantitative measure of the \( L_10 \) phase homogeneity [3].


This work has been done in collaboration with D. A. Gilbert, J. W. Liao, L. W. Wang, J. W. Lau, T. J. Klemmer, J. U. Thiele, and C. H. Lai, supported by the NSF (DMR-1008571).

12:27PM B30.00005 Magnetic anisotropy modified by strain effects in \( Y_2Fe_4B \), Yoshiro Goehda, Tokyo Institute of Technology, Yokohama, ZAHRAM TORBATIAN, TAISUKE OZAKI, SHINJI TSUNEYUKI, The University of Tokyo — In exhibiting the magnetic anisotropy energy (MA) mainly arises from the spin-orbit coupling interaction. Here, throughout an ab initio study we show that direct exchange coupling in Fe alloyed with B is responsible for the symmetry breaking in an octahedral crystal field. Our magnetic-anisotropy decomposition identified dominant magnetic site and orbital couplings. Our method will enable us to study the anisotropy at microstructure interfaces. [1] Z. Torbatian, T. Ozaki, S. Tsuneyuki, and Y. Goehda, Appl. Phys. Lett. 104, 242403 (2014).

[1] This work was supported by ESICMM and the K computer.

12:39PM B30.00006 Tuning magnetic properties of metallic nanostructures on semi-insulating substrates, Oleg Brovko, Valeri Stepanyuk, Max Planck Institute of Microstructure Physics, Halle, Germany — In the past two decades, the properties of metallic nanostructures on metallic surfaces have been studied in minute detail and possibilities to tune them have been explored both experimentally and theoretically. [1] Recently the focus has been shifting towards insulating or semi-insulating substrates, [2] the reason being that while on metallic surfaces the magnetism of nanostructures is determined by the coupling of the localized magnetic moment of the ad-structure to a bath of itinerant electrons of the substrate, on insulating substrates the spin is largely isolated and often exhibits emergent quantum properties. In this work we simulate semi-insulating substrates open an additional possibility of adjusting the coupling of the ad-structure spin to the substrate. In the present contribution we show the possibility to tune magnetic properties of metal nanostructures and their interaction among each other on such semi-insulating substrates as thin decoupling CuN, h-BN and MgO layers. As a means of tuning we focus on adsorption site tailoring and exposure to external electric field. [1] O. Brovko et al., JPCM 26, 093001 (2014). [2] S. Loth et al., Science 335, 196 (2012), T. Schuh et al., Nano Lett. 12, 4805 (2012)

12:51PM B30.00007 Effects of exchange interactions on magnetic anisotropy and spin-dynamics of adatoms on metallic surfaces, Pedro Ruiz Diaz, Max Planck Institute of Microstructure Physics, Oleg Stepanyuk, Physics Department, Moscow State University, Valeri Stepanyuk, Max Planck Institute of Microstructure Physics — A common belief is that magneto-crystalline anisotropy energy (MA) mainly arises from the spin-orbit coupling interaction. Here, throughout an ab initio study we show that direct exchange interactions (Eex) together with substrate-mediated interactions rules the MA nature in Co inter-acting adatoms supported on Cu(001) and Pt(001) surfaces. MA exhibits a non-trivial behavior and is found to be strongly sensitive to Eex, magnetic order and substrate composition. Oscillatory magnetization switching is also revealed. Further, by means of a stochastic method, for the first time to our knowledge, the spin-dynamics of these single-spin systems assessed in the hysteresis loops is presented. Insights about the interplay between Eex and MA which determines the onset of the magnetization curves and their shape are discussed.

1:03PM B30.00008 ABSTRACT WITHDRAWN

1:15PM B30.00009 A New Method Based on RF Impedance Technology and Soft Ferromagnetic Ribbons for Real-Time Corrosion Monitoring, Izabella Berman, Jagannath Devkota, Harinaran Srikanth, Mahn-Huong Phan, None — Development of a quick, cheap, and reliable technique to estimate the concentration of corrosive chemicals has been of technological interest for safety in industries and the environment for many years. Here we present a new approach for real-time monitoring of chemical corrosion based on the radio-frequency (RF) impedance technology and soft ferromagnetic ribbons. The impedance \( Z \), resistance \( R \), and reactance \( X \) of a commercial METGLAS®2714A ribbon was measured in real time for \( 5 \mu l \) of drop-casted HNO\(_3\) of various concentrations. Variations in the concentration of the drop-casted acid were assessed by considering the difference of \( \Delta Z \) in the Z, R, and X with and without the acid treatment. The measurements performed at 0.2 MHz showed a large linear increase in the \( \Delta Z \) and \( \Delta R \) with the acid concentration which is ideal for developing highly sensitive chemical sensors. Since the ribbon used is commercially available at low cost and the measurement system is quick and low power consuming, the proposed sensor can be used as an easy, quick, and low-cost chemical probe in industries and environmental safety purposes.

[1] Department of Physics, University of South Florida

1:27PM B30.00010 Stochastic magnetization dynamics of biochemically bound magnetic nanoparticles, Daniel Reeves, Department of Physics and Astronomy, Dartmouth College, John Weaver, Department of Physics and Department of Radiology, Dartmouth College — Understanding the dynamics of magnetic nanoparticles in applied magnetic fields is critical for biosensing and therapeutic applications. In biological environments, the nanoparticles may clump together and the resultant dynamics are interesting and important. We show simulation schemes using stochastic Langevin equations that describe the particle rotations in various conditions and suggest ways to improve the applications. Biochemical binding is described in terms of changes of the size distribution from network theory perspective. Also, using log-normally size distributed particles, a master variable is derived that contains all the significant variables. This compacts the parameter space, quickens simulation, and improves intuition. An approximate closed form solution to the magnetization harmonics in an oscillating field is given in terms of this variable using the Langevin function.
1:39PM B30.00011 Iron oxide nanoparticles with controlled morphology for advanced hyperthermia

ZOHREH NEMATI PORSOKHOU, HAFSA KHURSHID, Univ of South Florida-physics, JAVIER ALONSO MESSA, Univ of South Florida-physics and BC Materials (Spain), MANH-HUONG PHAN, HARIRHAN SRIKANTH, Univ of South Florida-physics — Magnetic nanoparticles (NPs) are interesting for a wide range of applications. In biomedicine, they have been exploited for use in drug delivery, magnetic resonance imaging, and magnetic hyperthermia. While magnetic hyperthermia, using NPs to convert electromagnetic energy into heat to destroy the cancer cells, represents a novel cancer treatment technique, a poor heating conversion efficiency of the existing NPs restricts its practical use. Different strategies have been proposed to overcome this limitation, mainly by tuning the size, saturation magnetization and effective anisotropy of the NPs. Here we report a magnetic hyperthermia study on Fe3O4 NPs, where the effective anisotropy was tuned by varying particle morphology from the spherical to octopod shape. The Fe3O4 NPs were synthesized using a thermal decomposition method. Transmission electron microscopy (TEM) and high-resolution TEM images show high crystalline monodisperse nanoparticles. X-ray diffraction patterns confirm the presence of Fe3O4 phase. Hyperthermia experiments indicate that the octopod possesses a higher SAR as compared to their spherical counterpart. Our findings provide an effective approach to improve the SAR of NPs by manipulating the shape anisotropy of the nanoparticles.

1:51PM B30.00012 Magneto-impedance based detection of magnetically labeled cancer cells and bio-proteins

J. DEVKOTA, Department of Physics, University of South Florida, M. HOWELL, S. MOHAPATRA, Department of Molecular Medicines, University of South Florida, T.H. NHUNG, Institute of Physics, Vietnam Academy of Science and Technology, P. MUKHERJEE, H. SRIKANTH, M.H. PHAN, Department of Physics, University of South Florida — A magnetic biosensor with enhanced sensitivity and immobilized magnetic markers is essential for a reliable analysis of the presence of a biological entity in a fluid. Based on conventional approaches, however, it is quite challenging to create such a sensor. We report on a novel magnetic biosensor using the magneto-impedance (MI) effect of a Co-based amorphous ribbon with a microhole-patterned surface that fulfills these requirements. The sensor probe was fabricated by patterning four microholes, each of diameter 2 µm.H. PHAN, Department of Physics, University of South Florida — Magnetic nanoparticles (NPs) are being considered as therapeutic tools for cancer treatments. Most of the existing NPs, where the effective anisotropy was tuned by varying particle morphology from the spherical to octopod shape. The Fe3O4 NPs were synthesized using a thermal decomposition method. Transmission electron microscopy (TEM) and high-resolution TEM images show high crystalline monodisperse nanoparticles. X-ray diffraction patterns confirm the presence of Fe3O4 phase. Hyperthermia experiments indicate that the octopod possesses a higher SAR as compared to their spherical counterpart. Our findings provide an effective approach to improve the SAR of NPs by manipulating the shape anisotropy of the nanoparticles.

2:03PM B30.00013 Comparison of Coil Designs for Transcranial Magnetic Stimulation on Mice

PRIYAM RASTOGI, RAVI HADIMANI, DAVID JILES, Department of Electrical and Computer Engineering, Iowa State University — Transcranial magnetic stimulation (TMS) is a non-invasive treatment for neurological disorders using time varying magnetic field. The electric field generated by the time varying magnetic field is used to depolarize the brain neurons which can lead to measurable effects. TMS provides a surgical free method for the treatment of neurological brain disorders like depression, post-traumatic stress disorder, traumatic brain injury and Parkinson’s disease. Before using TMS on human subjects, it is appropriate that its effects are verified on animals such as mice. The magnetic field intensity and stimulated region of the brain can be controlled by the shape, position and current in the coils. There are a few reports on the designs of the coils for mice. In this paper, different types of coils are developed and compared using an anatomically realistic mouse model derived from MRI images. Parameters such as focality, depth of the stimulation, electric field strength on the scalp and in the deep brain regions, are taken into account. These parameters will help researchers to determine the most suitable coil design according to their need. This should result in improvements in treatment of specific disorders.


11:15AM B31.00001 The Relationship Between Torsion and Anisotropic Exchange Coupling in a Tb(III)-Radical Complex

MICHAEL L. BAKER, TAKUYA TANAKA, Tohoku University, SEIKO KAWAMURA, KENJI NAKAJIMA, J-PARC, TAKAYUKI ISHIDA, The University of Electro-Commun., HIROYUKI NOJIRI, Tohoku University — The incorporation of paramagnetic ligands within anisotropic rare earth ion clusters has provided significant advance to the design of single molecule magnets with large blocking temperatures [1]. The exchange interaction in such systems is complex, difficult to probe, and little is known about structural relations. Inelastic neutron scattering and sub-THz electronic paramagnetic resonance are used complimentary to investigate the large exchange interaction between a rare earth - radical pair in the Tb(hfac)3(2pyNO) complex [2]. Two molecular species exhibiting different Tb-O-N-C torsion angles of the paramagnetic 2pyNO ligand are compared. Antiferromagnetic Ising type 2p – 4f exchange is determined for a low torsion angle (3.8 degrees) species. A different species with a larger torsion angle (15.8 degrees) is found to have weaker antiferromagnetic exchange and a non-degenerate ground state doublet. The origin of degeneracy lifting is due to an in-plane ferromagnetic component to the exchange matrix originating from 2p – 5d charge transfer rather than a Dzyaloshinski-Moriya interaction.


11:27AM B31.00002 Magnetic Behavior of a Dy8 Molecular Nanomagnet

QING ZHANG, MYRIAM SARACHIJK, City College of New York, MICHAEL BAKER, City College of New York and New York University, YIZHANG CHEN, ANDREW KENT, New York University, THEOCHRIS STAMATATOS, Brock University, Ontario — As part of a study of quantum tunneling in a newly synthesized family of dysprosium-based molecular magnets that exhibit a chiral spin structure, we report initial investigations of the magnetic response of a Dy8 cluster with the formula (Et2N)2[Dy8O(μ4-O)2(NO3)10(H2O)2]·2MeCN [1]. The molecular complex contains triangular arrangements of exchange coupled Dy(III) ions [2]. The compound forms an approximate snub-square Archimedeans lattice unit. The measured magnetization of this network of four triangles suggests the presence of multiple spin chiral vortices. Single crystal susceptibility and magnetization measurements indicate the presence of a hard-axis direction and an easy plane. These principal orientations have been investigated in magnetic fields up to 5 Tesla for temperatures between 1.8 and 100 K using a SQUID-based Quantum Design MPMS magnetometer. Complex easy plane magnetic hysteresis loops emerge at lower temperatures measured using Hall probe magnetometry at sub 1 K temperatures. The analysis of these measurements will be discussed and compared with results of theoretical calculations. [1] D. I. Alexandropoulos, et al., Inorg. Chem. 53, 5420 (2014). [2] J. Luzon, et al., Phys. Rev. Lett. 100, 247201 (2008).

1 Work supported by ARO W911NF-13-1-1025 (CCNY), NSF-DMR-I309202 (NYU); the synthesis of the Dy8 cluster was supported by NSERC (Discovery grant to Th.C.S.).
11:39AM B31.00003 Magnetic Properties of Electrically Contacted Fe₄ Molecular Magnets
JACOB BURGESS, MPSD and MPI FKF, Germany, LUIGI MALAVOLTI, VALERIA LANZILOTTO, MATTEO MANNINI, FREDERICO TOTTI, SILVIYA NINOVA, Dept of Chem, UniFi and INSTM, Florence, Italy, SHICHAO YAN, DEUNG-JANG CHOI, STEFFEEN ROLF-PISSARCZYK, MPSD and MPI FKF, Germany, ANDREA CORNIA, Dept of Chem and Geo Sciences, UniMoRE and INSTM, Italy, ROBERTA SESSOLI, Dept of Chem, UniFi and INSTM, Florence, Italy, SEBASTIAN LOTH, Max Planck Institute for the Structure and Dynamics of Matter (MPSD), Hamburg and Max Planck Institute for Solid State Research (MPI FKF), Stuttgart — Single molecule magnets (SMMs) are often large and fragile molecules. This poses challenges for the construction of SMM based spintronics. Device geometries with two electronic leads contacting a molecule may be explored via scanning tunneling microscopy (STM). The Fe₄ molecule [1] stands out as a robust, thermally evaporable SMM, making it ideal for such an experiment. Here we present the first STM investigations of individual Fe₄ molecules thermally evaporated onto a monolayer of Cu₂N on a Cu (100) crystal. Using inelastic electron tunneling spectroscopy (IETS), spin excitations in single Fe₄ molecules can be detected at meV energies. Analysis using a Spin Hamiltonian [2] allows extraction of magnetic properties of individual Fe₄ molecules, and investigation of the influence of the electronic leads. The tip and sample induce small changes in the magnetic properties of Fe₄ molecules, making Fe₄ a promising candidate for the development of spintronics devices based on SMMs.

1. [Nature 468, 417 (2010)].
2. [Nano Letters 12, 518 (2012)].

11:51AM B31.00004 Single-Molecule Toroics in Ising-type lanthanide molecular clusters
LVIIU CHIBOTARU, KU Leuven — The toroidal magnetic moment [1] is an antisymmetric combination of second-order magnetic moments, possessing distinct symmetry from first-order electromagnetic moments due to the sign change under both space and time inversion. It has been observed for the first time in LiCoPO₄ as a homogeneous distribution of toroidal polarization [2], which was also the first evidence for the fourth fundamental form of ferroic order, the ferrotoroidicity [3]. Recently an almost net toroidal moment has been detected in Dy₃ triangles, implying the existence of toroidal quantum states in these complexes [4]. Single-molecule toroics (SMTs) are defined, by analogy with single-molecule magnets (SMMs), as bistable molecules with toroidal magnetic state, which seem to be most promising for future applications in quantum computing and information storage and as molecular multiferroic materials with magnetoelectric effect. The key features offering advantages to CMTs as potential units for storage and processing of information are (i) their insensitivity to external homogeneous magnetic fields and a remarkably weak magnetic interaction between themselves and (ii) the possibility to manipulate the toroidal states by electrical means (charge currents and variable electric fields). In this interdisciplinary research area that spans chemistry, physics and material sciences, synthetic chemists have already produced SMT systems suitable for detailed experimental study, while ab initio calculations have proven their reliability in the description of toroidal magnetization [6]. In this presentation, I will review the emerging field of SMTs with particular focus on how recent studies tend to address the issue of toroidal arrangement of local magnetic moment on the metal sites. Nine lanthanide-based SMTs will be presented showing, in particular, that the assembly of wheel-shaped complexes with the high symmetry of the molecule unit and combining strong intermetallic dipolar interactions with strong axial ferrotoroidicity [3]. Recently an almost net toroidal moment has been detected in Dy₃ triangles, implying the existence of toroidal quantum states in these complexes [4]. Single-molecule toroics (SMTs) are defined, by analogy with single-molecule magnets (SMMs), as bistable molecules with toroidal magnetic state, which seem to be most promising for future applications in quantum computing and information storage and as molecular multiferroic materials with magnetoelectric effect. The key features offering advantages to CMTs as potential units for storage and processing of information are (i) their insensitivity to external homogeneous magnetic fields and a remarkably weak magnetic interaction between themselves and (ii) the possibility to manipulate the toroidal states by electrical means (charge currents and variable electric fields). In this interdisciplinary research area that spans chemistry, physics and material sciences, synthetic chemists have already produced SMT systems suitable for detailed experimental study, while ab initio calculations have proven their reliability in the description of toroidal magnetization [6].


12:27PM B31.00005 Spontaneous Magnetic Deflagration of Mn₁₂tBuAc in a Transverse Field
YIZHANG CHEN, A. D. KENT, New York University, QING ZHANG, M. P. SARACHIK, City College of New York, MICHAEL L. BAKER, New York University & City College of New York, D. A. GARANIN, Lehman College of CUNY, NAJAH MHESN, CHRISTOS LAMPROPOULOS, University of North Florida — Magnetic deflagration has been triggered in molecular magnets with a swept longitudinal magnetic field [1], acoustic waves [2], and by applying a heat pulse [3-4]. In this work we report a study of the conditions for the spontaneous ignition of magnetic deflagration in the axially symmetric single molecule magnet Mn₁₂tBuAc. The onset of spontaneous deflagration shows clear resonant features in the Hₓ ⊗ Hₐ plane; here Hₓ is the longitudinal magnetic field, the bias that reduces the height of the magnetic anisotropy barrier, and Hₐ is the field transverse to the easy axis that mixes spin states on opposite sides of the anisotropy barrier. Consistent with expectations, the conditions (Hₓ, Hₐ) for spontaneous ignition vary with temperature. We show that the speed of the deflagration fronts are strongly reduced near quantum tunneling resonances due to magnetic relaxation prior to spontaneous deflagration events.

1. Yoko Suzuki *et al.*, *PRL* 95, 147201 (2005);
2. A. Hernández-Mínguez *et al.*, *PRL* 99, 217205 (2005);
3. S. McHugh *et al.*, *PRB* 76, 172410 (2007);

1. Work supported by NSF-DMR-1309202 (NYU); ARO W911NF-13-1-0125 (CCNY); DMR-1161571(Lehman College); Cottrell College Science Award from the Research Corporation for Science Advancement (UNF).

12:39PM B31.00006 Understanding and controlling the magnetic interaction between Ln(III) bis-(phenthalocyanine)’s “Double Decker” molecular nanomagnets and a magnetic substrate
ANDREA CANDINI, SIMONE MAROCCO, VALDIS CORRADINI, FILIPPO TROIANI, VALERIO BELLINI, Istituto Nanoscienze - CNR, Italy, ROBERTO BIAGI, VALENTINA DE RENZI, UMBERTO DEL PENNINO, MARCO AFFRONTE, Università di Modena e Reggio Emilia, Italy, SVETLANA KLYATSKAYA, MARIO RUBEN, Karlsruhe Institute of Technology (KIT), Germany, DAVID KLAR, HEIKO WENDE, University of Duisburg-Essen, Germany — Understanding and controlling the interaction between molecules and substrate is of crucial importance for the realization and implementation of molecular devices. Here we present the study by means of XAS and XMCD of the magnetic coupling between LnPc2 “Double Decker” (Ln = Tb, Dy, Er) molecular nanomagnets sublimated in situ on top of a Ni(111) single crystal. We find an antiferromagnetic exchange coupling between the molecules and the Ni substrate. The observed dependence of the coupling strength on the specific Ln ion is explained by the analysis of the Ln spin-polarized density of states as calculated by DFT. This allows us to identify the microscopic origin of the magnetic interaction between the Ln ions and the molecule environment which happens by the mediation of the organic part of the molecule. This result will be particularly relevant also for the investigation of molecular spintronics devices employing TbPc₂ molecules. Finally, we show how this interaction can be further tuned by the insertion of a graphene layer.

1. A. Candini et al., paper submitted (2014)
12:51PM B31.00007 Pushing the Limits of Magnetic Anisotropy in a Mononuclear Ni(II) Single-Molecule Magnet: a High-Field EPR Study, LAKSHMI BHASKARAN, Department of Physics, Florida State University (NHMFL), Tallahassee, Florida, USA, KATIE MARRIOTT, MARK MURRIE, Department of Chemistry, University of Glasgow, Scotland, UK, STEPHEN HILL, Department of Physics, Florida State University (NHMFL), Tallahassee, Florida, USA — Single-Molecule Magnets (SMMs) are potential candidates for nanoscale magnetic information storage, where slow magnetization dynamics (bistability) is realized at low temperatures due to a magnetic anisotropy barrier separating the “spin-up” and “spin-down” states of the SMMs. Here, we report spectroscopic evidence for a huge easy-axis anisotropy in a trigonal bipyramidal (TBP) [NiII(3dabco)2] complex with an orbitally degenerate ground state. Single-crystal EPR studies were carried out in a 35T resistive magnet at the NHMFL. A very strong angle-dependence of the spectrum was observed within a few degrees of the hard plane, suggesting a huge zero-field-splitting (zfs) parameter, |D|>300 cm⁻¹, associated with first order spin-orbit coupling. This value is considerably larger than previously reported for a NiII TBP complex [1], and is thought to be due to the rigidity of the ligand that prevents Jahn-Teller type effects that can reduce D [2]. This is confirmed by the small value of the rhombic parameter, |E|= 0.66 cm⁻¹.

1:03PM B31.00008 Observation of Highly Forbidden Single-Photon Transitions in a Ni₄ Single-Molecule Magnet¹, YIMING CHEN, Amherst College and University of Massachusetts at Amherst, MOHAMMAD D. ASHEKEZARI, Amherst College, RAFAEL CASSARO, University of Massachusetts at Amherst, JONATHAN FRIEDMAN, Amherst College — We report electron-spin resonance experiments on a crystal of the single-molecule magnet (SMM) [Ni(hmp)(dmb)Cl]₂ (hereafter Ni₄), which is an S=4 system with large uniaxial anisotropy. At 115.4 GHz and low magnetic fields (below the anisotropy field for the SMM), we observe two weak resonances that correspond to highly forbidden transitions between magnetic sublevels, one corresponding to Δm = 0 and another corresponding to Δm = −1. The interpretation of the observed transitions is confirmed by following how the peak positions change with the angle between the sample’s easy axis and the applied field. The selection rules forbidding these transitions are lifted by tunneling between m states. The observed forbidden transitions can be viewed as tunneling-assisted direct single-photon transitions between spin states. Equivalently, the forbidden transitions can be interpreted as resonant tunneling between one spin state of the molecule and the dressed state of another spin state. The forbidden transitions have much narrower line widths than the allowed transitions, which suggests that the lines are not inhomogeneously broadened by local fields. Assuming homogeneous broadening, we infer a decoherence time T₂ of ~0.5 ns.

¹Work supported by NSF under grant no. DMR-1310135.

1:15PM B31.00009 Single Molecule Metamagnetism and the Single Energy Scale Model, BELLAVE SHIVARMA, University of Virginia, PRADEEP KUMAR, University of Florida, RICHARD WINPENNY, University of Manchester, MICHAEL OSOFSKY, Naval Research Labs, V. CEILLI, University of Virginia — Measurements of the magnetization isotherms at low temperatures are used to extract the linear, χ₁ and third order, χ₃, magnetic susceptibilities of two distinct single molecule magnets (SMM), (UO₂⁻L₁)₃ and Cr₆F₁₁. In (UO₂⁻L₁)₃ the behavior of χ₃ is consistent with a peak appearing at a temperature T₀ which is ~ 0.5 T₁; the temperature at which a peak in χ₁ is observed. In Cr₆F₁₁ a peak in χ₁ is not present neither is a peak in χ₃ observed. Nevertheless, a simple phenomenological model with only a single energy scale, is able to account for the two distinct behaviors in the linear and nonlinear magnetic response of these two SMMs.

1:27PM B31.00011 Role of spin-orbit fluctuations in spin decoherence, MATHEW MARTENS, Florida State University, National High Magnetic Field Lab, JOHAN VAN TOL, National High Magnetic Field Lab, NARESH DALAL, Florida State University, SYLVAIN BERTAINA, Aix-Marseille University, CNRS, IM2NP UMR7334, 13397 cedex 20, Marseille, France, IRINEL CHIORESCU, Florida State University, National High Magnetic Field Lab — We performed a systematic study of the decoherence mechanism in the molecular compound K₆[As⁶⁺O₁₂D₂O] · 8D₂O, in short V₁₅ utilizing high-field electron spin resonance at 120 GHz, 241 GHz, and 336 GHz. This system has shown important quantum effects such as coherent spin oscillations as well as interesting out-of-equilibrium spin dynamics due to phonon bottlenecking. The spectra of a single V₁₅ crystal were measured and linewidths as a function of orientation, temperature, and field were extracted. By analyzing the shape and orientation anisotropy of the linewidths, we study how fluctuations in each term of the spin Hamiltonian contribute to the spin decoherence with much attention given to the spin-orbit coupling that generates g-factor anisotropy. Our conclusion is that fluctuations in the spin-orbit coupling can play an important role in the linewidth of a spin resonance.

³This work was supported by NSF Grant No. DMR-1206267 and CNRS-PICS CoDyLow. The NHMFL is supported by Cooperative Agreement Grant No. DMR-0654118 and the state of Florida.

³Martens et. al., PRB 89, 2014

⁴S. Bertain et. al., Nature (London) 466, 2010

⁵I. Chiorescu et. al., PRL 84, 2000

1:39PM B31.00011 Low Temperature Scanning Tunneling Spectroscopy of isolated Mn₁₂-Ph Single Molecule Magnets, K. REAVES, Dept of Materials Science and Engineering and Physics and Astronomy, Texas A&M University; WPI-AIMR, Tohoku University, Sendai, Japan, P. HAN, K. IWAYA, H. HITORUGI, D. PACKWOOD, WPI-AIMR, Tohoku University, Sendai, Japan, H. G. KATZGRABER, Dept of Materials Science and Engineering and Physics and Astronomy, Texas A&M University, Santa Fe Institute, H. ZHAO, K.R. DUNBAR, Dept of Chemistry, Texas A&M University, K. KIM, W. TEIZER, Dept of Materials Science and Engineering and Physics and Astronomy, Texas A&M University; WPI-AIMR, Tohoku University, Sendai, Japan — We study Mn₁₂O₁₂(C₆H₅COO)₁₅(H₂O)₄ (Mn₁₂-Ph) single-molecule magnets on a Cu(111) surface using scanning tunneling microscopy and scanning tunneling spectroscopy at cryogenic temperatures (T<6K). We report the observation of Mn₁₂-Ph in isolation and in thin films, deposited through in situ vacuum spray deposition onto clean Cu(111). The tunneling current of isolated Mn₁₂-Ph, normalized with respect to the Cu background, shows a strong bias voltage dependence within the molecular interior. The qualitative features of these I vs.V curves differ by spatial location in several intriguing ways (e.g. fixed junction impedance with increasing bias voltages). We explore these normalized I vs. V curves and present a phenomenological explanation for the observed behaviors, corresponding to the physical and electronic structure within the molecule.

¹Funding from WPI-AIMR
1:51PM B31.00012 Quantum coherence in Mn-based single molecule magnets . C. ABEYWARDANA, F.H. CHO, University of Southern California, A. MOWSON, G. CHRISTOU, University of Florida, S. TAKAHASHI, University of Southern California — As spin systems in solids, single-molecule magnets (SMMs) form a unique class of materials that have a high-spin, and their spin state and interaction can be easily tuned by changing peripheral organic ligands and solvate molecules. In addition, it has been shown that an individual or a small ensemble of SMMs can be transferred to surface with retention of their magnetic behavior. SMM is therefore a promising system for fundamental quantum science and for applications to dense and efficient quantum memory, computing, and molecular spintronics devices. In spite of diverse interests on quantum properties in SMMs, decoherence properties that ultimately limit such behaviors have not been understood yet. Until now, coherent manipulation of spin states in SMMs has been experimentally demonstrated only in a few SMMs [1-2]. In this presentation, we investigate quantum coherence in Mn-based SMMs using a high-frequency pulsed EPR technique, which has a significant advantage to quench the spin decoherence due to electron spins [3].


2:03PM B31.00013 Interface Effects in Spin-crossover (SCO) Thin Films on Au(111). SUMIT BENIWAL, XIN ZHANG, University of Nebraska - Lincoln, PATRICK ROSA, JEAN-FRANCOIS LETARD, TATIANA PALAMARCIC, Universite de Bordeaux, BERNARD DOUDIN, Universite Louis Pasteur Strasbourg, PETER DOWBEN, AXEL ENDEERS, University of Nebraska - Lincoln — Thin films of the SCO molecules [Fe(H_2B(pz)_2)(bipy)] on Au(111) are investigated. The growth mode is determined by low temperature scanning tunneling microscopy, whereas chemical and electronic properties are determined with X-ray photoemission spectroscopy (XPS) and inverse photoemission spectroscopy (IPES). The role of substrate in determining the electronic structure is determined from thickness and temperature dependent XPS. Thin films exhibit coexistence of Fe(II) and Fe(III) oxidation states, which is different from the Fe(II) oxidation state in bulk. The fraction of molecules in the Fe(II) state increases with film thickness, which suggests that the molecules at the interface are in the Fe(III) state. Cooling the films to 100 K triggers an irreversible transition from Fe(III) to Fe(II). This transition coincides with spin phase transition, where shift of the conduction band edge away from the Fermi level is observed in IPES. These results demonstrate that thin films of this complex have different phase transition behavior as compared to bulk-like samples and underline that substrate interaction is a powerful parameter to control their structural conformation, spin state as well as electronic properties.

Monday, March 2, 2015 11:15AM - 12:15PM — Session B32 GMAG DMP: Focus Session: Transition Metal Oxides I 207B - 11:15AM B32.00001 Probing functional perovskites through scanning transmission electron microscopy and first-principles theory1. STEPHEN PENNYCOOK, National University of Singapore — The aberration-corrected scanning transmission electron microscope (STEM) can provide real space imaging and spectroscopy at atomic resolution with a new level of sensitivity to chemical and electronic properties that ultimately limit such behaviors have not been understood yet. Until now, coherent manipulation of spin states in SMMs has been experimentally demonstrated only in a few SMMs [1-2]. In this presentation, we investigate quantum coherence in Mn-based SMMs using a high-frequency pulsed EPR technique, which has a significant advantage to quench the spin decoherence due to electron spins [3].


11:51AM B32.00002 Spin-state blockade in Te⁶⁺-substituted electron-doped LaCoO₃¹. KEISUKE TOMIYASU, SHUN-ICHI KOYAMA, MASANORI WATAHlKI, MIKA SATO, KAZUKI NISHIHARA, MITSUGI ONODERA, KAZUAKI IWASA, TSUTOMU NOJIMA, Tokohu Univ, YUICHI YAMASAKI, HIROHITO NAKAO, YOICHI MURAKAMI, KEN — Perovskite-type LaCoO₃ (Co²⁺: d⁶) is a rare inorganic material with sensitive and characteristic responses among low, intermediate, and high spin states. For example, in insulating nonmagnetic low-spin states below about 20 K, light hole doping (Ni substitution) induces much magnetization than expected; over net 10µB/hole (5µB/Ni) for 1µB/hole (1µB/Ni), in which the nearly isolated dopants locally change the surrounding Co low-spin states to magnetic ones and form spin molecules with larger total spin [1-4]. Further, the former is isotropic, whereas the latter exhibits characteristics anisotropy probably because of Jahn-Teller distortion [2]. In contrast, for electron doping, relatively insensitive spin-state responses were reported, as in LaCo(Ti⁴⁺)O₃, but are not clarified, and are somewhat controversial. Here, we present macroscopic measurement data of another electron-doped system LaCo(Te⁶⁺)O₃ and discuss the spin-state responses. – Refs. [1] S. Yamaguchi et al., PRB (1996). [2] K. Tomiyasu et al., PRB (2013). [3] A. Podlesnak et al., PRL (2008). [4] Y. Ju et al., J. Supercond. Nov. Magn. (2013).

1. This study was financially supported by Grants-in-Aid for Young Scientists (B) (No. 22740209 and 26800174) from the MEXT of Japan.

12:03PM B32.00003 Crystal Fields as a Probe of the Valence Transition in Pr-based Cobaltites . D. PHELAN, S. ROSENKRANZ, Argonne National Laboratory, D.M. PAJEROWSKI, NIST Center for Neutron Research, C. LEIGHTON, University of Minnesota — Upon cooling, a unique first-order metal-insulator transition (MIT) has been observed in cobaltite perovskites at certain compositions with Pr on the A-site; this is strongly suspected as a consequence of electron transfer from Pr³⁺ ions to hybridized Co-O orbitals. Here we discuss the crystal field levels of Pr³⁺ and Pr⁴⁺ ions which we have investigated using inelastic neutron spectroscopy as a function of temperature for three samples: one insulating, one metallic, and one that undergoes the MIT. We show that the insulating compound, PrCoO₃₋δ, contains Pr⁴⁺ ions (J=4) whose ground state multiplet is split into nine singlets, and we extract its crystal field parameters. In the hole-doped metal, Pr₀.₇Ca₀.₃CoO₃₋δ, which also contains Pr⁴⁺ ions, the crystal field levels maintain the same energy-level structure but are noticeably broadened. The scattering from the Pr⁴⁺ crystal fields, though present, is diminished in the sample that undergoes the MIT (Pr₀.₆₉Y₀.₀₇Ca₀.₃CoO₃₋δ), consistent with a decrease in the concentration of Pr⁴⁺; moreover, the levels are severely broadened. The experiments illustrate the inhomogeneous charge distribution that occurs around the Pr sites upon substitution.

1. Research sponsored by the US DOE-BES-MSED, ERC starting investigator award and Fundación Caja de Madrid.

2. This study was financially supported by Grants-in-Aid for Young Scientists (B) (No. 22740209 and 26800174) from the MEXT of Japan.
12:15PM B32.00004 Spatial Magnetic Phase Separation in the Oxygen Deficient Perovskite SrCoO$_{1-x}$O$_x$. Z.H. ZHU, Physics Department at University of Connecticut, F.J. RUECKERT, Wentworth Institute of Technology, J.I. BUDNICK, W.A. HINES, B.O. WELLS, Physics Department at University of Connecticut, CH. NIEDERMAYER, Laboratory for Neutron Scattering at Paul Scherrer Institut, B. DABROWSKI, Department of Physics at Northern Illinois University — We report here the unique local structure of the magnetically phase separated perovskite SrCoO$_{1-x}$O$_x$ by means of transverse field (TF) and zero field (ZF) muon spin rotation. Previously we reported samples of SrCoO$_3$ and SrCoO$_2$, both have unique magnetic and crystallographic phases, whereas samples of intermediate composition have multiple magnetic transitions but a single structural phase (Appl. Phys. Lett. 99, 052503 (2011)). Muon measurements establish that the intermediate compounds show spatially separated, distinct magnetic phases – true magnetic phase separation. In addition, the two magnetic phases evolve with temperature in a way indicating that the two phases remain coupled.

3Work at UConn was supported by NSF contract # DMR-0907197.

12:27PM B32.00005 Atomic-resolution scanning transmission electron microscopy study of the valence state transition in (Pr$_{0.85}$Y$_{0.15}$)$_{0.75}$Ca$_{0.3}$CoO$_3$, ROBERT KLIE, AHMET GULEC, University of Illinois at Chicago, DANIEL PHELAN, CHRIS LEIGHTON, University of Minnesota — The observation of a first-order magnetic/electronic transition in certain Pr-based perovskite cobaltites, such as Pr$_{0.5}$Ca$_{0.5}$CoO$_3$, has attracted significant attention. A simultaneous metal to insulator transition, a sharp drop in the magnetic moment and a change in the electronic structure has been reported to occur below $T_{MI}$. It was suggested that the low-temperature phase is stabilized by a shift of the mixed valence Co$^{3+}$/Co$^{4+}$ toward pure Co$^{3+}$, enabled by a valence change of Pr$^{3+}$ to Pr$^{4+}$. We present an atomic-scale study of (Pr$_{1-y}$Y$_y$)$_{0.75}$Ca$_{0.3}$CoO$_3$ using atomic-resolution imaging, electron energy-loss spectroscopy and in-situ cooling experiments in a scanning transmission electron microscope. The valence state transition in (Pr$_{1-y}$Y$_y$)$_{0.75}$Ca$_{0.3}$CoO$_3$ occurs at a transition temperature $T_{MI}$ ~ 135K for $y = 0.15$ and the in-situ cooling experiments are conducted at 90 K. At room temperature, we find oxygen vacancy ordering associated with a Co valence state ordering and we will demonstrate that the electron transfer occurs from Pr to Co below the transition temperature. The oxygen vacancy ordering disappears as a result of the Co valence state transition. The effects of oxygen mobility, sample homogeneity and the impact on the observed transition will be discussed.

1This work is supported by a grant from the National Science Foundation (NSF-DMR1408427).

12:39PM B32.00006 Brownmillerite CaCoO$_{2.5}$: Synthesis, Re-entrant Structural Transitions and Magnetic properties 1 JUNJIE ZHANG, HONG ZHENG, CHIRSTOS MALLIAKAS, JARED ALLRED, YANG REN, QING'AN LI, TIAN-HENG HAN, JOHN MITCHELL, Argonne Natl Lab. — Cobalt oxides attract both fundamental and technological attention due to their physical properties including thermoelectricity, giant magnetoresistance, superconductivity and multiferroicity [1]. Here we report the first synthesis of CaCoO$_{2.5}$, single crystals using a high pressure optical-image floating zone technique. We find that it is an ordered oxygen-deficient perovskite of the brownmillerite type, and it undergoes an unprecedented re-entrant structural phase transitions (Pcmb→P2/c11→P12/1/m→Pcm) with decreasing temperature. We describe its temperature-dependent structural, thermal, and magnetic properties, including AFM ordering near 240 K, with a weakly spin canted ferromagnet ground state below 140 K. The magnetic response of CaCoO$_{2.5}$ depends markedly on the cooling rate and field history. Magnetization data also imply the potential of a distinct, field-induced phase arising uniquely from the P12/1/m structure, revealed as kinetically trapped by a rapid-cooling protocol.

1Work in the Materials Science Division at Argonne National Laboratory was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Division of Materials Science and Engineering.

12:51PM B32.00007 Neutron Scattering Study on the Spin-1/2 Triangular-Lattice Antiferromagnet Ba$_2$CoSb$_2$O$_9$. JIE MA, Oak Ridge National Laboratory, Y. KAMIYA, iTHES Research Group and Condensed Matter Theory Laboratory, RIKEN, Japan, TAO HONG, H.B. CAO, G. EHLERS, Oak Ridge National Laboratory, Z.L. DUN, University of Tennessee, Knoxville, W. TIAN, Oak Ridge National Laboratory, C.D. BATISTA, Los Alamos National Laboratory, H.D. ZHOU, University of Tennessee, Knoxville, M. MATSUDA, Los Alamos National Laboratory, OAK RIDGE NATIONAL LABORATORY TEAM, iTHES RESEARCH GROUP AND CONDENSED MATTER THEORY LABORATORY, RIKEN, JAPAN COLLABORATION, UNIVERSITY OF TENNESSEE, KNOXVILLE COLLABORATION, LOS ALAMOS NATIONAL LABORATORY COLLABORATION — Ba$_2$CoSb$_2$O$_9$ is a spin-1/2 triangular-lattice antiferromagnet with uniform bond length that has attracted a lot of attention in the past decade. This compound is recognized as an ideal material to study the interplay between frustration, low-dimensionality, and strong quantum fluctuations. Both neutron diffraction and inelastic neutron scattering measurements were performed on Ba$_2$CoSb$_2$O$_9$ by obtaining the neutron scattering technique. According to our unpolarized and polarized neutron diffraction measurements, the Co$^{2+}$ magnetic moments form a 120 degree structure in the easy ab-plane. The intra- and inter-plane exchange interactions were determined by fitting the measured spin-wave dispersion with an S=1/2 XXZ model.

1Work at BNL supported by Office of Basic Energy Sciences, US DOE, under Contract No. DE-AC02-98CH10886.

1:03PM B32.00008 Anisotropic dispersion of charge stripe fluctuations in La$_{1.75}$Sr$_{0.25}$NiO$_4$. JOHN TRANQUADA, RUIDIAN ZHONG, GENDA GU, Brookhaven Natl Lab, DMITRY REZNIK, U. Colorado, BARRY WINN, ORNL — It has recently been demonstrated that charge stripe fluctuations can be detected in La$_2$Sr$_2$NiO$_6$ by inelastic neutron scattering at temperatures close to the charge-ordering transition [1]. The next step is to characterize the dispersion of these excitations. To do this, we have studied a crystal with $x = 0.25$ using the HYSPEC instrument at the Spallation Neutron Source. The clearest picture has been obtained at a temperature of 160 K, where spin order is absent while the charge order is weak but finite. The effective observation window is limited to $E < 8$ meV, as acoustic phonons dispersing from neighboring Bragg peaks obscure the weak signal of interest at higher energies. Measuring about the charge-order peak at wave vector (4.4,3,0), where $q* = 1.150$ Å$^{-1}$, we observe a dispersion with a velocity of ~ 20 meVÅ along the stripe-modulation direction, but no clear dispersion in the orthogonal direction. The detected velocity has the scale of lattice, rather than purely electronic, excitations.


1Work at BNL supported by Office of Basic Energy Sciences, US DOE, under Contract No. DE-AC02-98CH10886.

1:15PM B32.00009 ABSTRACT WITHDRAWN —
11:27PM B32.00010 Low-energy description of rare-earth nickelates. OLEG PEIL, University of Geneva, ALASKA
SUBEDI, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, ANTOINE GEORGES, College de France, Paris — We propose a simple low-energy theory of rare-earth nickelates that involves only two \( e_g \) orbitals per nickel site. We show that this theory, in particular, captures all important features of the metal-insulator transition of nickelates. In the monoclinic insulating state, bond-length disproportionation splits the manifold of \( e_g \) bands, leading to a modulation of the effective on-site energy. We show that, when subject to a local Coulomb repulsion \( U \) and Hund’s coupling \( J \), the resulting bond-disproportionated state is a paramagnetic insulator for a wide range of interaction parameters. Furthermore, we find that when \( U - 3J \) is small or negative, a spontaneous instability to bond disproportionation takes place for large enough \( J \). In the metallic phase, on the other hand, this negative effective coupling results in the suppression of the orbital polarization of \( e_g \) states, consistent with experiments and earlier calculations. This minimal theory emphasizes that a small or negative charge-transfer energy, a large Hund’s coupling, and a strong coupling to bond-disproportionation are the key factors determining the physics of nickelates. Finally, we discuss particular experimental consequences of this theoretical picture.

11:39PM B32.00011 Exchange and Magnetic Anisotropic Interactions of Magnetic Ions in Antiferromagnetic Materials, \( \text{Nd}_4\text{CuO}_4 \), ALEXANDER BAZHAN, P.L.Kapitza Institute for Physical Problems, RAS, Kosygin str, 2, Moscow, Russia — Investigations of magnetic ions interactions, based on theory of crystallographic and magnetic symmetry, which indicate quadratic forms of thermodynamic potentials, presented in irreducible representations of interacting magnetic moments, described by antiferromagnetic and magnetic vectors, which determine antiferromagnetic orderings, are caring out using vector v.s.magnetometer, in example, of non collinear antiferromagnetic orderings of four \( \text{Cu} \) ions in magnetic unit cells in \( \text{Nd}_4\text{CuO}_4 \) of tetragonal symmetry, applying in HTS. Magnetic field dependencies of three separate components of samples magnetic moments directly indicate magnetic moments orientations, determined by magnetic ions interactions. Transformations of non collinear antiferromagnetic orderings of \( \text{Cu} \) ions in magnetic fields \( H_0 \sim 42kOe \) and \( H_2 \sim 8.4kOe \), at fields orientations along \([100]\) and \([110]\) axis, \( T \sim 1.8K \), which are discussing using representations, determined by two antiferromagnetic vectors in equations of magnetic states, can be used in investigations, when two dimensional correlated electrons systems are introduced in such materials, before HTS.

2:03PM B32.00013 ABSTRACT MOVED TO W32.00006 —

Monday, March 2, 2015 11:15AM - 1:27PM — Session B33 GPC: Focus Session: The Physics of Climate

11:15AM B33.00001 A Test for Periodic and Quasi-Periodic Fluctuations in Past Climate Change Data, JAMES OTTO, JAMES ROBERTS, University of North Texas — In this work the temperature fluctuations for a number of proxy data sets were analyzed to test for periodic and quasi-periodic fluctuations in climate changes in the past. The data sets analyzed identify temperature functions which could be modeled using amplitude and frequency modulated sinusoidal waves. Data for the past 2000 years were tested and they show select periods of 11 years, 100 years, 300 years and 600 years. Longer term data (million years) indicate periods of 21000 and 41000 years as predicted by Milankovitch.

11:27AM B33.00002 Nonlinear/Non-Gaussian Data Assimilation\(^1\), JUAN RESTREPO, Department of Mathematics, Oregon State University — Data and models, with their inherent uncertainties and errors, are blended within a Bayesian framework with the aim of improving estimates of dynamic processes. This process, called data assimilation, is said to be responsible for significantly better weather/climate forecasts. Nonlinear/non-Gaussian processes, however, pose special conceptual and computational challenges. In the context of generic transport problems of importance in climate and weather a strategy which I have been investigated involves adding physically based constraints, leading to smaller but higher quality ensembles with which to produce estimates. I will describe some of the tradeoffs and their implications on filtering and forecasting.

\(^1\)Supported by NSF and BP/GoMRI

11:39AM B33.00003 The Role of Radiation in Organizing Tropical Convection\(^1\), SHARON SESSIONS, STIPO SENTIC, MICHAEL HERMAN, DAVID RAYMOND, New Mexico Institute of Mining and Technology — Convective organization regulates the radiation emitted to space, and therefore is important for the global heat budget. Organized convection—regions of intense convection surrounded by large cloud-free regions—permit more longwave radiation to escape and therefore may constitute a net cooling effect, while more scattered convection promotes greenhouse warming. Models which simulate the spontaneous organization of deep tropical convection—self-aggregation—suggest that radiative cooling in response to water vapor content is essential for convection to spontaneously organize. Multiple equilibria—steady states which maintain persistent precipitating convection or are completely dry—in small domains with weak temperature gradients (WTG) are analogous to dry and moist regions in large scale simulations of convective self aggregation. We explore the role of radiative cooling in multiple equilibria. Interactive radiative cooling suppresses convection in the dry state and it permits multiple equilibria over a larger parameter range. However, multiple equilibria still exist with fixed radiative cooling. This suggests that while interactive radiation is conducive for organizing convection, it is not essential. This study elucidates radiation’s role in convective organization.

\(^1\)Work supported by the NSF

11:51AM B33.00004 Thermodynamics of Hurricanes, KERRY EMANUEL, MIT — No abstract available.
12:27PM B33.00005 Stratified shear flow instability: Application to oceanic overflows, ROBERT ECKE, Los Alamos National Laboratory, PHILIPPE ODIER, Ecole Normale Superieure Lyon — The Earth’s thermohaline circulation provides major oceanic transport of heat and salinity and is an important determining factor in the climate of nearby land areas. We address the stability of overflow currents of heavier water moving into a region of less heavy quiescent fluid using experimental measurement of wall bounded stratified boundary currents under controlled laboratory conditions. In these currents, the stratification acts to stabilize the flow whereas the shear associated with the moving current produces turbulent kinetic energy fluctuations. We derive an expression for the potential for dissipation of these fluctuations. Our experimental measurements using particle-image velocimetry and laser-induced fluorescence allow the simultaneous acquisition of velocity and density fields, respectively. Rather than using traditional time-averaged statistics, we consider the stability of unperturbed sections of the interface and use a measure of the overturning or mixing called the Thorpe length. We present evidence for universal behavior in the normalized Thorpe length probability distribution and the general properties of the system under increasingly stable conditions. We relate these properties to realistic circumstances in the ocean.

12:39PM B33.00006 Eliminating Major Tornadoes in Tornado Alley, R. TAO, Temple Univ — In my recent paper, I propose that major tornadoes in Tornado Alley can be eliminated by building east-west ranged walls, 300 meter high and 50 meter wide. The work has received much attention, but some meteorologists are against the idea, claiming that the major tornadoes in Tornado Alley are not related to the collisions between northbound warm air flow and southbound cold air flow because supercells are not at the collision front. In this talk, we will show that wind tunnel experiments and airplane wing tip vortices clearly demonstrate that vortices produced by air mass collisions are usually not at the collision front because of the extremely volatile condition over there; they are either near the ends or at sides of the collision fronts. When the warm and moist wind collides with the cold wind violently in Tornado Alley, similarly, the supercell storms cannot be right at the collision fronts, but are near the ends or at sides of the collision fronts. While only a small portion of vortices in the warm air side may have a chance to develop into tornadoes, the major tornadoes in Tornado Alley indeed start from the air mass clashes. If we can weaken such violent air mass collisions, we will eliminate the major tornadoes in Tornado Alley.

12:51PM B33.00007 Random Focusing of Tsunami Waves, HENRI-PHILIPPE DEGUELDER, JAKOB J. METZGER, RAGNAR FLEISCHMANN, THEO GEISEL, Max Planck Institute for Dynamics and Self-Organization, Goettingen — When waves propagate through a weakly scattering, correlated random medium, the consecutive effects of small focusing events give rise to the phenomenon called branched flow, producing patterns of high-energy fluctuations. These structures can be found in the depth profile of the ocean floor, we investigate how it affects tsunami propagation and derive the typical length scale on which the highest waves are to be expected. We show that as a consequence of this effect the inaccuracies in the current knowledge of the ocean floor topography can prevent reliable tsunami forecasts on medium to large length scales.

1:03PM B33.00008 Energy Dissipation when Internal Wave Beams Reflect from a Slope, BRUCE RODENBORN, Centre College, DANIEL KIEFER, Center for Nonlinear Dynamics, University of Texas at Austin, HEPENG ZHANG, Jiao Tung University, HARRY L. SWINNEY, Center for Nonlinear Dynamics, University of Texas at Austin — Internal wave reflection from a uniform sloping boundary is often analyzed using linear or a weakly nonlinear inviscid theory. Under these assumptions for a linearly stratified fluid, Thorpe and Tabaei et al. derived predictions for the boundary angle where second harmonic generation should be most intense. We previously conducted experiments and simulations that found that the angle that maximizes second harmonic generation is given instead by an empirical geometric relationship between the wave beam and boundary angle. In the previous study, we used integrated kinetic energy as a measure of beam intensity. We compare these results with a method using energy flux. We also study the energy flux into and out of a surface above the reflection region $E_{\text{out}}/E_{\text{in}}$ and find high rates of energy dissipation $O(90\%)$. The rates remain high even for weakly nonlinear wave beams and with the viscosity reduced by an order of magnitude.

1:15PM B33.00009 Lamination in Atmospheric Ozone: A Diagnostic for Tracer Transport Mechanisms, KENNETH MINSCHWANER, Department of Physics, New Mexico Institute of Mining and Technology, GLORIA MANNEY, NorthWest Research Associates, LUIS TORRES, Department of Physics, New Mexico Institute of Mining and Technology — An understanding of ozone variability in the upper troposphere (from ~5 km altitude up to the tropopause level) is critical to assessing the radiative forcing of climate by ozone, and for evaluating the impact of transport on regional air quality. Part of this variability arises in fine-layered (~0.2 to ~2 km) structures seen in vertical profile measurements of ozone. These laminae are also generally limited on horizontal scales (10’s to 100’s of km), leading to spatial ozone variability observed on quasi-horizontal coordinate surfaces. Given the relatively long photochemical time constants for ozone in the upper troposphere, most of the observed variability arises from transport rather than photochemistry. There are a wide range of dynamical processes that can generate ozone laminae in the upper troposphere, such as gravity and Rossby waves, convective lofting and detrainment of either high or low ozone amounts from the boundary layer, and intrusions of air masses with high ozone concentrations from the stratosphere. Here, we examine the range of observed laminae characteristics and describe methods for tracing the origins of tropospheric ozone laminae.

Monday, March 2, 2015 11:15AM - 1:27PM – Session B34 GERA: Electrochemical Reactions 210A -
**11:15AM B34.00001 Modeling the Voltage Dependence of Electrochemical Reactions at Solid-Solid and Solid-Liquid Interfaces in Batteries**, KEVIN LEUNG, Sandia National Laboratories — Electrochemical reactions at electrode/electrolyte interfaces are critically dependent on the total electrochemical potential or voltage. In this presentation, we briefly review ab initio molecular dynamics (AIMD)-based estimate of voltages on graphite basal and edge planes [1], and then apply similar concepts to solid-solid interfaces relevant to lithium ion and Li-air batteries. Thin solid films on electrode surfaces, whether naturally occurring during power cycling (e.g., undesirable lithium carbonate on Li-air cathodes) or are artificially introduced, can undergo electrochemical reactions as the applied voltage varies. Here the onset of oxidation of lithium carbonate and other oxide thin films on model gold electrode surfaces is correlated with the electronic structure in the presence/absence of solvent molecules. Our predictions help determine whether oxidation first occurs at the electrode-thin film or electrolyte-thin film interface. Finally, we will critically compare the voltage estimate methodology used in the fuel cell community [2] with the lithium cohesive energy calibration method broadly applied in the battery community, and discuss why they may yield different predictions.

Our results supported by Nanostructures for Electrical Energy Storage (NEES), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DESC0001160. Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.


**11:51AM B34.00002 Carbon composites with metal nanoparticles for Alcohol fuel cells**, LAKSHMAN VENTRAPRAGADA, Clemson University, R.S. SIDDHARDHA, Sri Sathy Sai Institute of Higher Learning, RAMAKRISHNA PODILLA, Clemson University, V.S. MUTHUKUMAR, Sri Sathy Sai Institute of Higher Learning, STEPHEN CREAGER, A.M. RAO, Clemson University, SAI SATHISH RAMA-MURTHY, Sri Sathy Sai Institute of Higher Learning — Graphene due to its high surface area and superior conductivity has attracted wide attention from both industrial and scientific communities. We chose graphene as a substrate for metal nanoparticle deposition for fuel cell applications. There are many chemical routes for fabrication of metal-graphene composites, but they have an inherent disadvantage of low performance due to the usage of surfactants, that adsorb on their surface. Here we present a design for one pot synthesis of gold nanoparticles and simultaneous deposition on graphene with laser ablation of gold strip and functionalized graphene. In this process there are two natural advantages, the nanoparticles are synthesized without any surfactants, therefore they are pristine and subsequent impregnation on graphene is linker free. These materials are well characterized with electron microscopy to find their morphology and spectroscopic techniques like Raman, UV-Vis. for functionality. This gold nanoparticle decorated graphene composite has been tested for its electrocatalytic oxidation of alcohols for alkaline fuel cell applications. An electrode made of this composite showed good stability for more than 200 cycles of operation and reported a low onset potential of 100 mV more negative, an important factor for direct ethanol fuel cells.

This work was supported by Nanostructures for Electrical Energy Storage (NEES), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences. Our results provide insight into metal ion storage mechanisms on two-dimensional materials and also suggest a route to preparing bare MXene nanosheets. Moreover, stable multilayer adsorption is predicted for Mg and Al, which significantly increases their theoretical capacities. High capacities and good rate capabilities, while bare MXenes show better performance. Our experiments clearly demonstrate the feasibility of Na- and K-ion intercalation into terminated MXenes. Moreover, stable multilayer adsorption is predicted for Mg and Al, which significantly increases their theoretical capacities. Our results provide insight into metal ion storage mechanisms on two-dimensional materials and also suggest a route to preparing bare MXene nanosheets.

This work was supported as part of the Fluid Interface Reactions, Structures and Transport (FIRST) Center, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences.

**12:03PM B34.00003 Prediction and Characterization of MXenes for non-lithium ion battery anodes**, PAUL KENT, YU XIE, HOULONG ZHUANG, Oak Ridge National Lab, YOHAN DALL’AGNESE, Université Paul Sabatier, Toulouse, France, MICHAEL NAGUIB, Oak Ridge National Lab, MICHEL BARSOUIM, YURY GOGOTSI, Drexel University — Rechargeable non-lithium-ion (Na+, K+, Mg2+, Ca2+, and Al3+) batteries have attracted great attention as emerging low-cost and high energy-density technologies for energy storage applications. However, their development is hindered by the limited performance of high choice of MXene electrode materials. Building on our previous work for lithium-ion applications, here we show that MXene nanosheets, a class of two-dimensional transition-metal carbides, may serve as high-performing anodes for non-lithium-ion batteries by combined first-principles simulations and experimental measurements. Both O-terminated and bare MXenes are shown to be promising anode materials with high capacities and good rate capabilities, while bare MXenes show better performance. Our experiments clearly demonstrate the feasibility of Na- and K-ion intercalation into terminated MXenes. Moreover, stable multilayer adsorption is predicted for Mg and Al, which significantly increases their theoretical capacities. Our results provide insight into metal ion storage mechanisms on two-dimensional materials and also suggest a route to preparing bare MXene nanosheets.

This work was supported as part of the Fluid Interface Reactions, Structures and Transport (FIRST) Center, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences.

**12:15PM B34.00004 Positive lithiation potential on functionalized Graphene sheets**, RAJIV KUMAR CHOUGHAN, PUSHPA RAGHANI, Boise State University, Boise, ID 83725, USA — Designing lithium batteries with high capacities is major challenge in the field of energy storage. As an alternative to the conventional graphitic anode with a capacity of ~372 mAh g⁻¹, we look at the adsorption of lithium on 2D graphene oxide (GO) sheets. We have included van-der-waals’s interaction in our calculation and compared with literature showing its importance in Li binding on Graphene sheets. In comparison to the negative lithiation potential in pristine graphene sheets, we were able to get positive lithiation potential by introducing functional groups such as epoxy(-O-) and hydroxy(-OH) on graphene. Also the non-stoichiometric nature of GO provides better potential to increase the lithiation potential in compare to the defects induced graphene 2D sheet. Dramatic charge redistribution within the sheet due to presence of highly electronegative oxygen plays an important role in increasing the capacity.

This work was supported as part of the Fluid Interface Reactions, Structures and Transport (FIRST) Center, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences.

**12:27PM B34.00005 Simulating Electric Double Layer Capacitance by Using Lattice Boltzmann Method**, NING SUN, DILIP GERSAPPE, Department of Materials Science and Engineering, Stony Brook University, Stony Brook, NY, 11794, USA — By using the Lattice Boltzmann Method (LBM) we studied diffuse-charge dynamics in electrochemical systems. We use the LBM to solve Poisson-Nernst-Planck equations (PNP) and Modified Poisson-Nernst-Planck equations (MPNP). The isotropic permittivity of electrolyte is modeled using the Booth field. The results show that both steric effect (MPNP) and isotropic permittivity (Booth model) can have large influence on diffuse-charge dynamics, especially when electrolyte concentration or applied potential is high. This model can be applied to simulate electric double layer capacitance of super capacitors with complex geometry and also incorporate other effects such as heat convection in a modular manner.

**12:39PM B34.00006 ABSTRACT WITHDRAWN**

**12:51PM B34.00007 ABSTRACT WITHDRAWN**
1:03PM B34.00008 Role of site-disorder in energy materials: case of Li$_x$Nb$_2$O$_5$ pseudocapacitor and $\beta$-Li$_3$PS$_4$ solid electrolyte$^\dagger$. P. GANESH, ANDREW A. LUBIMTSEV, GOPI K.P. DATHAR, JONATHAN ANCHELL, PAUL R.C. KENT, ADAM J. RONDIÈRE, BOBBY G. SIMPTER, Center for Nanophase Materials Science. Oak Ridge National Laboratory — In this study, we will present computational studies to elucidate the importance of site-disorder in energy materials. We will specifically focus on two recently discovered materials: a Li-ion intercalation pseudocapacitor Li$_x$Nb$_2$O$_5$ (Nature Materials, 12 518 (2013)) and a Li-ion solid-electrolyte. ($\textit{JACS}$, 135 975 (2013)). A combination of theoretical methods, such as density functional theory (DFT) based cluster-expansion, basin hopping, ab initio molecular dynamics, and nudged-elastic-bands calculations were employed to understand the origin of intercalation pseudocapacitance in the niobate-system. ($\textit{J. Materials Chem.}$ 114951 (2013)). It was found that having multiple sites with similar energies for ion-adsorption, lead to a site-occupancy disorder that eventually lead to a capacitative slope in the voltage profile over the entire range of ion intercalation, as seen in experiments. A similar site-occupancy induced sublattice melting in the $\beta$-Li$_3$PS$_4$ solid-electrolyte, which when “frozen” to RT, lead to high Li-ion conductivity. (G.K.P.Dathar et al, submitted (2014)). Further, we will elucidate how to take advantage of this control over site-disorder to better engineer improved energy materials for batteries and fuel-cells.

$^\dagger$(PG, GKPD, PRCK, AJR, BGS) were supported by the CNMS at ORNL, (AAL and JA) were supported by the DOE-HERE program. Computations were performed at NERSC.

1:15PM B34.00009 Al-Air Batteries: Fundamental Thermodynamic Limitations from First Principles Theory$^\dagger$, LEANNE D. CHEN, JENS K. NOERSKOV, ALAN C. LUNTZ, SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory/Stanford University — The Al-air battery possesses high theoretical specific energy (4140 Wh/kg) and is therefore an attractive candidate for vehicle propulsion applications. However, the experimentally observed open-circuit potential is much lower than what thermodynamics predicts, and this potential loss is widely believed to be an effect of corrosion. We present a detailed study of the Al-air battery using density functional theory. The results suggest that the difference between bulk thermodynamic and surface potentials is due to both the effects of asymmetry in multi-electron transfer reactions that define the anodic dissolution of Al and, more importantly, a large chemical step inherent to the formation of bulk Al(OH)$_3$ from surface intermediates. The former results in an energy loss of 3%, while the latter accounts for 14—29% of the total thermodynamic energy depending on the surface site where dissolution occurs. Therefore, the maximum open-circuit potential of the Al anode is only $\approx 1.87$ V vs. SHE in the absence of thermal excitations, contrary to $\approx 2.34$ V predicted by bulk thermodynamics at pH 14.6. This is a fundamental limitation of the system and governs the maximum output potential, which cannot be improved even if corrosion effects were completely suppressed.

$^\dagger$Supported by the Natural Sciences and Engineering Research Council of Canada and the ReLiable Project (#11-116792) funded by the Danish Council for Strategic Research

Monday, March 2, 2015 11:15AM - 2:15PM – Session B35 DAMOP: Circuit QED, Optomechanics and Hybrid Systems 210B -

11:15AM B35.00001 Experimental Study of Short-time Brownian Motion, JIANYONG MO, AKARSH SIMHA, DAVID RIEGLER, MARK RAIZEN, The University of Texas at Austin — We report our progress on the study of short-time Brownian motion of optically-trapped microwaves. In earlier work, we observed the instantaneous velocity of microwaves in gas and in liquid, verifying a prediction by Albert Einstein from 1907. We now report a more accurate test of the energy equipartition theorem for a particle in liquid. We also observe boundary effects on Brownian motion in liquid by setting a wall near the trapped particle, which changes the dynamics of the motion. We find that the velocity autocorrelation of the particle decreases faster as the particle gets closer to the wall.

11:27AM B35.00002 Loading an Optical Trap with Diamond Nanocrystals Containing Nitrogen-Vacancy Centers from a Surface, JEN-FENG HSU, PENG JI, M. V. GURUDEV DUTT, BRIAN R. D’URSO, Univ of Pittsburgh — We present a simple and effective method of loading particles into an optical trap. Our primary application of this method is loading photoluminescent material, such as diamond nanocrystals containing nitrogen-vacancy (NV) centers, for coupling the mechanical motion of the trapped crystal with the spin of the NV centers. Highly absorptive material at the trapping laser frequency, such as tartrazine dye, is used as media to attach nanodiamonds and burn into a cloud of air-borne particles as the material is swept near the trapping laser focus on a glass slide. Particles are then trapped with the laser used for burning or transferred to a second laser trap at a different wavelength. Evidence of successful loading diamond nanocrystals into the trap presented includes high sensitivity of the photoluminescence (PL) to the excitation laser and the PL spectra of the optically trapped particles.

11:39AM B35.00003 Investigations of a voltage-biased microwave cavity for quantum measurements of nanomechanical resonators$^1$, FRANCISCO ROUXINOL, HUGO HAO, MATT LAHAYE, Syracuse Univ — Quantum electromagnetic systems incorporating superconducting qubits have received extensive interest in recent years due to their promising prospects for studying fundamental topics of quantum mechanics such as quantum measurement, entanglement and decoherence in new macroscopic limits, also for their potential as elements in technological applications in quantum information network and weak force detector, to name a few. In this presentation we will discuss our efforts toward to devise an electromechanical circuit to strongly couple a nanomechanical resonator to a superconductor qubit, where a high voltage dc-bias is required, to study quantum behavior of a mechanical resonator. Preliminary results of our latest generation of devices integrating a superconductor qubit into a high-Q voltage biased microwave cavities are presented. Developments in the circuit design to couple a mechanical resonator to a qubit in the high-Q voltage bias CPW cavity is discussed as well prospects of achieving single-phonon measurement resolution.

$^1$National Science Foundation under Grant No. DMR-1056423 and Grant No. DMR-1312421

11:51AM B35.00004 A broadband reflective filter for applying dc biases to high-Q superconducting microwave cavities$^1$, YU HAO, FRANCISCO ROUXINOL, MATT LAHAYE, Syracuse Univ — The integration of dc-bias circuitry into low-loss microwave cavities is an important technical issue for topics in many fields that include research with qubit- and cavity-coupled mechanical system, circuit QED and quantum dynamics of nonlinear systems. The applied potentials or currents serve a variety of functions such as maintaining the operating state of device or establishing tunable electrostatic interactions between devices (for example, in order to couple a nanomechanical resonator to a superconducting qubit to generate and detect quantum states of a mechanical resonator). Here we report a bias-circuit design that utilizes a broadband reflective filter to connect to a high-Q superconducting coplanar waveguide (CPW) cavity. Our design allows us to apply dc-voltages to the center trace of CPW, with negligible changes in loaded quality factors of the fundamental mode. Simulations and measurements of the filter demonstrate insertion loss greater than 20 dB in the range of 3 to 10 GHz. Transmission measurements of the voltage-biased CPW show that loaded quality factors exceeding $10^5$ can be achieved for dc-voltages as high as $V=\pm 20$V for the cavity operated in the single photon regime.

$^1$National Science Foundation under Grant No. DMR-1056423 and Grant No. DMR-1312421
12:03PM B35.00005 Superconducting Coplanar Waveguide Resonators For A Hybrid Rydberg Atom-Superconductor Interface. MATTHEW BECK, JONATHAN PRITCHARD, JOSHUA ISAACS, MARK SAFFMAN, ROBERT MCDERMOTT, University of Wisconsin, Madison — Superconducting qubits achieve fast gate times (∼1 ns); however, coherence times are relatively short (∼10 μs). In contrast, atomic qubits based on Rydberg atoms achieve long coherence times of order 1 s, but are limited by slow gate times (∼1 μs). Combining these disparate technologies in a hybrid quantum processor would provide both a long-lived memory and the ability to run computations quickly. Here we describe the design, fabrication, and characterization of superconducting coplanar waveguide resonators optimized to achieve strong coupling between the resonator mode and a single trapped Cs Rydberg atom. We discuss the dependence of resonator quality factor and coupling strength on device geometry and describe the integration of superconducting thin-film processing with MEMS-style thick film fabrication in order to increase the spatial extent of the resonator’s electric field.

12:15PM B35.00006 Microwave frequency electromagnetic coupling to a thin membrane at one end of a cylindrical cavity. ALESSANDRO CASTELLI, LUIS MARTINEZ, Univ of California - Merced, JERRY SPEER, None, JAY SHARPING, RAYMOND CHIAO. Univ of California - Merced — We demonstrate coupling of an 11.1 GHz radio frequency (RF) TE011 cylindrical cavity mode to the mechanical motion of a silicon nitride (Si3N4) membrane. The membrane is driven into motion through radiation pressure forces arising from the transverse magnetic field present at the membrane boundary. We use a cylindrical aluminum cavity where one end consists of a 500-nm thick Si3N4 membrane that has been sputtered with 300 nm of niobium (Nb). Cavity frequency tuning is controlled via an aluminum plunger attached to a micrometer at the other end of the cavity. The membrane is driven into motion by modulating the amplitude of the RF signal at the membrane’s resonant frequency in the KHz range. The membrane’s displacement is measured by means of a Michelson interferometer. We compare results from experimental runs utilizing both square and circular membrane geometries. This experiment shows that the TE011 mode gives rise to radiation pressure on the ends of a cylindrical cavity and demonstrates the feasibility of future work using high Q superconducting RF cavities to realize a dynamical Casimir effect (DCE) due to the membrane’s motion at GHz frequencies.

12:27PM B35.00007 Motional sideband asymmetry in a quantum electro-mechanical device. AARON WEINSTEIN, CHAN U LEI, EMMA WOLLMAN, Caltech. JUNHO SUH, KRISS, ANJA METELMANN, AASH CLERK, McGill University, KEITH SCHWAB, Caltech — Quantum electro-mechanical systems offer a unique opportunity to probe quantum noise properties in macroscopic devices, properties which ultimately stem from Heisenberg’s uncertainty relations. A simple example of this is expected to occur in a microwave parametric transducer, where mechanical motion generates motional sidebands corresponding to the up and down frequency-conversion of microwave photons. Due to quantum vacuum noise, the rates of these processes are expected to be unequal. We measure this fundamental imbalance in a microwave transducer coupled to a radio-frequency mechanical mode, cooled near the ground state of motion. We also discuss the subtle origin of this imbalance: with linear detection of the output light field, the imbalance is most naturally attributed to the quantum fluctuations of the electromagnetic field.

12:39PM B35.00008 Tailoring the flow of light and sound in an optomechanical array. MICHAEL SCHMIDT, VITTORIO PEANO, FLORIAN MARQUARDT, University of Erlangen-Nuernberg — Recent progress in the field of optomechanics may soon allow the realization of optomechanical arrays, i.e. periodic arrangements of optical and vibrational modes whose interaction can be tuned in-situ by a laser. The most promising implementation is based on a simple setting, a dielectric slab with a suitable pattern of holes. The flow of light and sound in such a device could be tailored by engineering the laser wavefront, e.g. creating effective potential landscapes, tuning the phonon hopping range, or creating artificial gauge fields. We show that photons and phonons on a honeycomb lattice will produce an optically tunable Dirac-type band structure. Transport in such a system can exhibit transmission through an optically created barrier, similar to Klein tunneling, but with interconversion between light and sound.

12:51PM B35.00009 Testing Time Reversal Symmetry in Artificial Atoms. FREDERICO BRITO, Unio de Sao Paulo, FRANCISCO ROUXINOL, MATTHIEU LAHAYE, Syracuse University, AMIR CALDEIRA, Universidade Estadual de Campinas — Over the past several decades, a rich series of experiments has repeatedly verified the quantum nature of superconducting devices, leading some of these systems to be regarded as artificial atoms. In addition to their application in quantum information processing, these “atoms” provide a test bed for studying quantum mechanics in macroscopic limits. Regarding the last point, we present here a feasible protocol for directly testing time reversal symmetry in a superconducting artificial atom. Time reversal symmetry is a fundamental property of quantum mechanics and is expected to hold if the dynamics of the artificial atom strictly follow the Schrödinger equation. However, this property has yet to be tested in any macroscopic quantum system. The test we propose is based on the verification of the microreversibility principle, providing a viable approach to verify quantum work fluctuation theorems - an outstanding challenge in quantum statistical mechanics. For this, we outline a procedure that utilizes the microreversibility test in conjunction with numerical emulations of Gibbs ensembles to verify these theorems over a large temperature range.

1:03PM B35.00010 Theory of on-chip integrated microwave-to-optical quantum coherent converter. CLEMENT JAVERZAC-GALY, KIRILL PLEKHANOV, LASZLO TOTH, ALEXEY FEOFANOVI, TOBIAS J. KIPPPENBERG, Ecole Polytechnique Federale de Lausanne — We present a proposal for implementing a direct quantum electro-optical converter based on a nonlinear optical microresonator. The hybrid system combines planar superconducting microwave circuits and integrated nonlinear ultrahigh-Q crystalline whispering gallery mode (WGM) optical microresonator. It features low footprint and scalability. The electro-optical dynamics of the device is similar to that of a cavity quantum optomechanical system and Pockels effect is used as the coupling interaction. We simulate the system and show that high-conversion performance can be achieved with current technology. On-chip, such integrated device holds promise for use in large-scale quantum applications as a first direct microwave-to-optical quantum repeater.

1:15PM B35.00011 Ultrahigh Q Bulk Acoustic Wave Cavities at the Quantum Limit. MICHAEL TOBAR, MAXIM GORYACHEV, EUGENE IVANOV, FRANK VAN KANN, The University of Western Australia, SERGE GALLIOU, FEMTO-ST — A Fabry-Perot cavity is an optical resonator, which can store photons for milliseconds and enhance interaction between light and matter. The acoustics analogue (phonon trapping), is the Bulk Acoustic Wave device (in thin film or crystal lattice). Measurements provide the ultimate material loss regimes, minimizing clamping losses and achieving record high Q products [1], allowing observation of various loss mechanisms such as Landau-Rumer, phonon-phonon dissipation and Rayleigh phonon scattering, as well as previously non-observed non-linear effects [2]. This presentation will summarize our recent work towards cooling such modes to the ground state and operating the device at the Quantum Limit [3]. This includes the first measurements of the Nyquist noise near at 4K [4], as well as details on using such devices to test fundamental physics [5]. [1] M Goryachev etal, Observation of rayleigh phonon scattering through excitation of extremely high overtones in low-loss cryogenic acoustic cavities for hybrid quantum systems, PRL, 111 085502 2013 [2] M Goryachev etal, Jump chaotic behaviour of ultra low loss bulk acoustic wave cavities, APL 105 063501 2014 [3] M Goryachev etal, Effects of geometry on quantum fluctuations of phonon-trapping acoustic cavities, NJP 16 063007 2014 [4] M Goryachev etal, Observation of the Fundamental Nyquist Noise Limit in an Ultra-High Q-Factor Cryogenic Bulk Acoustic Wave Cavity, APL 105 153505 2014 [5] M Goryachev etal, Gravitational wave detection with high frequency phonon trapping acoustic cavities, PRD 2014

1 Funded by ARC Grant No. CE110001013.
1:27PM B35.00012 Coherent coupling between ferromagnetic magnon and superconducting qubit. YUTAKA TABUCHI, SEICHIRO ISHINO, ATSUSHI NOGUCHI, TOYOICHI ISHIKAWA, REKISHU YAMAZAKI, KOJI USAMI, RCAST, The University of Tokyo, YASUNOBU NAKAMURA, RCAST, The University of Tokyo, CEMS, RIKEN — Coherent coupling between paramagnetic spin ensembles and superconducting quantum circuits is now widely studied for quantum memories and microwave-to-optical quantum transducers. Since those applications require strong coupling and sufficiently long coherence time simultaneously, collective excitation (magnon) in yttrium iron garnet (YIG), a typical ferromagnetic insulator, is an alternative promising candidate. The material is known to have a high spin density and a narrow ferromagnetic-resonance (FMR) linewidth. Recently, we achieved strong coupling between a 3D microwave cavity and the uniformly precessing spin mode. In this talk, we step forward to the control and measurement of magnons using superconducting circuits. We demonstrate coherent coupling between a magnon excitation in a millimeter-sized ferromagnetic sphere and a superconducting qubit, in which the interaction is mediated by a microwave cavity. We observe the coupling strength exceeding the damping rates, revealing that the system is in the strong coupling regime. Furthermore, we study a tunable coupling scheme using a microwave drive and the time-domain control of magnons. Our approach provides a versatile tool for control and measurement of the magnon excitations in the quantum regime.

1:39PM B35.00013 Novel techniques for strong coupling between spin ensembles and cavity resonators. DANIEL CREEDON, MAXIM GORYACHEV, WARRICK FARR, JEAN-MICHEL LE FLOCH, YAOHUI FAN, NATÁLIA CARVALHO, MICHAEL TOBAR, ARC Centre of Excellence for Engineered Quantum Systems, University of Western Australia, MIKHAIL KOSTYLEV, Magnetisation Dynamics and Spintronics Group, School of Physics, University of Western Australia, STEFANIA CASTELLETTO, ARC Centre of Excellence for Engineered Quantum Systems, RMIT University, Melbourne, PAVEL BUSHEV, Universität des Saarlandes, Saarbrücken, Germany — Spins in solids are a promising physical subsystem for the realization of hybrid quantum systems. We focus on experiments coupling spins to three dimensional cavities, a system where it is critical to achieve operation in the strong coupling regime. This has been achieved using two approaches: coupling to impurity ions in single-crystal Whispering Gallery photonic resonators, and by using a novel field focusing re-entrant cavity. The first approach has allowed us to investigate various impurities in sapphire, quartz, and YAG, as well as iron group ions in YSO. This method is characterised by relatively narrow photon linewidths, higher filling factors and lower impurity concentration. The second approach allowed strong coupling to P1 impurities in diamond and operation in the ultra-strong coupling regime with magnons in YIG. This method is designed to achieve spatial separation of the cavity magnetic and electric fields, relatively high filling factors with sub-mm crystals of any shape and a high concentration of magnetic ions, as well as arbitrary engineering of the cavity spectrum and field distribution.

2:03PM B35.00015 High-frequency and multi-mode operation of substrate-free micromembrane resonator. SUNGWAN CHO, Korea Research Institute of Standards and Science, MYUNG RAE CHO, Seoul National University, SANG GOON KIM, JUNHO SUH, Korea Research Institute of Standards and Science, YUN DANIEL PARK, Seoul National University, SEUNG-BO SHIM, Korea Research Institute of Standards and Science — Micromembrane mechanical resonator is fabricated from stoichiometric silicon nitride and its resonant motions are actuated with electrical field gradient pumping method. Using electrical field gradient force by electrode deposited near the suspended structure, micromembrane resonator can be actuated without electrical components on the movable component. We can drive and investigate multiple modes of micromembrane up to 32th mode with 78 MHz resonant frequency by optical measurement technique. This membrane can be applicable to optical system compatible with cavity without external driving technique.

Monday, March 2, 2015 11:15AM - 2:15PM — Session B36 DAMOP: Focus Session: Artificial Gauge Fields and Spin Orbit Coupling in Cold Atoms 211 - Martin Zwierlein, Massachusetts Institute of Technology

11:15AM B36.00001 Ultracold atoms in strong synthetic magnetic fields. WOLFGANG KETTERLE, MIT, Cambridge — The Harper Hofstadter Hamiltonian describes charged particles in the lowest band of a lattice at high magnetic fields. This Hamiltonian can be realized with ultracold atoms using laser assisted tunneling which imprints the same phase into the wavefunction of neutral atoms as a magnetic field does for electrons. I will describe our observation of a bosonic superfluid in a magnetic field with half a flux quantum per lattice unit cell, and discuss new possibilities for implementing spin-orbit coupling. Work done in collaboration with C.J. Kennedy, G.A. Siviloglou, H. Miyake, W.C. Burton, and Woo Chang Chung.

11:51AM B36.00002 Emergence of Quantum Liquid Crystals of Bosons in Kagome Lattices with Synthetic Gauge Fields. GUANYU ZHU, JENS KOCH, Northwestern University, IVAR MARTIN, Argonne National Laboratory — We consider a family of tight-binding models based on a kagome lattice with local synthetic gauge flux, which have a lowest flat band in the single particle spectrum. The flat band is spanned by eigenstates forming localized loops on the lattice, with the maximally compact loop states typically breaking the discrete rotational symmetry of the lattice. When populated by locally-interacting particles, the close packing of such maximally compact loop states leads to a nematic loop crystal ground state. If the particles are bosons, we show that mean field theory predicts that increasing filling beyond the close packing filling fraction leads to the formation of quantum liquid crystals including a nematic supersolid and a nematic superfluid phase with broken lattice rotation and \( U(1) \) symmetry.

12:03PM B36.00003 Strongly correlated atoms in artificial gauge fields. CIARÁN HICKEY, PRATIK RATH, ARUN PARAMEKANTI, Univ of Toronto — We study ultracold spinor atomic gases in an optical lattice in the presence of artificial gauge fields and a strong Hubbard repulsion. Using a combination of strong coupling approaches and novel numerical techniques, we explore exotic magnetic ground states and their thermal phase transitions induced by the interplay of momentum space topology and real space strong correlation effects.

12:15PM B36.00004 Realization of BEC on Cylindrical Surfaces with a Landau Gauge. BIAO HUANG, TIN-LUN HO, Ohio State Univ - Columbus — Landau’s famous solution of 2D electron gas on a cylindrical surface with the Landau gauge is one of the most important paradigm in condensed matter physics. Here, we point out the ways to create the Bose analog of this paradigm and discuss the property of a BEC in this setting. The synthetic “magnetic field” normal to the cylindrical surface is created through the Berry’s phase effects of bosons with hyperfine spins \( S \). As the strength of synthetic field increases, the vortex pattern on the surface undergo a sequence of transitions. These vortex patterns are very different from the triangular lattice array in rotating gases. They have dramatic signatures in time of flight measurements and can be revealed easily.

This work is supported by the NSF grant DMR-1309615, a MURI grant from ARO, and a grant from the NASA Fundamental Physics program.
12:27PM B36.00005 Synthetic magnetic fields in strained graphene-like optical lattices. BINBIN TIAN, University of Pittsburgh, MANUELE ENDRES, Max-Planck-Institut für Quantenoptik, DAVID PEKKER, University of Pittsburgh — Integer and fractional quantum hall effects are an area in which ultra cold atoms experiments could address long-standing problems of many-body physics. However there is a missing experimental ingredient: a good way to make “synthetic magnetic fields” for the neutral atoms that does not heat the atoms too quickly. Here we present a proposal for a solution by appealing to the physics of graphene. The motion of electrons in graphene is described by the Dirac equation. In the presence of strain the Dirac equation becomes modified as if there is a local magnetic field. We propose to use three laser beams to create a graphene-like optical lattice for ultra cold atoms. By mis-aligning the beams, we can encode a strain into the optical lattice and hence synthesize a uniform “magnetic” field. Using a tight binding model, we show that the synthetic magnetic field results in the formation of distinct Landau levels. These levels will persist in presence of a trap potential. The Landau levels can be detected using spectroscopic methods, like Bragg spectroscopy, or alternatively “kick” methods, like Bloch oscillations.

12:39PM B36.00006 Large Artificial Magnetic Fields Realized in a Synthetic Two-Dimensional Lattice, LAUREN AYCOCK, Joint Quantum Institute/ Cornell University/ National Institute of Standards and Technology/ University of Maryland, BEN STUHL, HSIN-I LU, DINA GENKINA, JQI/NSF/UMD, MARCELL GALL, JQI/NSF/UMD/Universitat Heidelberg, IAN SPIELMAN, JQI/NSF/UMD — We experimentally realize a large artificial magnetic field for a $^{87}$Rb Bose-Einstein condensate in a synthetic two-dimensional lattice [1]. This lattice combines a 1064nm 1D optical lattice along $\chi$ in real space while the 3 internal states of the manifold $F=1$ define a 3-site wide lattice in a second, synthetic dimension. These internal states are either RF- or Raman-coupled with a bichromatic light field allowing for tunneling in this synthetic dimension. The finite number of sites in this dimension naturally creates a hard walled potential ideal for studying edge states. The wavelength ratio between the optical lattice potential and the Raman coupling fields imprints a phase around each plaquette, creating a large, artificial magnetic field. We observe cyclotron orbits of the atoms and measure the edge state currents for opposite flux and varying group velocities. [1] A. Celi, P. Massignan, J. Ruseckas, N. Goldman, I. B. Spielman, G. Juzeliunas, and M. Lewenstein, Phys. Rev. Lett. 112, 043001 (2014)

12:51PM B36.00007 Striped Ferronematic ground states in a spin-orbit coupled spin-1 Bose gas, STEFAN NATU, XIAOPENG LI, WILLIAM COLE, University of Maryland and the Joint Quantum Institute — Motivated by recent experiments on spin-orbit coupled quantum gases, and the recent cooling to degeneracy of large spin atoms, we explore the ground state phase diagram of a spin-orbit coupled spin-1 Bose gas. A key new feature of large spin systems is the appearance of liquid crystalline order such as nematic or more exotic platicon solid order, which has no analog in solid state. Here we explore the interplay between spin order, translational symmetry breaking induced by spin-orbit coupling and these liquid crystalline order parameters in the experimentally relevant spin-1 system, finding a rich phase diagram. For repulsive spin-dependent interaction, we find a transition from a uniaxial ferronematic phase with XY spinor order but unique total density to a biaxial ferronematic phase with stripes in the total density. As a function of the quadratic Zeeman shift $\Omega$, for attractive spin dependent interactions, we find a transition from a ferromagnetic stripe phase which breaks translational symmetry in real space to a uniform ferromagnet for $\Omega>0$ and a uniform nematic phase for $\Omega<0$. We discuss the implications of our predictions to ongoing experiments on spin-orbit coupled large spin quantum gases.

1:03PM B36.00008 Spin-orbit coupled Fermi gas under sudden quench of Zeeman field, LIN DONG, Rice University, YING DONG, Hangzhou Normal University, MING GONG, The Chinese University of Hong Kong, HAN PU, Rice University — Motivated by recent efforts to achieve effective spin-orbit coupling in cold degenerate gases, we study the dynamical response of a spin-orbit coupled Fermi gas after a sudden quench of external Zeeman field. By solving the time-dependent Bogoliubov-de Gennes equation self-consistently, we have found three dynamical phases emerging from the time and the characteristic field strength, changing the above mentioned behavior of the order parameter. We further map out the phase diagram for the various dynamical states in the parameter space spanned by the initial and final values of the Zeeman field strength. In certain parameter regimes, the dynamical states possess nontrivial topological properties, manifested by the presence of the zero-energy edge state localized at a confining boundary. We present a detailed characterization of these phases.

1:15PM B36.00009 Bose-Einstein condensates with spin and orbital angular momentum coupling, KUEI SUN, CHUNLEI QU, CHUANWEI ZHANG, The University of Texas at Dallas — Spin-orbit coupling (SOC) plays a crucial role in many branches of physics. In this context, the recent experimental realization of the coupling between spin and linear momentum of ultra-cold atoms opens a completely new avenue for exploring new spin-related superfluid physics. Here we propose that another important and fundamental SOC, the coupling between spin and orbital angular momentum (SOAM), can be implemented for ultra-cold atoms using higher order Laguerre-Gaussian laser beams to induce Raman coupling between two hyperfine spin states of atoms. We study the ground state phase diagrams of SOAM coupled Bose-Einstein condensates (BECs) on a ring trap and explore their applications in gravitational force detection. We further investigate two-dimensional disk-shaped BECs with focus on the interplay between SOAM coupling, interaction, and external trapping. Our results provide the basis for further investigation of intriguing superfluid physics induced by SOAM coupling.

1 Supported by ARO (W911NF-12-1-0334) and AFOSR (FA9550-11-1-0313 and FA9550-13-1-0045)

1:27PM B36.00010 Berezinskii-Kosterlitz-Thouless Phase Transition in 2D Spin-Orbit Coupled Fulde-Ferrell Superfluids, YONG XU, CHUANWEI ZHANG, The University of Texas at Dallas — The experimental observation of traditional Zeeman-field induced Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) superfluids has been hindered by various challenges, in particular, the requirement of low dimension systems. In 2D, it is well known that finite temperature phase fluctuations lead to extremely small Berezinskii-Kosterlitz-Thouless (BKT) transition temperature, raising serious concern regarding the observability of 2D FFLO superfluids. Recently, it was shown that FFLO superfluids can be realized using a Rasha spin-orbit coupled Fermi gas subject to Zeeman fields, which may also support topological excitations such as Majorana fermions in 2D. Here we address the finite temperature BKT transition issue in this system, which may exhibits gapped, gapless, topological, and gapless topological FF phases. We find a large BKT transition temperature due to large effective superfluid densities, making it possible to observe 2D FF superfluids at finite temperature. In addition, we show that gapless FF superfluids can be stable due to their positive superfluid densities. These findings pave the way for the experimental observation of 2D gapped and gapless FF superfluids and their associated topological excitations at finite temperature.

1:39PM B36.00011 Superfluid Breakdown and Multiple Roton Gaps in Spin-Orbit Coupled Bose-Einstein Condensates on an Optical Lattice, DANIELE TONIOLÒ, JACOB LINDER, NTNU — Based on the results of Phys. Rev. A 89, 061605(R) (2014) I discuss the superfluid phases of a Rasha spin-orbit coupled Bose-Einstein condensate residing on a two-dimensional square optical lattice in the presence of an effective Zeeman field $\Omega$. At a critical value $\Omega = \Omega_c$, the single-particle spectrum $E_k$ changes from having a set of four degenerate minima to a single minimum at $k = 0$, corresponding to condensation at finite or zero momentum, respectively. I describe this quantum phase transition and the symmetry breaking of the condensate phases. The superfluid phase is discussed using the Bogoliubov theory, I present the phase diagram, the excitation spectrum and the sound velocity of the phonon excitations. A novel dynamically unstable superfluid regime occurring when $\Omega$ is close to $\Omega_c$ is analyzed using the Bogoliubov-de Gennes equation. In this regime a late time dynamic superfluid depletion is discussed. Moreover, I show that there are two types of roton excitations occurring in the $\Omega < \Omega_c$ regime and obtain explicit values for the corresponding energy gaps.
1:51PM B36.00012 Fermi Superfluids with Engineered Dispersion: A Consistent Treatment of Fluctuation Effects, BRANDON ANDERSON, CHIEN-TE WU, RUFUS BOYACK, KATHYRN LEVIN, James Franck Institute, University of Chicago — Recent experimental advances in cold atoms allows for the possibility of engineered dispersion that give rise to novel physics. For example, in systems with either spin-orbit coupling (SOC) or shaken optical lattices, momentum fluctuations can have energy cost that is quartic instead of quadratic at small momenta. The resulting density of states (DOS) will then more accurately resemble a system with lower dimension, leading to, e.g., enhanced depletion of Bose condensates or enhanced binding energy of Fermions. We consider the effects of the reduced DOS on the stability of fermionic superfluids in the presence of SOC or optical lattice shaking. We establish and characterize fluctuations associated with the standard mean field equations of the superfluid instability. This introduces bosonic degrees of freedom at a level beyond Gaussian fluctuations. Moreover, these bosons must necessarily condense in order for the fermionic superfluid to be stable. This is a non-trivial constraint for fermions, as seen from the observation that, e.g., Rashba SOC destroys a condensate instability. This introduces bosonic degrees of freedom at a level beyond Gaussian fluctuations. Moreover, these bosons must necessarily condense in order for the fermionic superfluid to be stable. This introduces bosonic degrees of freedom at a level beyond Gaussian fluctuations. Moreover, these bosons must necessarily condense in order for the fermionic superfluid to be stable.

This research was supported in part by AFOSR MURI program and The US Department of Energy Basic Energy Sciences (contract no. DE-AC02-07CH11358).

2:03PM B36.00013 Quantum phase transition in the interacting two-dimensional boson systems with Rashba spin-orbital coupling, CONGJUN WU, JIANDA WU, Univ of California - San Diego — The two-dimensional free bosons condensate at zero momentum at zero temperature. After turning on the Rashba spin-orbital coupling, the system displays a ring condensation in momentum space with highly degenerate quantum ground states [1]. It is pointed out that, after a mean-field treatment, the ring condensation will disappear when turning on and tuning the Zeeman coupling to a critical value, leading to a novel quantum phase transition in the system [2]. It is of great theoretical and experimental interests for the role the interaction plays in the system. Here we further explore the system via a relatively full treatment of the interaction. We find the presence of the interaction on one hand modifies the mean-field results, and on the other hand also drives the system undergoing quantum phase transition, leading to a new novel phase of “boson metal.”


11:15AM B37.00001 Overcoming erasure errors in quantum memories with multilevel systems, SRERAMAN MURALIDHARAN, Department of Electrical Engineering, Yale University, JIANMING WEN, LINSHU LI, LIANG JIANG, Department of Applied Physics, Yale University — We propose the usage of highly efficient error correcting codes of multilevel systems to encode quantum memories that suffer from erasure errors and introduce efficient hardware to repetitively correct these errors. Our scheme makes use of quantum polynomial codes to encode a quantum memory and generalized one-bit teleportation circuits for multilevel systems to repetitively correct photon erasure errors and operation errors in a fault-tolerant manner. We compare our scheme with earlier known schemes to encode quantum memories that use quantum parity codes and surface codes respectively and discuss the application of our encoded quantum memories for one-way quantum repeaters and show that they achieve a superior performance.

11:27AM B37.00002 Preserving flying qubit in single-mode fiber with Knill Dynamical Decoupling (KDD), MANISH GUPTA, Louisiana State Univ - Baton Rouge, ERIK NAVARRO, California State University, TODD MOULDER, JASON MUELLER, ASHKAN BALOUCHI, KATHERINE BROWN, HWANG LEE, JONATHAN DOWLING, Louisiana State Univ - Baton Rouge — The implementation of information-theoretic-crypto protocol is limited by decoherence caused by the birefringence of a single-mode fiber. We propose the Knill dynamical decoupling scheme, implemented using half-wave plates, to minimize decoherence and show that a fidelity greater than 96% can be achieved even in presence of rotation error.

11:39AM B37.00003 Multipulse dynamical decoupling-like protocol for controlling the light emission line of a two-level system, HERBERT F. FOTSO, Ames Laboratory, ADRIAN FEIGUIN, Northeastern University, VIACHESLAV DOBROVITSKI, Ames Laboratory — Emission lines of quantum systems in solids, such as quantum dots or color centers, are often significantly affected by the coupling to the solid-state environment, so that the frequencies of the emitted light slowly but uncontrollably fluctuates over time [1,2]. These fluctuations impede the photonic-based quantum information processing schemes (e.g. the two-photon interference, where the frequencies of the photons should stay close), and impair the protocols using the stationary-to-flying-qubit conversion. We present a possible solution for this problem, which employs optical pulses applied to the emitting system, which stabilize the position of the emission line at the desired location. Modeling the emitter as a two-level system, we analyze performance of the scheme both analytically and numerically. We show that already a few pulses, with rather large inter-pulse delay, can stabilize the emission line. We discuss application of the proposed scheme for stabilization of the zero-phonon emission line of the NV centers in diamond, and the possible use of this scheme for facilitating the long-distance entanglement between the NV centers [3]. [1] K. M. Fu et al, PRL 103, 256404 (2009). [2] V. M. Acosta et al, PRL 108, 206401 (2012). [3] W. Pfaff et al, Science 345 6196, 532 (2014).

This work was supported by AFOSR MURI program and The US Department of Energy Basic Energy Sciences (contract no. DE-AC02-07CH11358).

11:51AM B37.00004 Irreducible normalizer operators and thresholds for degenerate quantum codes with sublinear distances, LEONID P. PRYADKO, ILYA DUMER, University of California, Riverside, ALEXEY A. KOVALEV, University of Nebraska—Lincoln — We construct a lower (existence) bound for the threshold of scalable quantum computation which is applicable to all stabilizer codes, including degenerate quantum codes with sublinear distance scaling. The threshold is based on enumerating irreducible operators in the normalizer of the code, i.e., those that cannot be decomposed into a product of two such operators with non-overlapping support. For quantum LDPC codes with logarithmic or power-law distances, we get threshold values which are parametrically better than the existing analytical bound [1] based on percolation. The new bound also gives a finite threshold when applied to other families of degenerate quantum codes, e.g., the concatenated codes. [1] A. A. Kovalev and L. P. Pryadko, PRA 87, 020304(R) (2013).

This research was supported in part by the NSF grant PHY-1416578 and by the ARO grant W911NF-11-1-0027.
quantum annealing with applications to hard optimization problems. We explore a variety of techniques for leakage resilience in topological codes. Our contributions are twofold. First, we develop a leakage model that differs in critical details from earlier models. Secondly, we use Monte-Carlo simulations to survey several syndrome extraction circuits. Third, given the capability to perform 3-outcome measurements, we present a dramatically improved syndrome processing algorithm. Our simulations show that simple circuits with one extra CNOT per qubit reduce the accuracy threshold by less than a factor of 4 when leakage and depolarizing noise rates are comparable. This becomes a factor of 2 when the decoder uses 3-outcome measurements. Finally, when the physical error rate is less than $2 \times 10^{-4}$, placing LRUs after every gate may achieve the lowest logical error rate. We expect that the ideas may generalize to other topological codes.

The D-Wave Two (DW2) device has demonstrated the effectiveness of using error correction and suppression for quantum annealers. As the size of a quantum system increases, the number of logical qubits that can be encoded into the ground subspace of a Hamiltonian comprising a sum of commuting terms increases. Since such Hamiltonians are gapped they are considered natural candidates for protection of quantum information and topological or adiabatic quantum computation. However, we prove that they cannot be used to this end in the 2-local case. By breaking the favorable assumption that the gap is infinite we show that single-site perturbations can generate a degeneracy splitting in the ground subspace of this type of Hamiltonians which is of the same order as the magnitude of the perturbation, and is independent of the number of interacting sites and their Hilbert space dimensions, just as in the absence of the protecting Hamiltonian. This splitting results in decoherence of the ground subspace, and we demonstrate that for natural noise models the coherence time is proportional to the inverse of the degeneracy splitting. With the help of active error correction, this scheme is fault-tolerant, in the sense that the computation time can be arbitrarily long for large enough lattice size. It is shown that the frequency of error correction and the physical resources needed can be greatly reduced by the constant energy gap.

Quantum error suppression with commuting Hamiltonians: Two-local is too local. We consider error suppression schemes in which quantum information is encoded into the ground subspace of a Hamiltonian comprising a sum of commuting terms. Since such Hamiltonians are gapped they are considered natural candidates for protection of quantum information and topological or adiabatic quantum computation. However, we prove that they cannot be used to this end in the 2-local case. By breaking the favorable assumption that the gap is infinite we show that single-site perturbations can generate a degeneracy splitting in the ground subspace of this type of Hamiltonians which is of the same order as the magnitude of the perturbation, and is independent of the number of interacting sites and their Hilbert space dimensions, just as in the absence of the protecting Hamiltonian. This splitting results in decoherence of the ground subspace, and we demonstrate that for natural noise models the coherence time is proportional to the inverse of the degeneracy splitting. With the help of active error correction, this scheme is fault-tolerant, in the sense that the computation time can be arbitrarily long for large enough lattice size. It is shown that the frequency of error correction and the physical resources needed can be greatly reduced by the constant energy gap.

Fault-tolerant Holonomic Quantum Computation in Surface Codes. We show that universal holonomic quantum computation (HQC) can be achieved by adiabatically deforming the gap-stabilizer Hamiltonian of the surface code, where quantum information is encoded in the degenerate ground space of the system Hamiltonian. We explicitly propose procedures to perform each logical operation, including logical state initialization, logical state measurement, logical CNOT, state injection and distillation, etc. In particular, adiabatic braiding of different types of holes on the surface leads to a topologically protected, non-Abelian geometric logical CNOT. Throughout the computation, quantum information is protected from both small perturbations and low weight thermal excitations by a constant energy gap, and is independent of the system size. Also the Hamiltonian terms have weight at most four during the whole process. The effect of thermal error propagation is considered during the adiabatic code deformation. With the help of active error correction, this scheme is fault-tolerant, in the sense that the computation time can be arbitrarily long for large enough lattice size. It is shown that the frequency of error correction and the physical resources needed can be greatly reduced by the constant energy gap.

Quantum Error Correction for Minor Embedded Quantum Annealing. We consider error correction schemes in which quantum information is encoded into the ground subspace of a Hamiltonian comprising a sum of commuting terms. Since such Hamiltonians are gapped they are considered natural candidates for protection of quantum information and topological or adiabatic quantum computation. However, we prove that they cannot be used to this end in the 2-local case. By breaking the favorable assumption that the gap is infinite we show that single-site perturbations can generate a degeneracy splitting in the ground subspace of this type of Hamiltonians which is of the same order as the magnitude of the perturbation, and is independent of the number of interacting sites and their Hilbert space dimensions, just as in the absence of the protecting Hamiltonian. This splitting results in decoherence of the ground subspace, and we demonstrate that for natural noise models the coherence time is proportional to the inverse of the degeneracy splitting. With the help of active error correction, this scheme is fault-tolerant, in the sense that the computation time can be arbitrarily long for large enough lattice size. It is shown that the frequency of error correction and the physical resources needed can be greatly reduced by the constant energy gap.

Comparing codes for error corrected quantum annealing. We consider error correction schemes in which quantum information is encoded into the ground subspace of a Hamiltonian comprising a sum of commuting terms. Since such Hamiltonians are gapped they are considered natural candidates for protection of quantum information and topological or adiabatic quantum computation. However, we prove that they cannot be used to this end in the 2-local case. By breaking the favorable assumption that the gap is infinite we show that single-site perturbations can generate a degeneracy splitting in the ground subspace of this type of Hamiltonians which is of the same order as the magnitude of the perturbation, and is independent of the number of interacting sites and their Hilbert space dimensions, just as in the absence of the protecting Hamiltonian. This splitting results in decoherence of the ground subspace, and we demonstrate that for natural noise models the coherence time is proportional to the inverse of the degeneracy splitting. With the help of active error correction, this scheme is fault-tolerant, in the sense that the computation time can be arbitrarily long for large enough lattice size. It is shown that the frequency of error correction and the physical resources needed can be greatly reduced by the constant energy gap.

Comparing codes for error corrected quantum annealing. We consider error correction schemes in which quantum information is encoded into the ground subspace of a Hamiltonian comprising a sum of commuting terms. Since such Hamiltonians are gapped they are considered natural candidates for protection of quantum information and topological or adiabatic quantum computation. However, we prove that they cannot be used to this end in the 2-local case. By breaking the favorable assumption that the gap is infinite we show that single-site perturbations can generate a degeneracy splitting in the ground subspace of this type of Hamiltonians which is of the same order as the magnitude of the perturbation, and is independent of the number of interacting sites and their Hilbert space dimensions, just as in the absence of the protecting Hamiltonian. This splitting results in decoherence of the ground subspace, and we demonstrate that for natural noise models the coherence time is proportional to the inverse of the degeneracy splitting. With the help of active error correction, this scheme is fault-tolerant, in the sense that the computation time can be arbitrarily long for large enough lattice size. It is shown that the frequency of error correction and the physical resources needed can be greatly reduced by the constant energy gap.
2:03PM B37.00015 ABSTRACT WITHDRAWN —

Monday, March 2, 2015 11:15AM - 2:15PM —
Session B38 GQI: Focus Session: Quantum Foundations and Technologies I 212B - Matthew Pusey, Perimeter Institute for Theoretical Physics

11:15AM B38.00001 Understanding Nature from Experimental Observations: A Theory Independent Test for Gravitational Decoherence . STEPHANIE WEHNER, TU Delft — Quantum mechanics and the theory of gravity are presently not compatible. A particular question is whether gravity causes decoherence - an unavoidable source of noise. Several models for gravitational decoherence have been proposed, not all of which can be described quantum mechanically. In parallel, several experiments have been proposed to test some of these models, where the data obtained by such experiments is analyzed assuming quantum mechanics. Since we may need to modify quantum mechanics to account for gravity, however, one may question the validity of using quantum mechanics as a calculational tool to draw conclusions from experiments concerning gravity. Here we use ideas from quantum information to propose an experiment to estimate gravitational decoherence whose conclusions hold even if quantum mechanics would need to be modified. We first establish a general information-theoretic notion of decoherence which reduces to the standard measure within any physical process for any physical theory satisfying only very mild conditions. Finally, we propose a concrete experiment using optomechanics to estimate gravitational decoherence in any such theory, including quantum mechanics as a special case. Our work raises the interesting question whether other properties of nature could similarly be established from experimental observations alone - that is, without already having a rather well formed theory of nature like quantum mechanics to make sense of experimental data. We conclude by discussing this possibility.

Joint work with C. Pfister, J. Kaniewski, M. Tomamichel, A. Mantri, R. Schmucker and G. Milburn

11:51AM B38.00002 A loophole-free Bell test with spin qubits in diamond1, ANAIS DREAU, BAS HENSEN, HANNES BERNIEN, ANDREAS REISERER, JUST RuitenBerg, MACHIEL BLOK, Kavli Institute of Nanoscience Delft, Delft University of Technology, MATTHEW MARKHAM, DANIEL TWITCHEN, Element Six, Ltd., Kings Ride Park, Ascot, Berkshire SL5 8BP, UK, STEPHANIE WEHNER, RONALD HANSON, Kavli Institute of Nanoscience Delft, Delft University of Technology, QUANTUM TRANSPORT GROUP TEAM2, ELEMENT 6 TEAM — One of the most intriguing phenomena in quantum physics is the entanglement of spatially separated objects. The benchmark to prove the fundamental non-locality of remote entanglement is provided by the famous Bell’s theorem. Nevertheless, all its experimental implementations to date open the door to loopholes that restrict the practical validity of this theorem. , we present our latest experimental results towards the realization of a Bell test, aimed to close the detection loophole and address the locality and free-will loopholes in a single experiment. Our qubits consist of the electronic spin associated with single NV center defects in diamond. An efficient remote entanglement protocol allows us to generate entangled qubit pairs between two labs separated by 1.3 km on the TU Delft campus. The moderate time (<3.5 us) required for high fidelity (>99%) qubit rotations and efficient (>97%) readout make our setup a good candidate to allow the experimental violation of Bell’s inequalities between two space-like separated entangled spins without relying on the fair sampling assumption.

1FOM, NWO, ERC, Kavli Institute of Nanoscience Delft, QUtech, STW
2Kavli Institute of Nanoscience Delft, Delft University of Technology
what the necessary requirements for speed-up in conventional quantum computing are. Between quantum and classical are much starker. By trying to identify which aspects of quantum theory are essential to this speed-up we can gain insight into applicable, kind of Turing machine. In this restricted setting results about quantum advantage become far easier to prove and the difference in capabilities factory can perform tasks which are impossible in the classical case. In some sense the Bernoulli factory can be considered as an alternate, although less superposition and mixture. We take a classical sampling problem, the Bernoulli coin factory, and explore a quantum version of it. We find that the quantum dependent subtleties of Huygens' principle. We will also discuss several implications of this effect in diverse scenarios ranging from quantum communication to quantum optical techniques.


The inspiration for the hypothesis was found as an undergrad at Princeton and the initial development was done as a grad student at Stanford.

ANDREY AKHMETELI, LTASolid Inc. — Is it possible to offer a “no drama” quantum electrodynamics, as simple (in principle) as classical electrodynamics – a theory described by a system of partial differential equations (PDE) in 3+1 dimensions, but reproducing unitary evolution of a quantum field theory in the Fock space? The following results suggest an affirmative answer: 1. The scalar field can be algebraically eliminated from scalar electrodynamics. 2. After introduction of a complex 4-potential (producing the same electromagnetic field (EMF) as the standard real 4-potential), the spinor field can be algebraically eliminated from spinor electrodynamics. 3. The resulting theories describe independent evolution of EMF and can be embedded into quantum field theories. Another fundamental result: in a general case, the Dirac equation is equivalent to a 4th order PDE for just one component, which can be made real by a gauge transform. Issues related to the Bell theorem and the connection with Barut’s self-field electrodynamics are discussed. A. Akhmeteli, Int’l Journal of Quantum Information, Vol. 9, Suppl., 17-26 (2011) A. Akhmeteli, Journal of Mathematical Physics, Vol. 52, 082303 (2011) A. Akhmeteli, quant-ph/1111.4630 A. Akhmeteli, European Physical Journal C, Vol. 73, 2371 (2013) (open access)

GELO NOEL TABIA, University of Tartu — In cryptography, the notion of a zero-knowledge proof was introduced by Goldwasser, Micali, and Rackoff [1]. An interactive proof system is said to be zero-knowledge if any verifier interacting with an honest prover learns nothing beyond the validity of the statement being proven. With recent advances in quantum information technologies, it has become interesting to ask if classical zero-knowledge proof systems remain secure against adversaries with quantum computers. The standard approach to show the zero-knowledge property involves constructing a simulator for a malicious verifier that can be rewinded to a previous step when the simulation fails. In the quantum setting, the simulator can be described by a quantum circuit that takes an arbitrary quantum state as auxiliary input but rewinding becomes a non trivial problem. Watrous proposed a quantum rewinding technique in the case where the simulation’s success probability is independent of the auxiliary input [2]. Here I present a more general quantum rewinding scheme that employs the quantum phase estimation algorithm. References: [1] S. Goldwasser, S. Micali, and C. Rackoff, SIAM J. Comput. 18(1) 186-208, 1989. [2] J. Watrous, SIAM J. Comput. 39(1) 25-58, 2009.

This work was funded by institutional research grant IUT72-1 from the Estonian Research Council and by the European Union through the European Regional Development Fund.

A Weak Value Based QKD Protocol Robust Against Detector Attacks. JAMES TROUPE, Applied Research Laboratories, University of Texas at Austin — We propose a variation of the BB84 quantum key distribution protocol that utilizes the properties of weak values to insure the validity of the quantum bit error rate estimates used to detect an eavesdropper. The protocol is shown theoretically to be secure against recently demonstrated attacks utilizing detector blinding and control and should also be robust against all detector based hacking. Importantly, the new protocol promises to achieve this additional security without negatively impacting the secure key generation rate as compared to that originally promised by the standard BB84 scheme. Implementation of the weak measurements needed by the protocol should be very feasible using standard quantum optical techniques.

Quantum Collect Calling. EDUARDO MARTIN-MARTINEZ, Institute for Quantum Computing / Perimeter Institute for Theoretical Physics — We show that it is possible to use a massless field in the vacuum to communicate in such a way that the signal travels slower than the speed of light and such that no energy is transmitted from the sender to the receiver. Instead, the receiver has to supply a signal-dependent amount of work to switch his detector on and off. This type of signalling is related to Casimir-like interactions and it is made possible by dimension —and curvature— dependent subtleties of Huygens’ principle. We will also discuss several implications of this effect in diverse scenarios ranging from quantum communication to Cosmology.

The Quantum Bernoulli Factory. HOWARD DALE, DAVID JENNINGS, TERRY RUDOLPH, Imperial College London — Understanding the difference between quantum mechanics and classical probability theory amounts to understanding the difference between superposition and mixture. We take a classical sampling problem, the Bernoulli coin factory, and explore a quantum version of it. We find that the quantum factory can perform tasks which are impossible in the classical case. In some sense the Bernoulli factory can be considered as an alternate, although less applicable, kind of Turing machine. In this restricted setting results about quantum advantage become far easier to prove and the difference in capabilities between quantum and classical are much starker. By trying to identify which aspects of quantum theory are essential to this speed-up we can gain insight into what the necessary requirements for speed-up in conventional quantum computing are.
1:39PM B38.00011 Certifying Unpredictable Randomness from Quantum Nonlocality, PETER BIERHORST, Tulane University — A device-independent quantum randomness protocol takes an initial random seed as input and then expands it to a longer random string. It has been proven that if the initial random seed is trusted to be unpredictable, then the longer output string can also be certified to be unpredictable by an experimental violation of Bell's inequality. It has furthermore been argued that the initial random seed may not need to be truly unpredictable, but only uncorrelated to specific parts of the Bell experiment. In this work, we demonstrate rigorously that this is indeed true, under assumptions related to "no superdeterminism/no conspiracy" concepts along with the no-signaling assumption. So if we assume that superluminal signaling is impossible, then a loophole-free test of Bell's inequality would be able to generate provably unpredictable randomness from an input source of (potentially predictable) classical randomness.

1:51PM B38.00012 Adaptive Quadrature Detection for Multicarrier Continuous-Variable Quantum Key Distribution, LASZLO KYONGYO, Budapest University of Technology, Hungarian Academy of Sciences, SANDOR IMRE, Budapest University of Technology — We propose the adaptive quadrature detection for multicarrier continuous-variable quantum key distribution (CVQKD). A multicarrier CVQKD scheme uses Gaussian subcarrier continuous variables for the information conveying and Gaussian sub-channels for the transmission. The proposed multicarrier detection scheme dynamically adapts to the sub-channel conditions using a corresponding statistics which is provided by our sophisticated sub-channel estimation procedure. The sub-channel estimation phase determines the transmittance coefficients of the sub-channels, which information are used further in the adaptive quadrature decoding process. We define the technique called subcarrier spreading to estimate the transmittance conditions of the sub-channels with a theoretical error-minimum in the presence of a Gaussian noise. We introduce the terms of single and collective adaptive quadrature detection. We also extend the results for a multiuser multicarrier CVQKD scenario. We prove the achievable error probabilities, the signal-to-noise ratios, and quantify the attributes of the framework. The adaptive detection scheme allows to utilize the extra resources of multicarrier CVQKD and to maximize the amount of transmittable information.

This work was partially supported by the DFG and the Hungarian National Project.

2:03PM B38.00013 Highly Efficient Long-Distance Quantum Communication: a Blueprint for Implementation, LINSHU LI, SRERAMAN MURALIDHARAN, Yale University, JUNGSANG KIM, Duke University, NORBERT LUTKENHAUS, University of Waterloo, MIKHAIL LUKIN, Harvard University, LIANG JIANG, Yale University — Quantum repeaters provide a way for long distance quantum communication through optical fiber networks. Transmission losses and operation errors are two major challenges to the implementation of quantum repeaters. At each intermediate repeater station, transmission losses can be overcome using either heralded entanglement generation or quantum error correction, while operation errors can be corrected via entanglement purification or quantum error correction. Depending on the mechanisms used to correct loss and operation errors respectively, three generations of quantum repeaters have been proposed. We present a quantitative comparison of different quantum repeater schemes by evaluating the time- and qubit-resource consumed simultaneously. We can identify the most efficient scheme for given technological capabilities, which characterized by fiber coupling efficiency, local gate fidelity, and local gate speed. Our work provides a roadmap for high-speed quantum networks across continental distances.

Monday, March 2, 2015 11:15AM - 2:15PM

Session B39 GQI: Superconducting Circuits: Decoherence

11:15AM B39.00001 Comparison of 2D transmon coherence for different capacitive shunt fabrication methods, JONILYN YODER, MIT Lincoln Laboratory, ARCHANA KAMAL, FEI YAN, MIT, THEODORE GUDMUNDSEN, MIT Lincoln Laboratory, PAUL WELANDER, SLAC National Accelerator Laboratory, SIMON GUSTAVSSON, MIT, DAVID HOVER, ANDREW KERMAN, ADAM SEARS, WILLIAM OLIVER, MIT Lincoln Laboratory — Improvements in superconducting qubit coherence times and reproducibility have been demonstrated using capacitive shunting. In this study, we present a side-by-side comparison of two distinct methods for preparing the aluminum shunt capacitor material for 2D transmon superconducting qubit devices. The first method involved in situ wafer outgassing prior to molecular beam epitaxy aluminum evaporation. The second method involved outgassing prior to electron gun aluminum evaporation. Materials analysis for each process will be detailed. Experimental results, including qubit coherence times and superconducting coplanar waveguide resonator internal quality factors, will be presented for representative devices prepared using both methods. This work is sponsored by the Assistant Secretary of Defense for Research and Engineering under Air Force Contract FA8721-05-0002. Opinions, interpretations, conclusions, and recommendations are those of the authors and are not necessarily endorsed by the United States Government.

11:27AM B39.00002 Optimizing Hardware Compatibility for Scaling Up Superconducting Qubits, MICHAEL FANG, Univ of California - Santa Barbara, BROOKS CAMPBELL, ZIJUN CHEN, BEN CHIARO, ANDREW DUNSWORTH, JULIAN KELLY, ANTHONY MEGRANT, CHARLES NEILL, PETER O'MALLEY, CHRIS QUINTANA, AMIT VAINSENCHER, JIM WINNER, TED WHITE, University of California, Santa Barbara, RAMI BARENDS, YU CHEN, AUSTIN FOWLER, EVAN JEFFREY, JOSH MUTUS, PEDRAM ROUSHAN, DANIEL SANK, Google, Santa Barbara. JOHN MARTINIS, University of California and Google, Santa Barbara — Since quantum computation relies on the manipulation of fragile quantum states, qubit devices must be isolated from the noisy environment to prevent decoherence. Custom made components make isolation from thermal and infrared radiation possible, but have been unreliable, massive, and show sub-ideal microwave performance. Infrared isolation for large scale experiments (≥ 8 qubits) was achieved with compact impedance matched microwave filters which attenuate stray infrared signals on cryogenic cables with only -25 dB reflection up to 7.5 GHz. In addition, a thermal anchoring system was designed to effectively transfer unwanted heat from more than 100 coaxial cables in the dilution refrigerator and yielded a 33 percent improvement in base temperature and 50% improvement in hold time.
11:39AM B39.00003 Experiments on Interaction of Quasiparticles with Two-Level-Systems in a Superconducting Phase Qubit

ALEXANDER BILMES, JÜRGEN LISENFELD, ANDREAS HEIMES, SEBASTIAN ZANKER, Gerd SCHÖN, Alexey Ustinov, Karlsruhe Inst of Tech (KIT), PI TEAM 1, FTP TEAM 2 — Two-Level-Systems (TLS) are one of the main sources of decoherence in superconducting qubits. Some individual and coherent TLS, present in the tunnel barrier of the qubit’s Josephson junction, can be coherently operated via the qubit. In the past, experiments on superconducting glasses indicated that quasiparticles may give rise to TLS energy loss similar to Korringa relaxation 1. We will present experiments in which we use a phase qubit to explore the interaction of single TLS with non-equilibrium quasiparticles. We have implemented in-situ quasiparticle injection by using an on-chip dc-SQUID that is pulse-biased beyond its critical current. The quasiparticle density is calibrated by measuring associated characteristic changes to the qubit resonance frequency and energy relaxation rate 2. The coherence times of individual TLS is measured in dependence of the non-equilibrium quasiparticle density and compared to thermally generated quasiparticles.


1PI, KIT, Wolfgang-Gaede-Strasse 1, 76131 Karlsruhe, Germany
2TFP, KIT, Wolfgang-Gaede-Strasse 1, 76131 Karlsruhe, Germany

11:51AM B39.00004 Characterization of a Scalable Chip Mount Using a 5 Xmon Qubit Chain

BROOKS CAMPBELL, Z. CHEN, B. CHIARO, A. DUNSWORTH, I.-C. HOI, J. KELLY, A. MEGRANT, C. NEILL, P. J. J. O’MALLEY, C. QUINTANA, A. VAINSENCHER, J. WENNER, T. WHITE, UC Santa Barbara, R. BARENDS, Y. CHEN, A. FOWLER, E. JEFFREY, J. MUTUS, P. ROUSHAN, D. SANK, Google, Santa Barbara, John M. Martinis, UC Santa Barbara and Google, Santa Barbara — Superconducting quantum computing technology has progressed to the point that experiments involving the full control more than ten qubits will be realized in the next few years. As such, a scalable chip mount, able to accommodate dozens of microwave signal lines, will likely become necessary since current Xmon technology requires two control lines per qubit. Additionally, understanding parasitic coupling of Xmon qubits to control lines will aid in the proper design of both chips and chip mounts for even higher density circuits. We will present coherence, gate fidelity, and qubit-cross-talk benchmark measurements from a high performance 5 Xmon chain in various chip mount designs and materials.

12:03PM B39.00005 Influence of Non-equilibrium Noise on Quantum Superconducting Devices

JEN-HAO YEH, Laboratory for Physical Sciences; Department of Physics, University of Maryland, Jay LeFebvre, Department of Physics, University of Maryland, BALADITYA SURI, SERGEY NOVIKOV, Laboratory for Physical Sciences; Department of Physics, University of Maryland, FREDERICK WELLSTOOD, Department of Physics, University of Maryland; Joint Quantum Institute, University of Maryland, Benjamin Palmer, Laboratory for Physical Sciences; Department of Physics, University of Maryland — Non-equilibrium noise from temperatures larger than T ~ 20 mK coupled to quantum superconducting devices can cause energy relaxation [1], dephasing [2], and initialization errors [1]. In particular at low temperatures, any dissipated power can drive the electrons out of equilibrium with the phonons and produce thermal noise. To understand thermal noise driven out of equilibrium, we have created both finite element simulations using COMSOL and some simple analytical models. Based on these thermal simulations and models as well as microwave simulations, we have designed and fabricated some devices to decrease the amount of non-equilibrium noise influencing our devices. The design of these devices as well as preliminary characterization using a transmon device will be discussed.


12:15PM B39.00006 Non-exponential energy decay and quasi-particle fluctuations in a superconducting flux qubit

SIMON GUSTAVSSON, FEI YAN, MIT, GIANLUIGI CATELANI, Forschungszentrum Jülich, Germany, Archana KAMAL, MIT, Jonas Bylander, Chalmers University of Technology, Sweden, Fumiki Yoshihara, NICT, Japan, Yasunobu Nakamura, The University of Tokyo, Tokyo, Terry Orlando, MIT, William Oliver, MIT Lincoln Laboratory — We measure pronounced non-exponential energy relaxation in a superconducting flux qubit, observing a decay function that exhibits a fast initial decay followed by a much slower decay for long times. When applying a sequence of pi pulses to the qubit and measuring the decay after the last pi pulse, we observe strong modifications to the decay function, including a slow-down of the fast initial decay and a three-fold increase of the 1/e-time. If we attribute the non-exponential decay to quasiparticle number fluctuations, we speculate that the improvements in T1 are due to a qubit-mediated shuffling of quasiparticles between the metallic islands of the device, which will eventually pump them away from the Josephson junctions to a larger ground plane where their contribution to qubit energy relaxation become negligible.

12:27PM B39.00007 Laser made from a superconducting lumped-element resonator and random defects

YANIV ROSEN, Laser Laboratory for Physical Sciences, College Park, MD, MOE KHALIL, Laboratory for Physical Sciences, College Park, MD and University of Maryland, College Park, MD, Alex Burin, Department of Chemistry, Tulane University, New Orleans, LA, Kevin Osborn, Laboratory for Physical Sciences, College Park, MD and Joint Quantum Institute, College Park, MD — Random two-level system defects in dielectrics absorb energy and limit the quality factors of superconducting qubits and resonators used in quantum computing applications. We have found a method to invert the population of these random defects and pass them through resonance with a lumped-element superconducting microwave resonator. Stimulated emission of the defects causes the internal quality factor of the resonator, measured by an injection locking tone, to cross through an infinitely large value before becoming negative. In the latter case the defects emit more than they absorb and the internal lasing threshold is reached. With further population inversion, amplification of the injection locking tone is observed.

12:39PM B39.00008 Investigation of Limiting Decoherence Mechanisms in Xmon Qubits

C. M. Quintana, UC Santa Barbara, R. Barends, Google, Santa Barbara, B. Campbell, UC Santa Barbara, Y. Chen, Google, Santa Barbara, Z. Chen, B. Chiaro, A. Dunssworth, UC Santa Barbara, A. G. Fowler, Google, Santa Barbara, I.-C. Hoi, UC Santa Barbara, E. Jeffrey, Google, Santa Barbara, J. Kelly, A. Megrant, UC Santa Barbara, J. Mutus, Google, Santa Barbara, C. Neill, P. J. J. O’Malley, UC Santa Barbara, P. Roushan, D. Sank, Google, Santa Barbara, A. Vainsencher, J. Wenner, T. C. White, A. N. Cleland, UC Santa Barbara, J. M. Martinis, University of California and Google, Santa Barbara — Xmon-style transmon qubits have demonstrated a high level of coherence and controllability, enabling high-fidelity quantum gates and measurement at the levels required for surface code error correction. However, decoherence is still a limiting factor for fidelities, and further improvements to coherence could significantly reduce the overhead required to build a fault-tolerant quantum computer. We report on relaxation and dephasing mechanisms relevant to the Xmon qubit. In particular, we discuss dielectric loss from stray Josephson junctions and the dependence of dephasing on qubit temperature.
1:03PM B39.00010 Collective modes in the fluxonium qubit. GIANLUIGI CATELANI, Forschungszentrum Julich PGI-2, GIOVANNI VIOLA, RWTH Aachen - IQI - In the fluxonium qubit, an array comprising a large number of identical Josephson junctions form a so-called superinductance. The superinductance is connected to a junction - the phase slip element - with a smaller Josephson energy and a different charging energy. We investigate the effects of unavoidable capacitive couplings to ground as well as non-linearities of the superinductance: they both introduce interactions between the low-energy qubit degree of freedom and higher-energy collective modes of the circuit. We also consider the role of the additional capacitances that are used to couple the qubit to a resonator for driving and read-out. We show that the interactions with the collective modes can affect not only the spectrum of the qubit but also its coherence.

1:15PM B39.00011 Spurious modes in 3D multi-qubit circuits. MARTIN SANDBERG, DOUGLAS MCCLURE, HANHEE PAIK, IBM T.J. Watson Research Center, Yorktown Heights, New York, 10598, USA, DANIELA F. BOGORIN, B.L.T. PLOURDE, Syracuse University, Physics Department, Syracuse, NY 13244 USA, OLIVER DIAL, BALEEGH ABDI, IBM T.J. Watson Research Center, Yorktown Heights, New York, 10598, USA - In superconducting 3D circuits coherence times exceeding 100 microseconds are readily achieved for qubits in single cavities. One approach to building more complex circuitry in the 3D architecture is to use "bridge" qubits that span into two adjacent cavities. It has been found that these qubits exhibit reduced coherence compared to single cavity qubits. Significant effort has been put into understanding and improving the coherence of the bridge qubit. So far the mechanisms behind the reduced coherence have remained somewhat unclear. Here we present simulations and measurements indicating that stray modes in the microwave environment are one contributing factor to the reduced coherence. One potential location of such stray modes is at the boundary regions between sections of the cavity enclosure, where both machining imperfections and dielectric layers such as oxides can prevent perfect electrical contact. As these systems are scaled up, the spectrum of the modes becomes increasingly dense, presenting an increasing challenge. We present multiple methods that can be implemented to mitigate these modes.

1:27PM B39.00012 Cavity-induced decoherence in a long-lived superconducting flux qubit. FEI YAN, ARCHANA KAMAL, Research Laboratory for Electronics, Massachusetts Institute of Technology, THEODORE GUDMUNDSEN, JONILYN YODER, MIT Lincoln Laboratory, SIMON GUSTAVSSON, MIT Lincoln Laboratory; Research Laboratory for Electronics, Massachusetts Institute of Technology, WILLIAM OLIVER, Research Laboratory for Electronics, Massachusetts Institute of Technology — We implement a circuit QED system with a capacitively shunted (C-shunt) flux qubit coupled to a transmission line resonator. The improved design substantially enhances qubit coherences, achieving T1 of 55us at degeneracy. Dephasing is also improved, giving a spin-echo decay of 40us. We found that the dephasing is limited by photon shot noise at a residual thermal photon population of 0.006. The driven-evolution T1rho-spectroscopy and free-evolution CPMG results both validate the finding.

1:39PM B39.00013 Quantum optical theory of electronic noise in coherent conductors. FARZAD QASSEMI, BERTRAND REULET, ALEXANDRE BLAIS, Université de Sherbrooke — We investigate the quantum properties of radiated electromagnetic field from a quantum conductor, i.e., a conductor where the electron transport is governed by quantum mechanics. In particular, using tools borrowed from quantum optics such as input-output theory and Lindblad master equations, we demonstrate how the electron shot noise in the conductor tailors the properties of radiated field, leading to nonclassical electromagnetic radiation. Our results allow us to calculate the outcome of any measurement on the electromagnetic field in terms of the statistical properties of the current in the conductor. As an example, we explain the existence of squeezing, recently observed by G. Gasse et al [1].

1:51PM B39.00014 Spectroscopy of Nanoscale Two-Level Systems in Insulating Films. BAHMAN SARABI, ARUNA RAMANAYAKA, Laboratory for Physical Sciences, FREDERICK WELLSSTOOD, University of Maryland,College Park, KEVIN OSBORN, Laboratory for Physical Sciences — Nanoscale tunneling two level systems (TLSs) are viewed as defects in dielectric films because they are parasitic to the performance of superconducting qubits and resonators. Using a calibrated and uniform dc electric field within a special superconducting resonator we modify the energy potential of random TLSs in amorphous insulating films and measure them. As the dc electric field is applied, TLS energies are observed near the tunneling energies from their double-well degeneracy. From these measurements, the dipole moment projected along the field axis is directly extracted for each TLS. The random distribution of projected dipole moments shows that there are multiple dipole sizes in a silicon nitride film. This contrasts other techniques which find a single dipole size in an amorphous film. Spectroscopic splittings are observed which arise from a coherent exchange of a single photon between a TLS and the resonator, and they allow an overconstrained validation of cavity quantum electrodynamics with a TLS. The method used to measure multiple dipole moments is believed to be generally useful for the classification of TLSs, which can be used to test and screen films fabricated for coherent superconducting devices.
Mechanism of charge recombination in organic-inorganic hybrid perovskite solar cells

Au Nanocluster assisted PCE improvement in PEDOT: PSS - Si Hybrid Devices

Co-Assembling P3HT/ZnO as Parallel-Lane Hybrid Nanowires for Photovoltaics Application

Fulleropyrrolidine interlayers lower cathode work function to raise organic solar cell efficiency
and demonstrate that we can utilize these strategies for the synthesis of block copolymers beyond P3HT-b-PFTBT. We investigated the chemical composition, structure and electrical characteristics of the polymers prepared by the different synthetic methods, which served as model systems to study fundamental questions regarding optoelectric properties and charge transfer. However, the synthesis of fully conjugated block copolymers remains a challenging issue in the field. We have optimized the two-step synthesis of P3HT-b-PFTBT, which is comprised of the two blocks. Our morphological studies thus support the proposed alloying model that was put forth originally.

The role of exciton ionization processes in bulk heterojunction organic photovoltaic cells. YUNLONG ZOU, RUSSELL HOLMES, Univ of Minn - Minneapolis — Dissociating photogenerated excitons into their constituent charges is essential for efficient photon conversion in organic semiconductors. Organic photovoltaics cells (OPV) widely adopt a heterojunction architecture where dissociation is facilitated by charge transfer at a donor-acceptor (D-A) interface. Interestingly, recent work on MoO3/C60 Schottky OPVs has demonstrated that excitons in C60 may also undergo bulk-ionization to generate photocurrent, driven by the built-in field at the MoO3/C60 interface. Here, we show that bulk-ionization processes also contribute to the photocurrent in bulk heterojunction (BHJ) OPVs with fullerene-rich compositions. The short-circuit current density (Jsc) in a MoO3/C60 Schottky OPVs shows almost no dependence on temperature down to 80 K. This characteristic of bulk-ionization allows the use of temperature-dependent measurements of Jsc to distinguish bulk-ionization from charge transfer at a D-A interface. For BHJ OPVs constructed using the D-A pairing of boron subphthalocyanine chloride (SubPc)-C60, bulk-ionization is found to contribute >10% of the total photocurrent and >30% of the photocurrent from C60. We further find that fullerene-rich SubPc-C60 BHJ OPVs show a larger open-circuit voltage (Voc) than evenly mixed BHJs due to the presence of bulk-ionization. This talk will examine the dependence of Jsc and Voc on the relative fraction of dissociation by charge transfer and bulk-ionization processes.

Novel solar energy harvesting options based on solution-processable inorganic/organic hybrid materials. NATALIE STINGELIN, Imperial College London — The growing demand for energy and increasing concerns for the effect of the excessive abuse of fossil fuels on the environment force the scientific world to search for alternative, clean and safe energy sources. Finding ways to harvest solar energy is one of the most appealing options. Here, we present a novel approach that exploits the versatile properties of recently developed, photoactive organic/inorganic hybrid fluids based on titanium oxide hydrates and polyalcohols for the production of versatile solar fuels. We will show that such systems can absorb light in the UV-near visible wave-length range. The sunlight’s energy is then converted into chemical energy in the form of reduced titanium species, which can be re-oxidised by oxygen when required. Therefore, the absorbed energy is stored as long as oxygen is excluded by the hybrid system. We, furthermore, demonstrate that once discharged, the fluid can be activated again by exposing it to sunlight and recycled – a property that is important technologically. The same hybrids can also be exploited to produce structures that permit efficient management of light. We will illustrate the potential of this class of materials based on some of our recent approaches to fabricate light-scattering and light-in-coupling structures, and discuss future opportunities they open up.

Dark current of organic heterostructure devices with insulating spacer layers. SUN YIN, Shandong University, China, WANYI NIE, ADITYA D. MOHITE, AVADH SAXENA, DARRYL L. SMITH, Los Alamos National Lab, P. PAUL RUUDEN, University of Minnesota — The dark current density at fixed voltage bias in donor/acceptor organic planar heterostructure devices can either increase or decrease when an insulating spacer layer is added between the donor and acceptor layers. The dominant current flow process in these systems involves the formation and subsequent recombination of an interfacial exciplex state. If the exciplex formation rate limits current flow, the insulating interface layer can increase dark current whereas, if the exciplex recombination rate limits current flow, the insulating interface layer decreases dark current. We present a device model to describe this behavior and illustrate it experimentally for various donor/acceptor systems, e.g. P3HT/LiF/C60.

Unpinning the Open-Circuit Voltage in Organic Solar Cells through Tuning Ternary Blend Active Layer Morphology. PETR KHYABICH, Princeton University, Department of Chemical and Biological Engineering, BARRY THOMPSON, University of Southern California, Department of Chemistry and Loker Hydrocarbon Research Institute, YUEH-LIN LOO, Princeton University, Department of Chemical and Biological Engineering — The use of ternary, as opposed to binary, blends having complementary absorption in active layers of organic bulk heterojunction solar cells is a simple approach to increase overall light absorption. While the open-circuit voltage (Voc) of such solar cells have generally been shown to be pinned by the smallest energy level difference between the donor and acceptor constituents, there have been materials systems, that when incorporated into active layers of solar cells, exhibit composition dependent and tunable Voc. Herein, we demonstrate that this Voc tunability in ternary blend solar cells is correlated with the morphology of the active layer. Chemical compatibility between the constituents in the blend, as probed by grazing-incidence X-ray diffraction (GIXD) measurements, affords Voc tuning. The constituents need not “co-crystallize”; limited miscibility between the constituents in the active layers of solar cells affords Voc tunability. Poor physical interactions between the constituent domains within the active layers, on the other hand, result in devices that exhibit an invariant Voc that is pinned by the smallest energy level difference between the donor(s) and the acceptor(s). Our morphological studies thus support the proposed alloying model that was put forth originally.

Synthesis and Structure of Fully Conjugated Block Copolymers Utilized in Organic Photovoltaics. YOUNGMIN LEE, MELISSA APLAN, QING WANG, ENRIQUE D. GOMEZ, Pennsylvania State Univ — Fully conjugated block copolymers have the potential to overcome many of the limitations of mixtures and blends as photoactive layers in solar cells; furthermore, they may serve as model systems to study fundamental questions regarding optoelectric properties and charge transfer. However, the synthesis of fully conjugated block copolymers remains a challenging issue in the field. We have optimized the two-step synthesis of P3HT-b-PFTBT, which is composed comprised of Grignard metathesis for polymerization of P3HT followed by chain extension through a Suzuki-Miyaura polycondensation. We find that the concentration of the Grignard reagent is critical for end-group control such that P3HT is terminated by H at one end and Br at the other. Furthermore, we can utilize an asymmetric feed ratio of monomers for the Suzuki-Miyaura reaction to minimize the amount of uncoupled homopolymers and to control the molecular weight of the second block. We investigated the chemical composition, structure and electrical characteristics of the polymers prepared by the different synthetic methods, and demonstrate that we can utilize these strategies for the synthesis of block copolymers beyond P3HT-b-PFTBT.
1:39PM B41.00011 Comparison of Reverse Leakage Current Density in Bilayer and Bulk Heterojunction Organic Photodetectors. XIN XU, ANANTH DODABALAPUR, University of Texas Austin — Soft materials such as organic semiconducting polymers and small molecules will allow the development of next generation photodetectors. Their ease of manufacturing and ability to be placed on flexible substrates allow new innovations such flexible camera elements. While organic photodetectors are structurally similar to their solar cell counterparts, their operation under reverse bias is an important difference which leads to differences in optimization. Reverse leakage current within photodetectors is a key metric in their performance. Minimizing these leakage currents is an important research goal for the advancement of organic photodetectors. We have examined different material systems such as ZnO/CuPc, ZnO/P3HT, and P3HT/PCBM. Using all of this data, we will present a broad picture on how to improve organic photodetector performance.

1We acknowledge support from the NASCENT NSF ERC.

1:51PM B41.00012 Analysis of Charge Carrier Transport in Organic Photovoltaic Active Layers. XU HAN, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — We present a systematic analysis of charge carrier transport in organic photovoltaic (OPV) devices based on phenomenological, deterministic charge carrier transport models. The models describe free electron and hole transport, trapping, and detrapping, as well as gerninate charge-pair dissociation and gerninate and bimolecular recombination, self-consistently with Poisson’s equation for the electric field in the active layer. We predict photocurrent evolution in devices with active layers of P3HT, P3HT/PMMA, and P3HT/PS, as well as P3HT/PCBM blends, and photocurrent-voltage (I-V) relations in these devices at steady state. Charge generation propensity, zero-field charge mobilities, and trapping, detrapping, and recombination rate coefficients are determined by fitting the modeling predictions to experimental measurements. We have analyzed effects of the active layer morphology for layers consisting of both pristine drop-cast films and of nanoparticle (NP) assemblies, as well as effects on device performance of insulating NP doping in conducting polymers and of specially designed interlayers placed between an electrode and the active layer. The model predictions provide valuable input toward synthesis of active layers with prescribed morphology that optimize OPV device performance.

2:03PM B41.00013 Ultrafast Measurement Confirms Charge Generation through Cold Charge Transfer States. BHJ CAUTAM, ROBERT YOUNTS, North Carolina State University, LIANG YAN, University of North Carolina at Chapel Hill, EVGENY DANILOV, HARALD ADE, North Carolina State University, WEI YOU, University of North Carolina at Chapel Hill, KENAN GUNDOGDU, North Carolina State University — The role of excess energy in generation and extraction of charges through charge transfer (CT) states in polymer solar cells is a subject of debate. There are reports suggesting increase of charge generation yield with excess energy based on ultrafast experiments. On the other hand time delayed collection field measurements shows that excess photon energy has no effect in photovoltaic efficiency. Here we resolved this discrepancy by studying the dynamics of CT excitons and polarons in blends of medium gap copolymers. We found that low-lying charge transfer (CT) excitons can generate charges over a long time period (nanosecond) and contribute photocurrent on the bulk heterojunction devices. By performing resonant CT excitation as well as above gap excitation transient absorption measurements we investigated that the charges are generated more efficiently through low-lying CT states in efficient devices independent of excitation energy.

3This work is supported by Office of Naval Research grant N000141310526 P00002

Monday, March 2, 2015 11:15AM - 2:15PM — Session B42 DPOLY: Focus Session: Block Copolymer Thin Films I 214B - Gila Stein, University of Houston

11:15AM B42.00001 Morphology of Conjugated Block Copolymers: Self-Assembly, Crystallization, and Phase Separation. RAFAEL VERDUSCO, William Marshall Rice University — All-Conjugated Block Copolymers comprised of donor and acceptor polymer blocks are currently under development for use in organic photovoltaic devices. An attractive feature of these materials is their potential to self-assemble into well-defined donor and acceptor domains. However, achieving self-assembled film structures requires additional processing and annealing due to the high crystallization temperature of conjugated polymers and low Flory-Huggins chi interaction parameter between polymer blocks. This talk will present experimental studies into the processing-dependent morphology of all-conjugated block copolymer films relevant for organic photovoltaic devices. Conjugated block copolymer films that contain poly(3-hexyl thiophene) (P3HT) as the donor block exhibit crystallization as the predominant feature. Even at relatively low mass contents, the P3HT block crystallizes in solvent cast films. The orientation of P3HT crystallites is face-on for as-cast or low-temperature annealed films, but under annealing at elevated temperature, the crystallite orientation flips to an edge-on orientation. This behavior is observed for a wide-range of acceptor polymer blocks. Analysis of films by grazing-incidence X-ray scattering shows that conjugated block copolymers exhibit poor mesoscale ordering in solvent cast or thermally annealed films. Under solvent annealing, periodic lamellae with characteristic domain size of 4 nm are observed. The domain size is independent of block copolymer molecular weight and composition, and we hypothesize is driven by a combination of crystallization and micro-phase segregation. Finally, we investigate the morphology of PTB7 block copolymers as compatibilizers for PTB7-fullerene blends. Addition of PTB7 block copolymers can increase or decrease domain sizes, and morphology is stable to long-term thermal annealing.

3This work was supported by the National Science Foundation (CBET-1264703) and the Welch Foundation for Chemical Research (R4440P)

11:51AM B42.00002 Polypeptoids: A model system for exploring sequence and shape effects on block copolymer self-assembly. RACHEL SEGALMAN, University of California, Santa Barbara — While our ability to understand the detailed relationship between block copolymer chemistry and mesoscopic self-assembly has made remarkable progress over the last many years, yet we are still limited to a relatively small number of blocks in terms of structure-property understanding. Thus, there is a need to explore self-assembly phase space with sequence using a model system. Polypeptoids are non-natural, sequence specific polymers that offer the opportunity to probe the effect of sequence on self-assembly with much simpler molecular interactions and more scalable synthesis than traditional polypeptides. In this talk, I will discuss the use of this model system to understand the role of sequence on chain collapse and globule formation in solution, polymer crystallization, and block copolymer self-assembly. I will then discuss potential application as surface active agents for anti-fouling.
12:27PM B42.00003 Morphology Development in Block Copolymer Thin Films via Direct Immersion Annealing , ARVIND MODI, SARANG BHAWAY, BRYAN VOGT, The University of Akron, ASHUTOSH SHARMA, IIT Kanpur, ALAMGIR KARIM, The University of Akron — Conventional methods of annealing thin block copolymer (BCP) films include Thermal Annealing and Solvent Vapor Annealing (SVA) processes. Both of the processes have demonstrated excellent control over morphologies and nanostructures. However, both have constraints including long annealing time duration and/or complicated setup requirement. We introduce Direct Immersion Annealing (DIA) of thin block copolymer (BCP) films involving immersion of polymer films directly into the solvent mixture composed of selective non-solvent and solvent for blocks. Non-solvent prevents the dissolution of films while the good solvent permeates the film and plasticizes the blocks. A fine control of swelling ratio can be achieved through an easy and robust control of solvent volume fractions. We studied cylindrical Poly(styrene-block-methyl methacrylate) system in detail and quantified the growth of correlation length ($\xi$) with time($t$) ($\xi \sim t^{\alpha}$). We observe a reduction in growth exponent ($\alpha$) with several fold increase in pre-exponential factor ($A$) compared to isotropic thermal annealing. We further demonstrate the extension of this strategy to systems with diverse range of $\chi$, molecular weight and other morphologies.

12:39PM B42.00004 Real-Time observation of PS-PDMS block copolymer self-assembly under solvent vapor annealing $^1$, WUBIN BAI, MIT, KEVIN YAGER, Brookhaven National Laboratory, CAROLINE ROSS, MIT — Solvent annealing provides a convenient way to produce microphase separation in films of block copolymers, but the morphology transition of the film during the solvent absorption, equilibrium solvent-BCP concentration and solvent desorption process are not well known. An in situ study of solvent annealing of polystyrene-block-polydimethylsiloxane (PS-PDMS, 16 kg/mol, fPDMS = 30%, period 17 nm) diblock copolymer was carried by synchrotron grazing-incidence small-angle X-ray scattering (GISAXS). The swollen film morphology was found to be strongly dependent on swelling ratio. A transition from the disordered state to a highly ordered state which contained multiple layers of in-plane cylinders was observed at a swelling ratio around 1.45 from samples with 100nm to 1000nm as-cast thickness. The rate of solvent absorption was found to be less important to the dried morphology, while the time of equilibrium solvent-BCP concentration stage was found to influence the orientation of self-assembled microdomains and the drying rate was found to affect the degree of structure deformation. The implications of the results to pattern generation for block copolymer directed self-assembly will be discussed.

$^1$Semiconductor Research Corporation, National Science Foundation

12:51PM B42.00005 The kinetics of swelling in block copolymer thin films during “solvo-microwave” and solvo-thermal annealing: The effect of vapour pressure , PARVANRH MOKARIAN-TABARI, University College Cork and Tyndall National Institute; Centre for Research on Adaptive Nanostructures, TIMOTHY COLLINS, CIAN CUMMINS, University College Cork and Tyndall National Institute, CLAUDIA DELGADO SIMÃO, OLIVIA SOTOMAYOR, ICN2, Campus de la UAB, Barcelona 08193, Spain, MICHAEL A. MORRIS, University College Cork and Tyndall National Institute; Centre for Research on Adaptive Nanostructures — Long annealing time associated with high chi block copolymers is a major disadvantage for their integration in industrial applications. Microwave-assisted microphase separation appears to offer considerable benefits in reducing annealing times for BCPs. However, despite the promise of this technique, little is known about the mechanism of how microwave irradiation might sponsor the molecular motion that accompanies microphase separation. In our earlier work we carried out an in situ temperature measurement during “solvo-microwave” annealing of poly(styrene-b-lactic acid) (PS-b-PLA) in presence of THF and also in the conventional oven. Comparing the results indicated that vapour pressure of THF might have a major role to achieve fast self-assembly (60 seconds) in PS-b-PLA film. Here, we study the kinetics of swelling by monitoring the pressure through in situ pressure experiments during “solvo-microwave” and solvo-thermal annealing. The preliminary data suggest that the rate at which the THF pressure increases is the key factor. This suggests that kinetics, i.e., the rate of film swelling and diffusion, affects the order and the coherence length of the pattern. We estimated the defect density in the patterns by our recently developed defect analysis software.

1:03PM B42.00006 Fluorine effects on morphology and surface energy of diblock copolymer thin films $^1$, UMESH SHRESTHA, DVORA PERAHIA, Clemson University, STEPHEN CLARSON, University of Cincinnati — The interfacial composition and structure formed by the segregation between the incompatible blocks in a diblock copolymer thin film influence the stability and response of the film to external stimuli. Introduction of fluorine enhances the interfacial energy as well as chemical and thermal stability of the polymer film. Here we follow the interfacial structure and response of Si containing diblock co-polymer poly trifluoro propyl methyl siloxane-poly(styrene) (PTEPSMS-PS) with the SiF fraction ranging from 0.3 to 0.5 in surface of the films as a function of temperature and solvent, using atomic force microscopy and contact angle measurement. We found that the tendency of the fluorine to migrate towards surface affects the surface energy while Si in backbone enhances the flexibility of the chains. Thin films prepared from selective good solvent for one of the blocks and good solvent for both blocks formed different structures compared to their melts. Correlation between morphology and volume fraction is dominant above the Tg of the polystyrene whereas below Tg limited effect is observed.

$^1$NSF DMR 0907390

1:15PM B42.00007 Perpendicularly oriented nanostructures by using star-shaped poly(methyl methacrylate)-block-poly(dimethylsiloxane) thin film , SANGSHIN JANG, KYUSEONG LEE, HONG CHUL MOON, JICHEOL PARK, JONGHEON KWAK, GUMHYE JEON, JIN KON KIM $^2$, Pohang Univ of Sci & Tech — Thin films of star-shaped 18-arm poly(methyl methacrylate)-block-poly(dimethylsiloxane) copolymers ((PMMA-b-PS)$_s$) with two different volume fraction of PS block (f$_{PS}$) (0.60 and 0.75). Interestingly, perpendicularly oriented lamellar and cylindrical domains were observed by atomic force microscopy (AFM) and grazing-incidence small-angle X-ray scattering (GISAXS), after thermal annealing without additional treatment such as random copolymer treatment or solvent annealing. Perpendicularly oriented nanostructures were also achieved for versatile substrates such as PS(OR PMMA)-brushed substrate, flexible substrate ( PEN) or gold-deposited substrate.

$^1$corresponding author

1:27PM B42.00008 Vertical Continuity and Alignment of Block Copolymer Domains by Kinetically Controlled Electrospray Deposition , HANQIONG HU, YOUNGWOO WOO, XUNDA FENG, CHINEDUM OSUJI, Yale University, OSUJI LAB TEAM — We report the fabrication of vertically aligned cylindrical block copolymer (BCP) domains using continuous electrospray deposition (ESD) onto bare wafer surfaces. The out-of-plane orientation of hexagonally packed styrene cylinders was achieved in a “fast-wet” deposition regime where rapid evaporation of solvent in droplets of polymer solution drove the vertical alignment of SBS domains. The deposition conditions were optimized such that thermally activated crosslinking of the polybutadiene matrix provided kinetic control of the morphology, locking in the vertical alignment and preventing relaxation of the system to its preferred parallel orientation on the non-treated substrate. Physically continuous and vertically oriented domains is achieved over several microns of film thickness. We describe the effects of flow rate, collection distance and substrate temperature on thin film morphology and demonstrate selective etching capabilities. The ability of ESD to fabricate well-ordered and aligned BCP films on non-treated substrates, the low utilization of material relative to spin-coating and the continuous nature of the deposition may open up new opportunities for BCP thin films. We are exploring ESD as a new platform for sequential deposition of BCPs with different functionalities.
1:39PM B42.00009 Edge effects and surface patterns in a quenched lamella forming block copolymer, ANDREW B. CROLL, PEGGY WILLENBRING, ALEXANDER WAGNER, North Dakota State Univ — Thin lamellar systems are well known to form structures when cast in a thickness that is not commensurate with a lamellar spacing. The structures have often been considered an ideal two-dimensional system and much has been learned of the patterns dynamics. This early work considered a uniform isotropic film in a region infinitely far from a boundary. Here we specifically consider the influence of a pre-existing boundary on the pattern formation process, and identify the emergence of a unique new lengthscale in the problem. Our work combines an idealized experimental system (polystyrene-poly(2-vinylpyridine) diblock near the order-to-disorder transition point) with precise numerical computation (a Lattice-Boltzmann model) in order to develop an understanding of the relative importance of the key physical phenomena underlying the results. The new lengthscale is found to be inversely proportional to both total film thickness and quench depth and offers unique opportunities to engineer structures extending beyond the 2D layer into the 3rd dimension.

1:51PM B42.00010 A Stable Hexagonally Modulated Lamellar (HML) Structure of Asymmetric Polystyrene-b-Poly(2-vinylpyridine) in Film Geometry, SUNGMIN PARK, Yonsei University, HYUNGJU AHN, Pohang Accelerator Laboratory, BYEONGDU LEE, Argonne National Laboratory, DU YEOL RYU, Yonsei University, YONSEI UNIVERSITY COLLABORATION, POHANG ACCELERATOR LABORATORY COLLABORATION, ARGONNE NATIONAL LABORATORY COLLABORATION — When a block copolymer (BCP) is confined in film geometry, the phase transitions would be different or shifted from those of the corresponding bulk. In this study, the phase transition of an asymmetric polystyrene-b-poly(2-vinylpyridine) (PS-b-P2VP) films in the presence of the strong interfacial interactions were investigated by grazing incidence small-Angle x-ray scattering (GISAXS) and transmission electron microscopy (TEM). The order-to-order transition (OOT) and order-to-disorder transition (ODT) in film geometry were influenced by the strong favorable forces between the P2VP block and substrate, resulting in the thickness-dependent phase diagram. The phase stability of a hexagonally modulated lamellar (HML) structure was identified in film geometry, and in the films below 10Lo it was extended over the entire temperature range even above the ODT temperature of the bulk.

2:03PM B42.00011 Adsorbed block copolymer nanolayers on solids, JENNIFER IMBROGNO, State Univ of NY-Stony Brook, MANI SEN, Department of Materials Science and Engineering, Stony Brook University, Stony Brook, NY 11794-2275, STEVEN KAHN, Department of Chemistry, University at Buffalo, The State University of New York, Buffalo, NY 14260-3000, SHOTARO NISHITSUJI, Department of Polymer Science and Engineering, Graduate School of Science and Engineering, Yamagata University, Yamagata, 992-8510, Japan, E. BHOJE GOWD, CSIR-NIIST, Trivandrum-695 019, Kerala, India, MAYA K. ENDOH, TADANORI KOGA, Department of Materials Science and Engineering, Stony Brook University, Stony Brook, NY 11794-2275 — Directed self-assembly of block copolymers (BCP) has been used as an advanced lithography method. In this study, we aim to shed light onto the structures of BCP at the polymer melt-solid interface. Polystyrene-block-poly(4-vinylpyridine) (PS-b-P4VP) block copolymer was used. Spin-cast 32 nm PS-b-P4VP films on silicon substrates were (i) thermally annealed at high temperature above Tg of the polymers or (ii) solvent vapor annealing with chloroform (non-selective solvent) and subsequent 1,4-dioxane (selective solvent). Using atomic force microscopy (AFM), we found perpendicular hexagonally packed cylinders at the topmost surface of the resultant PS-b-P4VP films regardless of the annealing processing. In addition, to study the adsorbed layer structure, we rinsed the annealed films with toluene and characterized the morphologies and film structures using grazing incidence small-angle X-ray scattering, X-ray reflectivity and AFM. The details will be discussed.

Monday, March 2, 2015 11:15AM - 2:15PM — Session B43 DPOLY: Focus Session: Fluids Under Confinement, Water at Interfaces and in Confinement 214C - Elisa Riedo, Georgia Institute of Technology

11:15AM B43.00001 Molecular Dynamics Simulations of Water Evaporation, CHENGYUAN WEN1, 2. Virginia Tech, GARY GREST3, Sandia National Laboratories, SHENGFENG CHENG4, Virginia Tech — The evaporation of water from the liquid/vapor interface is studied via large-scale molecular dynamics simulations for systems of more than a million atoms at 550K and 600K. The TIP4P-2005 water model whose liquid/vapor surface tension is in excellent agreement with experiments is used. Evaporative cooling at the interface is observed from temperature profiles determined from both translational and rotational kinetic energy. During evaporation, the density of water is slightly enhanced near the liquid-vapor interface. The velocity distribution of water molecules in the vapor phase during evaporation at various distances relative to the interface fit a Maxwell-Boltzmann distribution. While our results indicate an imbalance between evaporating and condensing water molecules, local thermal equilibrium is found to hold in addition to mechanical equilibrium.

1Department of Physics, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061, USA
2Sandia National Laboratories, Albuquerque, NM 87185, USA
3Department of Physics, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061, USA

11:27AM B43.00002 Structure of the Ice-Clathrate Interface, ANDREW NGUYEN, The University of Utah, MATTHEW KOC, TRICIA SHEPHERD, Westminster College, VALERIA MOLINERO, The University of Utah — In the laboratory, clathrates are customarily synthesized from ice and gas guest. It is not clear how and whether ice assists in the nucleation of clathrate hydrates. The structure of the ice-clathrate interface can help assess the role of ice in clathrate nucleation. However, only few studies have addressed the structure of the ice-clathrate interface. Here, we use molecular dynamic simulations to study the structure of the ice-clathrate interface. There is no lattice matching between any plane of ice and clathrate hydrates, therefore an interfacial transition layer has to form to connect the two crystals. We investigate the structure of the ice-clathrate interface produced by alignment and equilibration of the crystals, competitive growth of the two crystals from a common solution, and nucleation of hydrate in the presence of a growing ice front. We find that the interfacial transition layer between ice and clathrate has a width of two to three water layers and it is disordered in all cases. Water in the interfacial transition layer has tetrahedral order lower than either ice or clathrate and higher than liquid water under the same thermodynamic conditions.

1The work is supported by NSF grant number CHE-1012651
11:39AM B43.00003 Experimental evidence for empty cage methane clathrate hydrates grown using surfactants. JEFFREY BOTIMER, DEREK DUNN-RANKIN, PETER TABOREK, Univ of California - Irvine — Clathrate hydrates are non-stoichiometric ice-like crystalline compounds consisting of host water molecules forming a cage-like structure around guest molecules. The guest molecule is necessary for the stability of the hydrate. Surfactants have been shown to greatly enhance the kinetics of hydrate growth, which is important for many applications. We have built custom cells that allow in situ Raman and optical imaging of the growth of methane clathrate hydrates from liquid water. In our studies, above 0°C, we observe the formation of solid that precedes the absorption of methane gas required to form clathrate hydrates. Our research shows that sodium dodecyl sulfate (SDS) causes a fundamental change in the growth mechanism of methane hydrates, creating a temporary empty cage clathrate structure. This change is confirmed by in situ Raman spectroscopy and in situ NMR. Water uptake can simultaneously monitor the gas uptake, and the NMR signal of the growing hydrate in a high pressure NMR cell. The empty cage solid structure appears to be unique to surfactant assisted hydrate growth, and begins to disappear for low SDS concentrations (<25ppm).

Supported by the W. M. Keck Foundation.

11:51AM B43.00004 Formation of 1D adsorbed water structures on CaO(001), XUNHUA ZHAO, SASWATA BHATTACHARYA, LUCA M. GHIRINGHELLI, SERGEY V. LEVCHENKO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin — Understanding the interaction of water with oxide surfaces is of fundamental importance for basic and engineering sciences. Recently, a spontaneous formation of one-dimensional (1D) adsorbed water structures have been observed on CaO(001) [1]. Interestingly, at other alkaline earth metal oxides, in particular MgO(001) and SrO(001), such structures have not been found experimentally. We calculate the relative stability of adsorbed water structures on the three oxides using density-functional theory combined with the 

of one-dimensional (1D) adsorbed water structures have been observed on CaO(001) [1]. Interestingly, at other alkaline earth metal oxides, in particular MgO(001) and SrO(001), such structures have not been found experimentally. We calculate the relative stability of adsorbed water structures on the three oxides using density-functional theory combined with the ab initio atomistic thermodynamics. Low-energy structures at different coverages are obtained with a first-principles genetic algorithm. Finite-temperature vibrational spectra are calculated using ab initio molecular dynamics. We find a range of (T, p) conditions where 1D structures are thermodynamically stable on CaO(001). The orientation and vibrational spectra of the 1D structures are in agreement with the experiments [1]. The formation of the 1D structures is found to be actuated by a symmetry breaking in the adsorbed water tetramer, as well as by a balance between water-water and water-substrate interactions, determined by the lattice constant of the oxide.—[1] X. Shao, Y. Fujimori, M. Sterrer, H.-J. Freund, and N. Nilius, to be published.

12:03PM B43.00005 Characterization of the Mobility and Reactivity of Water Molecules on TiO2 Nanoparticles by 1H Solid-State Nuclear Magnetic Resonance1, XIAOLIANG WANG, LILI ZHU, Nanjing University, PINGCHUAN SUN, Nankai University, DONGSHAN ZHOU, GI XUE, Nanjing University — Understanding interfacial water behavior is essential to improving our understanding of the surface chemistry and interfacial properties of nanomaterials. Here we use 1H solid-state nuclear magnetic resonance (1H SSNMR), we successfully monitored ligand exchange reaction between oleylamine (OLA) and adsorbed water on titanium dioxide nanoparticles (TiO2 NPs). Three different types of interfacial waters with different reactivities were distinguished. The mobility of the adsorbed water molecules was characterized by dipolar filtered 1H SSNMR. Our experimental results demonstrate that the adsorbed water can be categorized into three different layers: rigid water species with restricted mobility closest to the surface of TiO2 NPs; less mobile water species weakly confined on TiO2 NPs; and water molecules with high mobility. Water in the third layer could be replaced by OLA, while water in the first and second layers remained intact. The finding that the interfacial water with the highest mobility has the strongest reactivity has guiding significance for tailoring the hydrophilic and hydrophobic properties of TiO2 NPs.

1 We gratefully acknowledge support from the Natural Science Foundation of China (No.21174062)

12:15PM B43.00006 Diffusive Dynamics of Water inside Hydrophobic Carbon Micropores Studied by Neutron Spectroscopy and MD Simulation, SOULEYMANE DIALLO, LUKAS VLOEK, EUGENE MAMONTOV, JONG KEUM, JIHUA CHEN, Oak Ridge National Laboratory, JOSEPH HAYES, American Technical Trading, DAVID WESOLOWSKI, ARIEL CHIALVO, Oak Ridge National Laboratory — Using neutron scattering, we have investigated the ambient pressure diffusive dynamics of water in microporous Kynol®TM= ACF-10 (with average micropore size of ~11.6 Å) from temperature T = 280 K in its stable liquid state down to T = 230 K into the metastable supercooled phase. The observed characteristic relaxation times and diffusion coefficients are found to be respectively higher and lower than those in bulk water, indicating a slowing down of the water mobility with decreasing temperature. Comparison between the experimental observations and complementary molecular dynamics simulations of a model system, in which we studied the diffusion of water within the 12 Å gap of two parallel graphene sheets will be presented.

12:27PM B43.00007 Quantum tunneling and vibrational dynamics of ultra-confined water, ALEXANDER I. KOLENSIKOV, LAWRENCE M. ANOVITZ, GEORGE EHLERS, EUGENE MAMONTOV, ANDREY PODLESNYAK, TIMOTHY R. PRISK, Oak Ridge National Laboratory, TN, ANDREW SEEL, ISIS Facility, UK, GEORGE F. REITER, University of Houston, TX — Vibrational dynamics of ultra-confined water in single crystals beryl, the structure of which contains ~ 5 Å diameter channels along the c-axis was studied with inelastic (INS), quasi-elastic (QENS), and deep inelastic (DINS) neutron scattering. The results reveal significantly anisotropic dynamical behavior of confined water, and show that effective potential experienced by water perpendicular to the channels is significantly softer than along them. The observed 7 peaks in the INS spectra (@ energies 0.25 to 15 meV), based on their temperature and momentum transfer dependences, are explained by transitions between the split ground equivalent positions across the channels. DINS study of beryl at T = 4.3 K shows narrow, anisotropic water proton momentum distribution with corresponding kinetic energy, E_p = 95 meV, which is much less than was previously observed in bulk water (~150 meV). We believe that the exceptionally small E_K in beryl is a result of water quantum tunneling \ delocalization in the nanometer size confinement and weak water-cage interaction.

The neutron experiment at ORNL was sponsored by the Sci. User Facilities Div., BES, U.S. DOE. This research was sponsored by the Div. Chemical Sci, Geosciences, and Biosciences, BES, U.S. DOE. The STFC RAL is thanked for access to ISIS neutron facilities.

1The neutron experiment at ORNL was sponsored by the Sci. User Facilities Div., BES, U.S. DOE. This research was sponsored by the Div. Chemical Sci, Geosciences, and Biosciences, BES, U.S. DOE. The STFC RAL is thanked for access to ISIS neutron facilities.

12:39PM B43.00008 Nanomechanical measurements of ionic effect on nanoconfined water, EDWARD KRAMKOWSKI, Wayne State University, SHAH KHAN, University of Peshawar, PETER HOFFMANN, Wayne State University — The behavior of liquid molecules confined to nanometer-scale spaces is a topic of particular interest to a variety of fields. From lab-on-a-chip medical device manufacturers to petroleum engineers involved in oil recovery, a wide range of researchers could benefit from a better understanding of the mechanics of nanconfined liquids. Previous research has shown that above a critical strain rate, a confined liquid exhibits a solid-like response that oscillates with a period roughly equal to the molecular diameter of the liquid being observed. This indicates that when a liquid is compressed at a rate faster than the molecules can diffuse in bulk out from between the confining surfaces, it dynamically solidifies into an anisotropic layered liquid. We have simultaneously monitored their uptake and their mechanical behavior. We believe that the exceptionally small E_K in beryl is a result of water quantum tunneling \ delocalization in the nanometer size confinement and weak water-cage interaction.

The neutron experiment at ORNL was sponsored by the Sci. User Facilities Div., BES, U.S. DOE. This research was sponsored by the Div. Chemical Sci, Geosciences, and Biosciences, BES, U.S. DOE. The STFC RAL is thanked for access to ISIS neutron facilities.
12:51PM B43.00009 Supressed Water Crystallization in Nano-Structured Physical Hydrogel. CLINTON WIENER, BRYAN VOGT, ROBERT WEISS, Univ of Akron — Suppressed water crystallization occurs in some organisms, such as the common wood frog, which allows it to hibernate in a frozen state without damage to its cells. Knowledge of the behavior of supercooled water and alternate ice forms may have many implications to many fields of science. Supercooled water by several degrees below the normal freezing point is often observed in hydrogels that have attractive interactions with water, e.g., hydrogen bonding. Repulsive confinement, such as in hydrophobic porous carbon, can have even more significant effects on the supercooling of the entrapped water. This talk describes the freezing behavior in nano-structured, hydrophobically modified poly(dimethyl acrylamide) hydrogels that possess attractive and repulsive interactions with water and are physically crosslinked by hydrophobic nanodomains. Three distinct water freezing regimes were observed in the hydrogel swollen to about 50% water by weight. Differential scanning calorimetry detected three crystallization exotherms at 254K, 244K, and 227K. Quasi-elastic neutron scattering experiments have shown that although the water mobility was suppressed at room temperature, the water remained significantly mobile below the normal freezing point of water. The talk will discuss how tuning the concentration of the hydrophobic composition of the hydrogel affects the porous length scales in the hydrogel, which may alter the state of water and the crystal form produced by supercooling.

1:03PM B43.00010 ABSTRACT WITHDRAWN

1:15PM B43.00011 Ice-like Behavior of Ultra-Confined Water1. TIMOTHY PRISK, ALEXANDER KOLESNIKOV, EUGENE MAMONTOV, LAWRENCE ANOVITZ. Oak Ridge National Laboratory — Water confined within microporous minerals presents an extreme example of fluid confinement, where the water molecule is trapped within cages or pore channels which are not much larger than the water molecule itself. Hemimorphite Zn$_4$SiO$_4$(OH)$_2$·H$_2$O is a microporous silicate mineral containing confined molecular water which interacts with the crystal structure by means of hydrogen bonding. The water molecule forms a supercooled hydrogen bonds with the hydroxyl groups, forming a system of two-dimensional ice within the pore channel. In this presentation, we report quasi-elastic and inelastic neutron scattering studies of water and hydroxyl proton dynamics within hemimorphite. The scattering data reveal strong anisotropy in the vibrational behavior of the water molecule, with the scissors and stretching normal mode motions occurring only on a single crystallographic plane. The effective density of states of the protons extracted from the scattering data reproduces the water contribution to the mineral’s heat capacity.

1:27PM B43.00012 The consequences of water in adhesion, friction and wetting2, ALI DHINOJWALA, ADRIAN DEFANTE, TARAK BURALI, MATTHEW BECKER, Univ of Akron — The interactions of hydrophobic surfaces are relevant to numerous processes in physical and biological sciences. We have used contact mechanics, contact angle measurements, and a biaxial friction cell to quantify adhesion, wetting and friction behavior in wet environments between two low energy surfaces. To gain an understanding of the role of water in these processes we have coupled these measurements with surface sensitive sum frequency generation to directly measure the contacting interface. These results provide a direct molecular probe to understand macroscopic phenomena.

1:39PM B43.00013 How different is water crystallization from polymer crystallization under confinement? . GEORGE FLOUDAS, University of Ioannina, YASUHITO SUZUKI, Max Planck Institute for Polymer Research, HATICE DURAN, TOBB University of Economics and Technology, MARTIN STEINHART, University of Osnabrueck, HANS-JUERGEN BUTT, Max Planck Institute for Polymer Research — The freezing mechanism of water under confinement can be fundamentally different from the bulk. Despite fundamental importance, the lack of well-defined confining media precluded a systematic investigation. Herein we employ self-ordered nanoporous aluminum oxide (AAO) which contains arrays of discrete, parallel and cylindrical nanochannels with uniform pore length and diameter to study the effect of confinement on water crystallization. By varying different parameters such as pore size, temperature and cooling rate, the respective conditions under which the hexagonal form (I$_h$) and the less common form of cubic ice (I$_c$) could be studied. We found a transition from homogeneous nucleation of I$_h$ to homogeneous nucleation of predominantly I$_c$, with decreasing pore diameter. Furthermore, the monotropic I$_c$ → I$_h$ transition commonly observed upon heating is suppressed inside pores having diameters ≤ 35 nm. These findings lead to the phase diagram of water under confinement. It contains a predominant cubic form, a form known to exist only in the upper atmosphere. There are many similarities between the freezing of water and the crystallization of polymers under confinement.

1:51PM B43.00014 Frictional energy barrier and blocking temperature in water molecules and carbon nanotubes system1. JIANWEI ZHANG, JIAJI LI, WENFENG LI, School of physics, Tongji University — Water transport through hydrophobic channels of single-walled carbon nanotubes has attracted a lot interests, especially, various potential applications of SWCNTs have been proposed for designing novel nanofluidic devices. By adopting Molecular dynamics method, we investigated mechanics and statistics properties of water molecules escaping from a confined single-walled carbon nanotube. From our numerical MD simulations and statistical model, we determined the friction energy barrier of water molecules in (10.10) SWCNT is 9.88 kcal/mol, and which is the minimal energy for flowing a water molecules in CNT. By only using friction energy barrier and relaxation time parameter, our model can fit all different situations MD simulation results. In order to describing the frictional lock behavior of water molecules, we introduced a new blocking temperature, below this temperature (391K for our system), water is locked in CNT due to friction energy barrier. We found that the blocking temperature is closely related to system response time, and it also shows a linear behavior to frictional energy barrier. Furthermore, we found several other interesting statistics results when a water molecules leaving SWCNTs.

2:03PM B43.00015 The Role of Water and Carbon Dioxide Intercalation on Na-Montmorillonite Swelling Behavior at Geological Carbon Sequestration Conditions1 MEYSAM MAKAREMI, KENNETH JORDAN, GEORGE GUTHRIE, EVGENIY MYSHAKIN, National Energy Technology Laboratory, and University of Pittsburgh, Pittsburgh, PA — Swelling of Na-montmorillonite in the environment relevant to geological CO$_2$ sequestration in deep underground formations is investigated by conducting classical Monte Carlo and molecular dynamics simulations. Both the binary (clay-water or clay–CO$_2$) and the ternary (clay-water–CO$_2$) systems containing the clay, water and carbon dioxide phases are simulated, and the free energy for clay swelling is calculated as a function of the interlayer distance. The calculations indicate that while water intercalates into the clay layer and forms stable monolayer and bilayer hydration states, in the absence of interlayer water adsorption of dry carbon dioxide is thermodynamically unfavorable. In the ternary system, two hydration states are observed with interlayer spacings corresponding closely to those of the pure water binary system. In addition, the simulations of the ternary system show that the incomplete first hydration state is more effective at adsorbing CO$_2$ molecules than is the incomplete second hydration state.

1This research conducted at the Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

2National Science Foundation, Akron Functional Materials Center

3This work was supported by NSFC No.11274240 and NO.51471119.
and Mechanisms II

214D -

that we can create an arbitrary number of well separated minima, i.e. shapes. With 3D printing, we bring these shape-shifting structures to life.

for motion, the 4-vertex, has two distinct branches of motion. By deriving a local combinatorial rule, we show that the number of branches in a tessellated sheet

of vertices of an origami structure have different impacts on different mechanical properties, and different origami designs could have different sensitivities to

designs. Through reliability and probabilistic analysis, we investigate the effect of randomness in origami structures on their mechanical properties. Dislocations

imperfections introduced during manufacturing, or non-uniform deformations under working conditions (e.g. due to non-uniform thermal effects). Therefore, the

large scale deployable shells. For instance, some origami-inspired designs have unique properties such as negative Poisson ratio and flat foldability. However,

the specific requirements of an engineering problem. The application of origami to structural design problems ranges from micro-structure of materials to

ancient paper folding art, has inspired many solutions to modern engineering challenges. The demand for practical applications motivates further

research. The new patterns are appropriate for a broad range of applications, from mechanical metamaterials to deployable and kinetic structures, at both

small and large scales.

22:17AM B44.00002 Origami Mechanics: Bistability and Isometries, MOKHTAR ADDA-BEDIA, FREDERIC LECHENAULT, Laboratoire de Physique Statistique de l’ENS, MORPHOGENESIS AND MULTISCALE PHENOMENA TEAM — Origami structures are usually seen as assemblies of rigid faces articulated around creases with hinge-like behaviour. Their deployment and degrees of freedom are purely kinematic, resulting only from the geometry of the crease network. However, in real folded structures, the base material can deform outside the creases. In such situations, face bending competes with crease actuation in a morphogenetic way. In order to rationalise this interplay, we investigate the mechanical behaviour of an infinite sheet on which one or more straight creases meet at a single vertex. We find that these structures generically exhibit bistability, in the sense that they can snap through from one metastable configuration to another. Furthermore, we uncover a new class of isometry of the plane, which corresponds to metastable states of a creased sheet for which the hoop stress vanishes, an instability mechanism that is also responsible for the wrinkling of thin plates.

11:39AM B44.00003 ABSTRACT WITHDRAWN —

11:51AM B44.00004 Topological mechanics: from metamaterials to active matter, VINCENZO VITELLI, Leiden University — Mechanical metamaterials are artificial structures with unusual properties, such as negative Poisson ratio, bistability or tunable acoustic response, which originate in the geometry of their unit cell. At the heart of such unusual behavior is often a mechanism: a motion that does not significantly stretch or compress the links between constituent elements. When activated by motors or external fields, these soft motions become the building blocks of robots and smart materials. In this talk, we discuss topological mechanisms that possess two key properties: (i) their existence cannot be traced to a local imbalance between degrees of freedom and constraints (ii) they are robust against a wide range of structural deformations or changes in material parameters. The continuum elasticity of these mechanical structures is captured by non-linear field theories with a topological boundary term similar to topological insulators and quantum Hall systems. We present several applications of these concepts to the design and experimental realization of 2D and 3D topological structures based on linkages, origami, buckling meta-materials and lastly active media that break time-reversal symmetry.

12:27PM B44.00005 Critical transition to bistability arising from hidden degrees of freedom in origami structures, ITAI COHEN, JESSE SILVERBERG, Physics, Cornell Univ., JUN-HEE NA, Polymer Science and Engineering, UMass Amherst, ARTHUR EVANS, Physics, UMass Amherst, BIN LIU, Physics, Cornell Univ., THOMAS HULL, Maths, Western New England University, CHRISTIAN SANTANGELO, Physics, UMass Amherst, ROBERT LANG, Lang Origami, RYAN HAYWARD, Polymer Science and Engineering, UMass Amherst — Origami, the traditional art of paper folding, is now being used to design responsive, dynamic, and customizable mechanical metamaterials. The remarkable abilities of these origami-inspired devices emerge from a predefined crease pattern, which couples kinematic folding constraints to the geometric placement of creases. In spite of this progress, a generalized physical understanding of origami remains elusive due to the challenge in determining whether local kinematic constraints are globally compatible, and an incomplete understanding of how bending and crease plasticity found in real materials contribute to the overall mechanical response. Here, we show experimentally and theoretically that the traditional square twist, whose crease pattern has zero degrees of freedom (DOF) and therefore should not be foldable, is nevertheless able to be folded by accessing higher energy scale deformations associated with bending. Due to the separation of bending and crease energy scales, these hidden DOF lead to a geometrically-driven critical bifurcation between mono- and bistability. The scale-free geometric underpinnings of this physical phenomenon suggest a generalized design principle that can be useful for fabricating micro- and nanoscale mechanical switches.

12:39PM B44.00006 A probabilistic approach to randomness in geometric configuration of scalable origami structures, KE LIU, GLAUCIO PAULINO, PAOLO GARDONI, University of Illinois at Urbana-Champaign — Origami, an ancient paper folding art, has inspired many solutions to modern engineering challenges. The demand for actual engineering applications motivates further investigation in this field. Although rooted from the historic art form, many applications of origami are based on newly designed origami patterns to match the specific requirements of an engineering problem. The application of origami to structural design problems ranges from micro-structure of materials to large scale deployable shells. For instance, some origami-inspired designs have unique properties such as negative Poisson ratio and flat foldability. However, origami structures are typically constrained by strict mathematical geometric relationships, which in reality, can be easily violated, due to, for example, random imperfections introduced during manufacturing, or non-uniform deformations under working conditions (e.g. due to non-uniform thermal effects). Therefore, the effects of uncertainties in origami-like structures need to be studied in further detail in order to provide a practical guide for scalable origami-inspired engineering designs. Through reliability and probabilistic analysis, we investigate the effect of randomness in origami structures on their mechanical properties. Dislocations of vertices of an origami structure have different impacts on different mechanical properties, and different origami designs could have different sensitivities to imperfections. Thus we aim to provide a preliminary understanding of the structural behavior of some common scalable origami structures subject to randomness in their geometric configurations in order to help transition the technology toward practical applications of origami engineering.

12:51PM B44.00007 Exponential Number of Shapes in Origami Metasheets, PETER DIELEMAN, Univ of Leiden / AMOLF, SCOTT WAITUKAITIS, Univ of Leiden, MARTIN VAN HECKE, Univ Leiden / AMOLF — The simplest possible fold pattern that allows motion, the 4-vertex, has two distinct branches of motion. By deriving a local combinatorial rule, we show that the number of branches in a tesselated sheet of such 4-vertices grows exponentially with the number of vertices. We introduce energy in the system by approximating the folds as torsional springs and show that we can create an arbitrary number of well separated minima, i.e. shapes. With 3D printing, we bring these shape-shifting structures to life.
1:03PM B44.00008 Topological modes bound to lattice dislocations in mechanical metamaterials. JAYSON PAULOSE, BRYAN CHEN, VINCENZO VITELLI, Lorentz Institute — The mechanical rigidity of frameworks – nodes connected by springs or rigid bars – underlies the structural integrity of bridges, the response of granular materials, and the design of metamaterials with unusual mechanical properties. A fundamental question governing rigidity is the existence of mechanisms: motions that do not significantly stretch or compress the constituent elements of the structure. We demonstrate a novel way to introduce approximate mechanisms at desired locations in a metamaterial, by exploiting the properties of a recently introduced class of topological metamaterials. These special periodic frameworks which exhibit localized edge modes, analogous to the electronic edge states of topological insulators. We show that dislocations in such metamaterials are associated with soft modes of topological origin. The existence of the modes is determined by the interplay between two Berry phases – the Burgers vector of the dislocation and a topological “polarization” characterizing the underlying lattice. Simple prototypes built out of triangular plates joined by hinges provide a visual demonstration of these modes.

1:15PM B44.00009 Wave Propagation in Origami-inspired Foldable Metamaterials. PAI WANG, SIJIE SUN, Harvard University, KATIA BERTOLDI, bertoldi@seas.harvard.edu — We study the propagation of elastic waves in foldable thin-plate structures. Both 1D systems of periodic folds and 2D Miura-Ori patterns are investigated. The dispersion relations are calculated by finite element simulations on the unit cell of spatial periodicity. Experimental efforts and considerations are also discussed. The characteristic propagating bands and bandgaps are found to be very sensitive to the folding angles. The existence of highly tunable bandgap makes the system suitable for potential applications including adaptive filters in vibration-reduction devices, wave guides and acoustic imaging equipment.

1:27PM B44.00010 Quantification of a Helical Origami Fold. ERIC DAI, Washington University in St. Louis, XIAOMIN HAN, ZI CHEN, Dartmouth College — Origami, the Japanese art of paper folding, is traditionally viewed as an amusing pastime and medium of artistic expression. However, in recent years, origami has served as a source of inspiration for innovations in science and engineering. Here, we present the geometric and mechanical properties of a twisting origami fold. The origami structure created by the fold exhibits several interesting properties, including rigid foldability, local bistability and finely tunable helical coiling, with control over pitch, radius and handedness of the helix. In addition, the pattern generated by the fold closely mimics the twist buckling patterns shown by thin materials, for example, a mobius strip. We use six parameters of the twisting origami pattern to generate a fully tunable graphical model of the fold. Finally, we present a mathematical model of the local bistability of the twisting origami fold. Our study elucidates the mechanisms behind the helical coiling and local bistability of the twisting origami fold, with potential applications in robotics and deployable structures.

1:39PM B44.00011 Associative memory through rigid origami. ARVIND MURUGAN, MICHAEL BRENNER, Harvard University — Mechanisms such as Miura Ori have proven useful in diverse contexts since they have only one degree of freedom that is easily controlled. We combine the theory of rigid origami and associative memory in frustrated neural networks to create structures that can “learn” multiple generic folding mechanisms and yet can be robustly controlled. We show that such rigid origami structures can “recall” a specific learned mechanism when induced by a physical impulse that only need resemble the desired mechanism (i.e. robust recall through association). Such associative memory in matter, seen before in self-assembly, arises due to a balance between local promiscuity (i.e., many local degrees of freedom) and global frustration which minimizes interference between different learned behaviors. Origami with associative memory can lead to a new class of deployable structures and kinetic architectures with multiple context-dependent behaviors.

1:51PM B44.00012 Hiding the weakness: structural robustness using origami design. BIN LIU, Physics Department, Cornell University, CHRISTIAN SANTANGELO, Department of Physics, University of Massachusetts, Amherst, ITAI COHEN, Physics Department, Cornell University — A non-deformable structure is typically associated with infinitely stiff materials that resist distortion. In this work, we designed a structure with a region that will not deform even though it is made of arbitrarily compliant materials. More specifically, we show that a foldable sheet with a circular hole in the middle can be deformed externally with the internal geometry of the hole unaffected. Instead of strengthening the local stiffness, we fine-tune the crease patterns so that all the soft modes that can potentially deform the internal geometry are not accessible through strain on the external boundary. The inner structure is thus protected by the topological mechanics, based on the detailed geometry of how the vertices in the foldable sheet are connected. In this way, we isolate the structural robustness from the mechanical properties of the materials, which introduces an extra degree of freedom for structural design.

2:03PM B44.00013 Untangling the mechanics versus topology of overhand knots. PEDRO REIS, MOHAMMAD JAWED, Massachusetts Institute of Technology, PETER DIELEMAN, Leiden University, BASILE AUDOLY, Sorbonne Universités, UPMC Univ Paris & CNRS — We study the interplay between mechanics and topology of overhand knots in slender elastic rods. We perform precision desktop experiments of overhand knots with increasing values for the crossing number (our measure of topology) and characterize their mechanical response through tension-displacement tests. The tensile force required to tighten the knot is governed by an intricate balance between topology, bending, friction, and contact forces. Digital imaging is employed to characterize the configuration of the contact braid as a function of crossing number. A robust scaling law is found for the pulling force in terms of the geometric and topological parameters of the knot. A reduced theory is developed, which predictively rationalizes the process.

Monday, March 2, 2015 11:15AM - 2:15PM — Session B45 DPOLY: Polymer Melts & Solutions I 216AB - Debra Audus, National Institute of Standards and Technology

11:15AM B45.00001 Domain Growth Kinetics in Stratifying Foam Films. YIRAN ZHANG, VIVEK SHARMA, Chemical Engineering, University of Illinois Chicago — Baking bread, brewing cappuccino, pouring beer, washing dishes, shaving, shampooing, whipping eggs and blowing bubbles all involve creation of aqueous foam films. Typical foam films consist of two surfactant-laden surfaces that are 5 nm – 10 micron apart. Sandwiched between these interfacial layers is a fluid that drains primarily under the influence of viscous and interfacial forces, including disjoining pressure. Interestingly, for certain low molecular weight surfactants, a layered ordering of micelles inside the foam films (thickness <100 nm) leads to a stepwise thinning phenomena called stratification. We experimentally elucidate the influence of these different driving forces, and confinement on drainage kinetics of horizontal stratifying foam films. Thinner, darker domains spontaneously grow within foam films. Quantitative characterization of domain growth visualized in a using Scheludko-type thin film cell and a theoretical model based on lubrication analysis, provide critical insights into hydrodynamics of thin foam films, and the strength and nature of surface forces, including supramolecular oscillatory structural forces.
11:27AM B45.00002 Atomic Simulations of Poly(N-isopropylacrylamide) Surfactants in Water, LAUREN J. ABBOTT, MARK J. STEVENS, Sandia National Laboratories — The amphiphilic polymer poly(N-isopropylacrylamide) (PNIPAM) displays a sharp phase transition at its LCST around 32 °C, which results from competing interactions of the hydrophobic and hydrophilic groups with water. This thermoresponsive behavior can be exploited in more complex architectures, such as block copolymers or surfactants, to provide responsive PNIPAM head groups. In these systems, however, changes to the hydrophobic/hydrophilic balance can alter the transition behavior. In this work, we perform atomistic simulations of PNIPAM-alkyl surfactants to study the temperature dependence of their structures. A single chain of the surfactant does not show temperature-responsive behavior. Instead, below and above the LCST of PNIPAM, the surfactant folds to bring the hydrophobic alkyl tail in contact with the PNIPAM backbone, shielding it from water. In addition to single chains, we explore the self-assembly of multiple surfactants into micelles and how the temperature-dependent behavior is changed. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

11:39AM B45.00003 Self-assembly of Giant Molecular Shape Amphiphiles in Solution, RONG WANG, SHIYING MA, Nanjing University — The self-assembly of giant molecular shape amphiphiles consisting of a hydrophilic head and one or more hydrophobic tails is investigated by dissipative particle dynamics. The morphology can transform from vesicles to worm-like cylinders and further to spheres by increasing the interaction parameter between the hydrophilic heads. The results are in agreement with the experimental observations. Through changing the interaction parameter between hydrophilic head and solvents, the length of hydrophobic tail and the size of hydrophilic head, the self-assembled aggregates exhibit a rich variety of morphological structures, such as, spheres, vesicles, worm-like cylinders, disk-like micelles and layered-rod-like micelles. Vesicles form for short hydrophobic tail, while disk-like micelles are taken shape for longer hydrophobic tail. As further increasing the diameter of hydrophilic head, large compound micelles are obtained for short hydrophobic tail, however layered-rod-like micelles form for longer tail. The simulation findings might be valuable for guiding the experimental studies and fascinating new possibility and applications in material science. This work was financially supported by NNSFC (21374041, 21207405), NBRPC (2010CB923303) and PCSIRT.

11:51AM B45.00004 Transition to Area-Dependent Dissipation in Droplet Spreading, KARI DALNOKI-VERESS, MARK ILTON, Department of Physics & Astronomy, McMaster University, Hamilton, Ontario, Canada, OLIVER BÄUMCHEN, Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077, Göttingen, Germany — We have studied the spreading dynamics of a liquid diblock copolymer in the pseudo-partial wetting regime, in which disordered droplets coexist with a wetting layer of the same liquid. Using optical microscopy, the relaxation time of the droplets is measured as they evolve towards an equilibrium contact angle. The relaxation is investigated as a function of the contact angle, droplet volume, and viscosity. In this unique system all three parameters can be systematically varied on the same sample and for both advancing and receding motion. The relaxation time of the droplets does not scale with the length of the contact line as is typically the case. Instead, the relaxation time depends on the contact area. We are able to describe the experiments with a model that assumes area-dependent dissipation with only two adjustable parameters.

12:03PM B45.00005 Patterning Polymer Films with Bidirectional Control of Marangoni Flow by Photochemically Manipulating Surface Tension, CHAE BIN KIM, DUSTIN JANES, SUNSHINE ZHOU, AUSTIN DU-LANEY, CHRISTOPHER ELLISON, University of Texas at Austin - McKetta Department of Chemical Engineering — Small variations in temperature or composition at a fluid interface, often spontaneously generated, can cause local changes in surface tension and promote dramatic movement of fluids through convective motion. This phenomenon, often referred as Marangoni convection, is typically experienced in everyday life as a macroscopic and seemingly stochastic phenomenon. One might imagine attempting to direct this process for reproducibly forming microscale and nanoscale patterns. While this might initially seem impractical, here we will report a photochemical strategy to harness the Marangoni convection as a versatile patterning method. Two photo-exposures with different irradiating wavelengths were applied to a solid, glassy styrene-acrylic copolymer thin film. Each photo-exposure imposes either a higher or lower surface energy in the light exposed regions without inducing topography on the flat film surface. Once this solid film is heated to a liquid state, however, bidirectional Marangoni-flows occur spontaneously from low-to-high surface tension regions.

12:15PM B45.00006 Coffee Stains from Drops with Receding Contact Lines1, JULIAN FREED-BROWN, University of Chicago — We present a framework for calculating the surface density profile of a coffee stain deposited by a drying drop with a receding contact line. For standard coffee stains, the fluid pins to the substrate, forces flow towards the exterior of the drop and deposits a thin, concentrated ring of particles. Unlike a pinned drop, a receding drop pushes fluid towards its interior and continuously deposits mass across its substrate as it evaporates. This gives rise to a new class of mountain-like morphologies that are not seen in the standard coffee ring effect but are reminiscent of recent experimental results. For a thin, circular drop with uniform evaporation, we calculate the surface density profile analytically and find that it diverges towards the center of the drop as $\rho \propto r^{-1/2}$, where $r$ is the distance from the center. We show that this divergence is softened due to solute interactions at the final stage of drying. Our framework can be extended numerically or analytically to investigate novel stain morphologies left by drying drops of different shapes and evaporation profiles.

12:27PM B45.00007 Supramolecular Structural Forces and Hydrodynamics of Stratifying Foam Films, VIVEK SHARMA, YIRAN ZHANG, SUBINUER YILIXIATI, Chemical Engineering, University of Illinois Chicago — Liquid foams are complex fluids, mostly formed by gas bubbles dispersed within a surfactant solution. The lifetime of foams depends critically on stability and drainage of thin film layers. Unlike a pinned drop, a receding drop pushes fluid towards its interior and continuously deposits mass across its substrate as it evaporates. This gives rise to a new class of mountain-like morphologies that are not seen in the standard coffee ring effect but are reminiscent of recent experimental results. For a thin, circular drop with uniform evaporation, we calculate the surface density profile analytically and find that it diverges towards the center of the drop as $\rho \propto r^{-1/2}$, where $r$ is the distance from the center. We show that this divergence is softened due to solute interactions at the final stage of drying. Our framework can be extended numerically or analytically to investigate novel stain morphologies left by drying drops of different shapes and evaporation profiles.

12:39PM B45.00008 Concentration Dependent Structure of Block Copolymer Solutions1, SOOHYUNG CHOI, Hongik University, FRANK S. BATES, TIMOTHY P. LODGE, University of Minnesota — Addition of solvent molecules into block copolymers can induce additional interactions between the solvent and both blocks, and therefore expands the range of accessible self-assembled morphologies. In particular, the distribution of solvent molecules plays a key role in determining the microstructure and its characteristic domain spacing. In this study, concentration dependent structures formed by poly(styrene-b-ethylene-alt-propylene) (PS-PEP) solution in squalane are investigated using small-angle X-ray scattering. This reveals that squalane is essentially completely segregated into the PEP domains. In addition, the conformation of the PS block changes from stretched to nearly fully relaxed (i.e., Gaussian conformation) as amounts of squalane increases.

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1 This work is part of a thesis project advised by Tom Witten. It was supported in part by the National Science Foundation’s MRSEC Program under Award Number DMR 0820054.
12:51PM B45.00009 Structure and flow properties of trilobic copolyelectrolyte hydrogels. SAMAN-VAYA SRIVASTAVA, MATTHEW TIRRELL, Univ of Chicago — Polyelectrolyte complexes (PEC) are dense, polymer-rich phases that form when oppositely charged polyelectrolyte chains spontaneously associate and phase separate in aqueous mediums. Bulk phase separation of the PECs can be evaded by combining one or both of the polyelectrolytes with a neutral polymer, thus engineering pathways for self-assembly of PEC based micelles and hydrogels with large-scale ordering of the nanoscale PEC domains. The PEC domains in these assemblies can encapsulate both hydrophobic and hydrophilic therapeutics and thus have tremendous potential in drug delivery, diagnostic and tissue engineering applications. This study will present insights on the equilibrium structure and self-assembly kinetics of PEC hybrid hydrogels through detailed rheology studies of self-assembled materials comprising of functionalized polylallyl glycidyl ethers (PAGE) connected to either single poly(ethylene glycol) (PEG) chain to form diblock copolymers or as functionalized end-groups on a trilobic copolymer with a PEG midblock. The effect of key parameters such as polymer concentration, polymer block lengths, salt, ionic strength, and degree of charge mismatch on the equilibrium material properties will be discussed, with a special emphasis on the temporal evolution of flow properties, and will lead to comparisons with the rheology models for associating polymers. Complementary studies with extensive static and dynamic light, X-ray and neutron scattering investigations will also be presented, thus providing a comprehensive structural description of these materials.

1:03PM B45.00010 Network structures of trilobic copolymer by two-step phase separation. MIKIHITO TAKENAKA, Kyotou University, RIKEN, AYANO INOUE, HIROKAZU HASEGAWA, Kyoto University — We investigated network structures of poly(styrene-b-polyisoprene-polydimethylsiloxiane (PS-PI-PDMS) trilobic copolymer formed solvent cast processes. The obtained morphologies were observed by 3D-TEM and SAXS. Two-step phase transition occurs during the self-assembling processes of PS-PI-PDMS in solvent cast processes, resulting in the morphologies such as OBDD and P-surface, which is not formed in the equilibrium state of trilobic copolymer.

1:15PM B45.00011 The Amphiphilic Character of Cellulose Molecules in True Solution in Solvent Mixtures Containing Ionic Liquid and its Utilization in Emulsification. SOFIA NAPSO, YACHIN COHEN, DMITRY REIN, RAFAIL KHALFAN, Technion, Israel, NOEMI SZEKELY, Forschungszentrum Juelich, Germany — Cellulose is the most abundant renewable material in nature that is utilized as a raw material for manufacturing of synthetic products. Although it is not soluble in common solvents, there is significant interest in the use of solvent mixtures containing ionic liquids (IL) and polar organic solvents for cellulose dissolution. We present evidence for true molecular dissolution of cellulose in binary mixtures of common polar organic solvents with an ionic liquid, using cryogenic transmission electron microscopy, small-angle neutron-, x-ray- and static light scattering. In particular, the measured low values of the molecular, gyration radius and persistence length indicate the absence of significant aggregation of the dissolved chains. We conjecture that the dissolved cellulose chains are amphiphilic. This can be inferred from the facile fabrication of cellulose-encapsulated colloidal oil-in-water or water-in-oil dispersions. This may be done by mixing water, oil and cellulose solution in an ionic liquid. A more practical alternative is to form first a hydrogel from the cellulose/ionic liquid solution by coagulation with water and applying it to sonicated water/oil or oil/water mixtures. Apparently the dissolution/ regeneration process affords higher mobility to the cellulose molecules so an encapsulation coating can be formed at the water-oil interface.

1:27PM B45.00012 The Effect of Illumination on the Gelation Process of Optoelectronic Materials. BRIAN MORGAN, MARK DADMUN, University of Tennessee — A tremendous amount of insight into the functionality of conjugated polymers in optoelectronic devices can be gained by the study of these materials as they progress through the gelation process. The nature of the percolated network structures formed directly affects exciton transport and device efficiency, thus precise knowledge of the evolution of structures provides crucial information towards improving device efficiency via processing techniques. Additionally, select optoelectronic polymers have exhibited reversibly altered physical properties such as viscosity upon exposure to white light, potentially indicative of temporary conformation changes. We have conducted a series of small angle neutron scattering experiments to probe the temperature-driven gelation process of the conjugated photoactive polymer poly(3-hexylthiophene-2,5-diyl) (P3HT) in both the presence and complete absence of white light. Fitting the resultant data indicates the creation and steady growth of cylindrical aggregates formed by the agglomeration of free chain P3HT as the growth process. Furthermore, clear differences between illuminated and non-illuminated gels are observed across multiple length scales, pointing towards an optically-induced variation in the gelation process.

1:39PM B45.00013 Effect of Water Concentration on the Molecular Structure of Polyacrylate Gels. SRIAMVIGNESH MANI, FARIDIN KHABAZ, RAJESH KHARE, Texas Tech Univ — Recent studies have suggested pervaporation to be an efficient alternative method of alcohol recovery compared to distillation based separation processes. The ability to tune the hydrophobic/hydrophilic character makes polyacrylate gels attractive candidate materials for separating water-alcohol mixture by pervaporation. Experimentally, it is observed that the amount of water absorbed in the gel i.e. the degree of swelling of the gel shows a large variation with polymer chemistry. Relatively few studies exist highlighting the effects of water concentration on the membrane separation efficiency which in turn is directly related to the internal molecular structure of the water rich membranes. In this regard, an all-atom molecular dynamics (MD) simulation is employed to study water structure in polyacrylate gels. As a first step, polyacrylate copolymer systems with varying degree of hydrophobicity are prepared using the simulated annealing polymerization technique. Atomistic structures of gels containing different amounts of water are also prepared. Effect of water content on the acrylate-water system microstructure is determined by characterizing the packing of water molecules as well as the hydrogen bonding in these systems. In addition, the change in dynamics of water molecules due to the interactions with polymer is captured by monitoring the auto-correlation function of their dipole vector.

1:51PM B45.00014 Polymer-Carbon Nanotube Composite Films at the Oil/Water Interface: Assembly and Properties. DAVID HOAGLAND, TAO FENG, THOMAS P. RUSSELL, Univ of Massachusetts Amherst — Efficient carbon nanotube assembly at the oil/water interface was achieved by dissolving cationic polymers in the oil phase and oxidized nanotubes in the water phase, the two components spontaneously forming salt bridges to produce a composite interfacial film of nanoscopic thickness. As seen by pendant drop tensiometry, parameters such as carbon nanotube and polymer concentration, pH, polymer molecular weight, and degree of nanotube oxidation all affect assembly strongly, with measured trends to be described and explained. The frequency-dependent elastic and viscous moduli of films in dilution were characterized by interfacial pendant drop rheology. Structural (fast, minutes) and adsorption/desorption (slow, tens of minutes) relaxations were both noted, and at frequencies intermediate to the two, almost insensitive to assembly parameters, the films displayed expected behaviors for 2D critical gels, i.e., at the crossover between fluid and solid. Tan(delta) was frequency-independent over one to two decades of frequency, and the modulus of linear stress relaxation was a power law in time. Films wrinkled by larger (nonlinear) strains recovered over the structural relaxation time.

1:51PM B45.00014 Polymer-Carbon Nanotube Composite Films at the Oil/Water Interface: Assembly and Properties. DAVID HOAGLAND, TAO FENG, THOMAS P. RUSSELL, Univ of Massachusetts Amherst — Efficient carbon nanotube assembly at the oil/water interface was achieved by dissolving cationic polymers in the oil phase and oxidized nanotubes in the water phase, the two components spontaneously forming salt bridges to produce a composite interfacial film of nanoscopic thickness. As seen by pendant drop tensiometry, parameters such as carbon nanotube and polymer concentration, pH, polymer molecular weight, and degree of nanotube oxidation all affect assembly strongly, with measured trends to be described and explained. The frequency-dependent elastic and viscous moduli of films in dilution were characterized by interfacial pendant drop rheology. Structural (fast, minutes) and adsorption/desorption (slow, tens of minutes) relaxations were both noted, and at frequencies intermediate to the two, almost insensitive to assembly parameters, the films displayed expected behaviors for 2D critical gels, i.e., at the crossover between fluid and solid. Tan(delta) was frequency-independent over one to two decades of frequency, and the modulus of linear stress relaxation was a power law in time. Films wrinkled by larger (nonlinear) strains recovered over the structural relaxation time.

1Support: NSF-sponsored UMass MRSEC and the US DoE Office of Basic Energy Science through contract DE-FG02-04ER46126


CHRISTOPHER JARZYNSKI, Univ of Maryland-College Park — Physical systems, including biological organisms, are capable of gathering information about their surroundings and acting in response to that information. When two physical systems interact with one another, each one affects and is affected by the other. It is often convenient to view such interactions in the context of measurement and feedback, with one system observing and exercising control over the other. I will discuss fundamental limits that thermodynamics places on such processes, when the systems are small and thermal fluctuations play an important role.

This research is supported by the U. S. Army Research Office under contract number W911NF-13-1-0399.

HONG QIAN, University of Washington, Department of Applied Mathematics — Adenosine triphosphate (ATP) molecule is used in living cells as a universal “energy currency.” The Gibbs free energy liberated from hydrolysis reaction of ATP to ADP + Pi is used for (a) biosynthesis, (b) ionic and neutral molecular pumping, and (c) mechanical movement. They are known collectively as the three major energy sinks at the cellular level. Using biochemical activities of various enzymes, a cell carries out information processing, known as signal transduction. Essentially all signal transduction reactions also require ATP (or GTP) hydrolysis. In the past, such energy dissipative reactions are considered as “futile.” However, it is clear that the free energy derived from a futile cycle is used to correct errors in biomolecular recognition, improve robustness in cell development, overcome Boltzmann’s equilibrium law of probability, and drive Maxwell’s demons (one notes that Gibbs’ chemical potential is a thermodynamic force without mechanical interpretation). The free energy involved in processing information will be explained in terms of stochastic entropy production — the central concept in irreversible and nonequilibrium steady-state (NESS) thermodynamics.

12:27PM B46.00003 A synthetic playground for non-equilibrium error correction and information processing , ARVIND MURUGAN, Harvard — Biological proofreading mechanisms can lower error rates well below Boltzmann statistics by consuming free energy. By abstracting the principles behind these biochemical mechanisms, we discuss the central ingredients needed for any complex reaction network to perform error correction and the inherent energy-error tradeoffs. We propose that such abstract principles can be implemented and tested in synthetic systems using DNA strand displacement reactions. Such DNA circuits can mimic biochemical models of proofreading because of two central features: 1. exquisite control over reaction kinetics, 2. a DNA analog of ATP hydrolysis. Indeed, such DNA circuits may be used to mimic any non-equilibrium information processing scheme seen in biochemistry, such as adaption and ultrasmall sensitivity in addition to error correction. We discuss the conceptual and practical benefits from having a well-controlled synthetic playground for non-equilibrium ideas.

1:03PM B46.00004 Experimental Demonstration of Information-to-Energy Conversion in Small Fluctuating Systems , MASAKI SANO, University of Tokyo — What is the relation between information and thermodynamics has been a long standing question in science. In 1867, J.C. Maxwell proposed a Gedanken experiment to demonstrate violation of the second law of thermodynamics by assuming a small creature called Maxwell’s demon which separates hot atoms from cold atoms. In 1929, L. Szilard formulated the idea of Maxwell for a more tractable setup in which a single particle is thermally moving in a box immersed in a heat bath. He succeeded to relate information entropy and the second law of thermodynamics in this Gedanken experiment. It has led to long and intense debates on the relation among thermodynamics, information, observation, and even computation until it was clarified recently. Nevertheless, experimental realization of information-energy-conversion has been elusive. Recently, we succeeded to demonstrate the information-energy-conversion by observing Brownian motion of colloidal particles and controlling them. We introduced a feedback control protocol based on the information of Brownian particle by electric fields and found that the particle rotates against the torque exerted by an external electric field and obtains free energy larger than the amount of work performed on it. By measuring detailed process, validity of a new nonequilibrium equality concerning the feedback control has been shown. Efficiency of information-energy conversion was evaluated in this feedback system. Moreover, I will discuss on possible generalization of this concept to information processing in cell chemotaxis.

This research is supported by the U. S. Army Research Office under contract number W911NF-13-1-0399.

1:39PM B46.00005 ABSTRACT WITHDRAWN —
A computational investigation of the role of behavioral heterogeneities on cell cluster motion. KATHERINE COPENHAGEN, Unv of California - Merced, NIR GOV, Weizmann Institute, AJAY GOPINATHAN, Univ of California - Merced — Collective motion of cells is a common occurrence in many biological systems, including tissue development, repair, and tumor formation. Recent experiments have shown that malignant B and T lymphocytes form clusters in a chemical gradient of CCL19 which display three different phases: translational, rotational, and random. Could these phases be due to interactions between cells as well as chemotaxis of individuals? If so what types of local interactions can lead to the three phases seen in experiment? We model cell clusters with a continuous two dimensional agent based model. To form a single cell cluster, which displays all three of the phases described above, cells interact with one another through a Lennard-Jones collision avoidance and cohesion interaction, and a long range spring interaction to prevent fracture. By changing the behaviors of individual cells depending on the number of cells they are contacting, we are able to create clusters that occupy these phases with varying likelihood. Our results show that heterogeneous behaviors of individuals based on local environment can lead to novel phases seen in experiments.

Optimal Intermittent Reorientation in Insect Navigation. ORIT PELEG, LAKSHMINARAYANAN MAHADEVAN, SEAS, Harvard University, APPLIED MATH LAB TEAM — The process of navigation is often accompanied by several cognitive demanding activities, such as motor control, locomotion planning, and multi-sensory acquisition and integration. Organisms with limited cognitive resources must therefore multitask and develop optimal schemes to dynamically allocate resources to the different tasks. An extreme example of task alternations during navigation is the hallmark of ball rolling dung beetles. The beetles need to roll their dung-ball along a straight path away from the dung pile where intense competition occurs [1]. Before initiating a roll, dung beetles climb on top of the ball and rotate about their vertical axis. This action serves as an orientation mechanism that allows them to set an initial bearing, and to regain this bearing if they experience an unintentional disturbance along the way [2]. We developed a model inspired by the beetle’s navigational scheme, where an agent performs a random walk intermittent by reorientation events, in which its heading direction is corrected. We show that the resultant paths are a characteristic of correlated diffusion in short time scale, and biased diffusion in the long time scale [3]. We identify optimal alternation schemes and characterize their robustness upon introducing noisy sensory acquisition and rough environmental conditions.

Self-righting behavior of cockroaches. CHEN LI, University of California, Berkeley, TONI WOHLR, University of Jena, HAN LAM, ROBERT FULL, University of California, Berkeley — Small insects must be able to right themselves from an upright-down orientation to survive. Previous studies described diverse self-righting strategies in insects. Here, we compare the self-righting behaviors in three cockroach species on a flat, rigid ground to begin to reveal what governs the choice of dominant behaviors. All species self-righted successfully (75 +/− 11 % probability) and quickly (as low as 140 ms and typically within 2 s). The smallest winged American cockroach, which has the most elongate, least flattened body, and longest legs, primarily pushed legs against the ground to roll its body to the side to self-right (relative frequency = 93%). The largest wingless Madagascar hissing cockroach with the shortest legs primarily (84%) hyperextended body to roll to the side and then rubbed its legs on the ground to self-right. The intermediate winged discoid cockroach, which has the least elongate, most flattened body, more often (57%) abducted wings and flexed body to raise center of mass and reduce ground contact and rotated about the wing edges to self-right. We hypothesize that, given morphological and physiological constraints, the gravitational potential energy landscape resulting from the animals’ body-appendage-ground interaction governs their dominant behaviors. Our study provides inspiration for robotics, as many current terrestrial robots have rigid, cuboidal bodies which hinder self-righting.

Tiger beetle’s pursuit of prey depends on distance. ROBERT NOEST, JANE WANG, Cornell University — Tiger beetles are fast predators capable of chasing prey under closed-loop visual guidance. We investigated their control system using high-speed digital recordings of beetles chasing a moving prey dummy in a laboratory arena. Analysis reveals that the beetle uses a proportional control law in which the angular position of the prey relative to the beetle’s body axis drives the beetle’s angular velocity with a delay of about 26 ms. The system gain is shown to depend on the beetle-prey distance in a pattern indicating three hunting phases over the observed distance domain. We show that to explain this behavior the tiger beetle must be capable of visually determining the distance to its target and using that to adapt the gain in its proportional control law. We will end with a discussion on the possible methods for distance detection by the tiger beetle and focus on two of them. Motion parallax, using the natural head sway induced by the walking gait of the tiger beetle, is shown to have insufficient distance range. However elevation in the field of vision, using the angle with respect to the horizon at which a target is observed, has a much larger distance range and is a prime candidate for the mechanism of visual distance detection in the tiger beetle.

Hierarchy and predictability in spontaneous behavior. GORDON BERMAN, WILLIAM BIALEK, JOSHUA SHAEVITZ, Princeton University — Animals perform a complex array of behaviors, from changes in body posture to vocalizations to other dynamic outputs. Far from being a disordered collection of actions, however, there is thought to be an intrinsic structure to the set of behaviors and their temporal organization. This structure has often been hypothesized to be hierarchical, with certain behaviors grouped together into modules that interact with other modules at time scales that are long with respect to that of an individual behavior. There have been few measurements, however, showing that a particular animal’s behavioral repertoire is organized hierarchically. This has largely resulted from an inability to measure the entirety of an animal’s behavioral repertoire or even to define precisely what a “behavior” is. In this talk, I will apply our novel method for mapping the behavioral space of animals to videos of freely-behaving fruit flies (D. melanogaster), showing that the organisms’ behavioral repertoire consists of a hierarchically-organized set of stereotyped behaviors. This hierarchical patterning results in the emergence of long time scales of memory in the system, providing insight into the mechanisms of behavioral control and patterning.

Environmental statistics and optimal regulation. DAVID SIVAK, Simon Fraser University, MATT THOMSON, University of California, San Francisco — The precision with which an organism can detect its environment, and the timescale for and statistics of environmental change, will affect the suitability of different strategies for regulating protein levels in response to environmental inputs. We propose a general framework—here applied to the enzymatic regulation of metabolism in response to changing nutrient concentrations—to predict the optimal regulatory strategy given the statistics of fluctuations in the environment and measurement apparatus, and the costs associated with enzyme production. We find: (i) relative convexity of enzyme expression cost and benefit influences the fitness of thresholding or graded responses; (ii) intermediate levels of measurement uncertainty call for a sophisticated Bayesian decision rule; and (iii) in dynamic contexts, intermediate levels of uncertainty call for retaining memory of the past. Statistical properties of the environment, such as variability and correlation times, set optimal biochemical parameters, such as thresholds and decay rates in signaling pathways. Our framework provides a theoretical basis for interpreting molecular signal processing algorithms and a classification scheme that organizes known regulatory strategies and may help conceptualize heretofore unknown ones.
12:27PM B47.00007 Quantification of Behavior During Drosophila Courtship. UGNE KLIABITE, GORDON BERMAN, Princeton University, JESSICA CANDE, DAVID STERN, Janelia Research Campus, HHMI, JOSHUA SHAEVITZ, Princeton University — Fruit flies display varying and species-specific behavioral repertoires, especially during highly stereotyped activities such as courtship. Interspecies differences in specific behaviors may arise from physical differences, e.g. a different type or speed of appendage motion, or higher-order changes such as differences in the frequencies of particular actions. One example is the use of wing-rowing by D. santomea males that is rarely, but sometimes, seen during D. yakuba courtship. We wish to study the complex interaction of two individuals during courtship. We extensively worked on mapping the postural dynamics of individual flies to analyze the simultaneous mapping of male and female behavior for hundreds of hours of courtship video data. Using this algorithm, we compare courtship behavior of dozens of targeted introgressions between D. yakuba and D. santomea to probe for differences in courtship and to determine which regions of the genome are responsible for this diversity.

12:39PM B47.00008 Intrinsic fluctuations and driven response of insect swarms, RUI NI, Yale University, JAMES G. PUCKETT, Gettysburg College, ERIC R. DUFRESNE, NICHOLAS T. OUELLETTE, Yale University — Much of our understanding of collective behavior in social animals comes from passive observations of animal groups. To understand the group dynamics fully, however, we must also characterize the response of animal aggregations to disturbances. Using three-dimensional particle tracking, we study both the intrinsic fluctuations of laboratory swarms of the non-biting midge Chironomus riparius and the response of the swarms to controlled external perturbations: the amplitude-modulated sound of male midge wingbeats. Although these perturbations have an insignificant effect on the behavior of individuals, we find that they can have a strong impact on the collective movement. Intriguingly, the response of the swarm is similar reminiscent to that of a passive equilibrium system to an external driving force, with microscopic fluctuations underlying combining to produce a macroscopic linear response over a wide range of driving frequencies.

12:51PM B47.00009 Measuring Whole-Brain Neural Dynamics and Behavior of Freely-Moving C. elegans, FREDERICK SHIPLEY, JEFFREY NGUYEN, GEORGE PLUMMER, JOSHUA SHAEVITZ, ANDREW LEIFER, Princeton University — Bridging the gap between an organism’s neural dynamics and its ultimate behavior is the fundamental goal of neuroscience. Previously, to probe neural dynamics, we have been limited to measuring from a limited number of neurons, whether by electrode or optogenetic measurements. Here we present an instrument to simultaneously monitor neural activity from every neuron in a freely moving Caenorhabditis elegans’ head, while recording behavior at the same time. Previously, whole-brain imaging has been demonstrated in C. elegans, but only in restrained and anesthetized animals (1). For studying neural coding of behavior it is crucial to study neural activity in freely behaving animals. Neural activity is recorded optically from cells expressing a calcium indicator, GCaMP6. Real time computer vision tracks the worm’s position in x-y, while a piezo stage sweeps through the brain in z, yielding five brain-volumes per second. Behavior is recorded under infrared, dark-field imaging. This tool will allow us to directly correlate neural activity with behavior and we will present progress toward this goal.


1Thank you to the Simons Foundation and Princeton University for supporting this research.

1:03PM B47.00010 Modulation of orthogonal body wave enables high maneuverability in sidewinding locomotion, HENRY ASTLEY, Georgia Institute of Technology, CHAOHUI GONG, MATT TRAVERS, Carnegie Mellon University, MIGUEL SERRANO, PATRICIO VELA, Georgia Institute of Technology, HOWIE CHOSEST, Carnegie Mellon University, JOSEPH MENDELSON III, DAVID HU, DANIEL GOLDMAN, Georgia Institute of Technology — To simplify control of high degree of freedom bodies, organisms may target a set of simple shape changes (a “template”). Recent work has revealed that the locomotion of sidewinder rattlesnakes can be described by a combination of horizontal and vertical body waves with a phase difference of ±π/2, representing a possible control template. These animals display high maneuverability which we hypothesize emerges from their ability to independently modulate these waves. Snakes used two distinct turning methods which we term differential turning (24° turn per cycle) and reversal turning (90°). Kinematic data suggested that during differential turning the animals imposed an amplitude modulation in the horizontal wave while in reversal turning they shifted the phase of the vertical wave by π. We tested these mechanisms in the robot, generating differential and reversal turning. Further manipulations of the two-wave system revealed a third turning mode, “frequency turning,” not observed in biological snakes which allowed the robot to execute large (127°) in-place turns. The two-wave system enables unprecedented maneuverability of high degree-of-freedom systems, revealing a practical benefits of the search for control templates.

1Zoo Atlanta

1:15PM B47.00011 Building spatially-structured biofilms with single-cell control using laser trapping, CHRISTOPHER RODENSEY, JAIME HUTCHISON, KARISHMA KAUSHIK, HENRY LE, DANIEL HURWITZ, Univ of Texas, Austin, YA-SUHIKO IRIE, Univ of Bath, VERNITA GORDON, Univ of Texas, Austin — Biofilms are sessile communities of microbes adhered to each other and to an interface. Biofilm infections are notoriously difficult to eradicate, and this arises in part from phenotypic changes due to the spatial structure of the biofilm. Spatial structure controls the microenvironment and intercellular associations, which in turn controls gene expression, virulence, and antibiotic resistance. There are few tools available for elucidating the role of spatial structure in biofilms. We present a method for controlling the positions of bacteria on a surface using optical trapping without impinging cell viability. Initial positions propagate into the developing biofilm, creating spatial structure. The native growth, motility, and surface adhesion of positioned cells are preserved, as shown for model organisms Pseudomonas aeruginosa and Staphylococcus aureus. We demonstrate statistically-significant effects of spatial structure on the growth of monoculture P. aeruginosa biofilms and for co-culture biofilms of P. aeruginosa and S. aureus. Because the laser trap we use is very basic and the other equipment required is inexpensive and standard, we believe that our technique will be a widely-useful tool for biological and physical collaborators at many types of institutions.

1:27PM B47.00012 Legless locomotion in lattices, PERRIN SCHIEBEL, Georgia Institute of Technology, JIN DAI, CHAOHUI GONG, Carnegie-Mellon University, MIGUEL M. SERRANO, Georgia Institute of Technology, JOSEPH R. MENDELSON III, Zoo Atlanta, HOWIE CHOSEST, Carnegie-Mellon University, DANIEL I. GOLDMAN, Georgia Institute of Technology — By propagating waves from head to tail, limbless organisms like snakes can traverse terrain composed of rocks, foliage, soil and sand. Previous research elucidated how rigid obstacles influence snake locomotion by studying a model terrain—symmetric lattices of pegs placed in hard ground. We want to understand how different substrate-body interaction modes affect performance in desert-adapted snakes during transit of substrates composed of both rigid obstacles and granular media (GM). We tested Chionactis occipitalis, the Mojave shovel-nosed snake, in two laboratory treatments: lattices of 0.64cm diameter obstacles arrayed on both a hard, slick substrate and in a GM of ~0.3mm diameter glass particles. For all lattice spacings, d, speed through the hard ground lattices was less than that in GM lattices. However, maximal undulation efficiencies $u_\eta$ (number of body lengths advanced per undulation cycle) in both treatments were comparable when $d$ was intermediate. For other $d$, $u_\eta$ was lower than this maximum in hard ground lattices, while on GM, $u_\eta$ was insensitive to $d$. To systematically explore such locomotion, we tested a physical robot model of the snake; performance depended sensitively on base substrate, $d$ and body wave parameters.
1:39PM B47.00013 Human pair walking behavior: evaluation of cooperation strategies. ULRICH DOBRAMYS, University of Oxford, KATARINA BODOVÁ, IST Austria, RICHARD KOLLAR, Comenius University Bratislava, RADEK ERBAN, University of Oxford — Human walkers are notoriously poor at keeping a direction without external cues: Experimental work by Souman et al. with blindfolded subjects told to walk in a straight line revealed intriguing circular and spiraling trajectories, which can be approximated by a stochastic process. In this work, motivated by pair walking experiments by Miglierini et al., we introduce an analysis of various strategies employed by a pair of blindfolded walkers, who are communicating via auditory cues, to maximize their efficiency at walking straight. To this end, we characterize pairs of strategies such as free walking, side-by-side walking and unconditional following from data generated by robot pair walking experiments (using computer vision techniques) and numerical simulations. We extract the mean exit distances of walker pairs from a corridor with finite width to construct phase portraits of the walking performance. We find intriguing cooperative effects leading to non-trivial enhancements of the efficiency at walking straight. ¹

¹The research leading to these results has received funding from the European Research Council under the European Community’s Seventh Framework Programme (FP7/2007-2013) / ERC grant agreement No. 239870; and from the Royal Society through a Research Grant.

1:51PM B47.00014 Pili-mediated Interactions between Neisseria Gonorrhoeae Bacteria are the Driving Mechanism of Microcolony Merging. WOLFRAM POENISCH, CHRISTOPH WEBER, Max Planck Institute for the Physics of Complex Systems, KHALED ALZURQA, HADI NASROLLAHI, NICOLAS BIAIS, Brooklyn College, NY, VASILY ZABURDAEV, Max Planck Institute for the Physics of Complex Systems, COLLECTIVE DYNAMICS OF CELLS TEAM, MECHANO-MICRO-BIOLOGY LAB TEAM — During the early infection with Neisseria gonorrhoeae the bacteria form microcolonies consisting of a few hundreds to a few thousands of cells. The formation of colonies is mediated by type IV pili, thin and long filaments that are also involved in the motion of single cells over a substrate. A related process causes attractive cell-cell-interactions. While the motion of single cells has been extensively studied during the past years, the physical principles driving the growth of these colonies are poorly understood. One key mechanism of colony growth is coalescence of smaller colonies. Therefore we experimentally examine the process of merging of two Neisseria gonorrhoeae colonies. We develop a theoretical microscopic model of single cells interacting solely by their pili. The experimental data and the results obtained from our model are in excellent quantitative agreement. We observe a fast initial approach of the two merging colonies within a few minutes, that is followed by a slow relaxation of the colony shape with a characteristic time of several hours. These findings suggest that pili-mediated interactions are the primary driving mechanism of the microcolony merging process.

2:03PM B47.00015 The growth and form of plant shoots. RAGHUNATH CHELAKKOT, SEAS, Harvard University, L. MAHADEVAN, SEAS. Department of organismic and evolutionary biology, Harvard university — Growing plant stems and shoots exhibit a variety of shapes that embody growth in response to various stimuli. We provide a quantitative biophysical theory for these shapes by accounting for the inherent observed passive and active effects: (i) the passive elastic deflection of the shoot due to its own weight, and (ii) the active controllable growth response of the shoot in its orientation relative to gravity, and (iii) proprioception, the shoot’s growth response to its own observable shape, which is itself determined by its elasticity and weight. A morphospace diagram in terms of two dimensionless parameters representing a scaled local active gravitropic sensitivity, and a scaled passive elastic sag shows how a variety of observed transient and steady morphologies with effective positive, negative and oscillatory gravitropic behaviors arise in a sentient growing filament naturally, without the need for ad-hoc complex spatio-temporal control strategies.


11:15AM B48.00001 ABSTRACT WITHDRAWN –

11:27AM B48.00002 Coarsening of protein clusters on subcellular drops exhibits strong and sudden size selectivity. AIDAN BROWN, ANDREW RUTENBERG, Dalhousie University — Autophagy is an important process for the degradation of cellular components, with receptor proteins targeting substrates to downstream autophagy machinery. An important question is how receptor protein interactions lead to their selective accumulation on autophagy substrates. Receptor proteins have recently been observed in clusters, raising the possibility that clustering could affect autophagy selectivity. We investigate the clustering dynamics of the autophagy receptor protein NBR1. In addition to standard receptor protein domains, NBR1 has a “J” domain that anchors it to membranes, and a coiled-coil domain that enhances self-interaction. We model coarsening clusters of NBR1 on the surfaces of a polydisperse collection of drops, representing organelles. Despite the disconnected nature of the drop surfaces, we recover dynamical scaling of cluster sizes. Significantly, we find that at a well-defined time after coarsening begins, clusters evaporate from smaller drops and grow on larger drops. Thus, coarsening-driven size selection will localize protein clusters to larger substrates, leaving smaller substrates without clusters. This provides a possible physical mechanism for autophagy selectivity, and can explain reports of size selection during peroxisome degradation.

11:39AM B48.00003 Mechanism of bacterial membrane poration by Antimicrobial Peptides. ANKITA ARORA, ABHIJIT MISHRA, Materials Science & Engineering, Indian Institute of Technology, Gandhinagar, India — Bacterial resistance to conventional antibiotics is a major health concern. Antimicrobial peptides (AMPs), an important component of mammalian immune system, are thought to utilize non-specific interactions to target common features on the outer membranes of pathogens; hence development of resistance to such AMPs may be less pronounced. Most AMPs are amphiphilic and cationic in nature. Most AMPs form pores in the bacterial membranes causing them to lyse, however, the exact mechanism is unknown. Here, we study the AMP CHRG01 (KSTGRRKSSRRKK), derived from human β defensin 3 (hBD3) with all Cysteine residues substituted with Serine. Circular Dichroism studies indicate that CHRG01 shows helicity and there is change in helicity as it interacts with the lipid membrane. The AMP was effective against different species of bacterial cells observed by SEM and AFM indicates AMP action by pore formation. Confocal microscopy studies on giant vesicles incubated with AMP confirm poration. The effect of this AMP on model bacterial membranes is characterized using Small Angle X-ray scattering and Fluorescence spectroscopy to elucidate the mechanism behind antimicrobial activity.
11:51 AM B48.00004 Dissecting EB1-microtubule interactions from every direction: using single-molecule visualization and static and dynamic binding measurements , BENJAMIN LOPEZ, Univ of California - Santa Barbara — EB1 is an important microtubule associating protein (MAP) that acts as a master coordinator of protein activity at the growing plus-end of the microtubule. We can recapitulate the plus-end binding behavior of EB1 along the entire length of a static microtubule using microtubules polymerized in the presence of the nonhydrolyzable GTP analogs GMPCPP and GTP\(^\gamma\)S instead of GTP. Through the use of single-molecule TIRF imaging we find that EB1 is highly dynamic (with a sub-second characteristic binding lifetime) and continuously diffusive while bound to the microtubule. We measure the diffusion coefficient, \(D\), through linear fitting to mean-squared displacement of individually labeled proteins, and the binding lifetime, \(\tau\), by fitting a single exponential decay to the probability distribution of trajectory lifetimes. In agreement with measurements of other diffusive MAPs, we find that \(D\) increases and \(\tau\) decreases with increasing ionic strength. We also find that \(D\) is sensitive to the choice of GTP analog: EB1 proteins bound to GTP\(^\gamma\)S polymerized microtubules have a \(D\) half of that found with GMPCPP polymerized microtubules. To compare these single-molecule measurements to the bulk binding behavior of EB1, we use TIRF imaging to measure the intensity of microtubules coated with EB1-GFP as a function of EB1 concentration. We find that EB1 binding is cooperative and the cooperative nature of EB1-microtubule binding leads to a decrease in \(D\) with increasing EB1 concentration. Interestingly, we also find an increase in \(\tau\) at high EB1 concentrations, consistent with attractive EB1-microtubule interactions driving the cooperativity. To further understand the cooperativity we estimate the interaction energy by measuring the association and dissociation rates (\(k_{\text{on}}\) and \(k_{\text{off}}\) respectively) at different concentrations of EB1.

12:27PM B48.00005 A Compete-and-Survive Mechanism Explains the Single FtsZ-Ring Formation , GANHUI LIM, LI-PING XIONG, George Washington University — Cytokinesis is a critical step in cell reproduction. In bacterial cells, this process is mediated by the cytoskeletal Z ring which is assembled from FtsZ filaments that are “anchored” to the cell membrane through ZipA/FtsA molecules. Fluorescence Recovery after Photobleaching experiments have shown that the Z ring is highly dynamic, with recovery half time of \(\sim 30\) seconds, yet has a rather persistent overall structure. But it is unclear how a single narrow dynamic Z ring emerges from a big pool of cytoplasmatic FtsZ molecules. Here, we developed a rule-based molecular model with FtsZ and ZipA/FtsA molecules, by explicitly considering the elementary assembling events of molecules and their diffusion. Our model can not only efficiently reproduce the Z ring but also obtained experimentally observed statistical properties, but provide a convenient way to combine biochemical dynamic and physical assembling processes within the same spatiotemporal modeling framework. In agreement with experiments, we showed that the spontaneous self-assembling process relies on the molecular “stoichiometry”: either high or low FtsZ to ZipA/FtsA ratios would result in multiple Z rings or aggregated bundles. Our in silico FRAP experiment further yields a recovery half time comparable to experimental results. These results indicate that the rapid turnover dynamics prevents the FtsZ molecules from being sequestered by small FtsZ bundles dispersed over the membrane, allowing single Z ring to emerge and mature. This dynamic colonolization mechanism provides cells a simple way for spatial regulation.

12:39PM B48.00006 Characterizing the statistical properties of protein surfaces , JI HYUN BAK, ANNE-FLORENCE BITTOL, WILLIAM BIALEK, Princeton University — Proteins and their interactions form the body of the signaling transduction pathway in many living systems. In order to ensure the accuracy as well as the specificity of signaling, it is crucial that proteins recognize their correct interaction partners. How difficult, then, is it for a protein to discriminate its correct interaction partner(s) from the possibly large set of other proteins it may encounter in the cell? An important ingredient of recognition is shape complementarity. The ensemble of protein shapes should be constrained by the need for maintaining functional interactions while avoiding spurious ones. To address this aspect of protein recognition, we consider the ensemble of proteins in terms of their three-dimensional shapes, more precisely in terms of their solvent-excluded surfaces. We take into account all high-resolution structures from E.coli non-DNA-binding cytoplasmic proteins that can be retrieved from the Protein Data Bank. We aim to characterize the statistical properties of the ensemble of protein surfaces, including the dimensionality of the space of surfaces.

12:51PM B48.00007 Microfluidic free-flow electrophoresis for the discovery and characterisation of calmodulin binding partners , THERESE HERLING, University of Cambridge, SARA LINSE, Lund University and University of Cambridge, TUOMAS KNOWLES, University of Cambridge — Non-covalent and transient protein-ligand interactions are integral to cellular function and malfunction. Key steps in signalling and regulatory pathways rely on reversible non-covalent protein–protein binding or ion chelation. Here we present a microfluidic free-flow electrophoretic method for detecting and characterising protein-ligand interactions in solution. We apply this method to probe the binding of calmodulin, a central protein to calcium signalling pathways. In this study we characterise the specific binding of calmodulin to phosphorylase kinase, a known target, and create a kinase, which we identify as a putative binding partner through high-throughput screening and surface plasmon resonance experiments. We verify the interaction between calmodulin and creatine kinase in solution using free-flow electrophoresis and investigate the effect of calcium and sodium chloride on the calmodulin-ligand binding affinity in free solution without the presence of a potentially interfering surface. Our results demonstrate the general applicability of quantitative microfluidic electrophoresis to characterise binding equilibria between biomolecules in solution.

1:03PM B48.00008 Atomic force microscopy based nanoassay: a new method to study \(\alpha\)-Synuclein-dopamine bioaffinity interactions , STEFANIA CORVAGLIA, Elettra-Sincrotrone Trieste S.C.p.A., BARBARA SANAVIO, IFOM, Italy, BARBARA SORCE, ETH-Zurich, ALESSANDRO BOSCO, Elettra-Sincrotrone Trieste S.C.p.A., STEFANIA SABELLA, PIERPAOLO POMP, Istituto Italiano di Tecnologia, Lecce, Italy, GIACINTO SOLE, University of Udine, Italy, LOREDANA CAVALISI, Elettra-Sincrotrone Trieste S.C.p.A. — Intrinsically Disordered Proteins (IDPs) are characterized by the lack of well-defined 3-D structure and show high conformational plasticity. For this reason, they are a strong challenge for the traditional characterization of structure, supramolecular assembly and biorecognition phenomena. We show here how the fine tuning of protein orientation on a surface turns useful in the reliable testing of biorecognition interactions of IDPs, in particular \(\alpha\)-Synuclein. We exploited atomic force microscopy (AFM) for the selective, nanoscale confinement of \(\alpha\)-Synuclein on gold to study the early stages of \(\alpha\)-Synuclein aggregation and the effect of small molecules, like dopamine, on the aggregation process. Capitalizing on the high sensitivity of AFM topographic height measurements we determined, for the first time in the literature, the dissociation constant of dopamine-\(\alpha\)-Synuclein addsucts.

1:15PM B48.00009 Non-covalent interactions between ATP and RecA DNA-repairing proteins: DFT and semiempirical calculations , JORGE RODRIGUEZ, Department of Physics and Astronomy, Purdue University — The role of Bacterial RecA in the structural maintenance of genomes and the genetic information they carry has been established. In particular, the RecA DNA-repairing protein from \(D\). Radiodurans, a radiation-resistant bacteria, is crucial for the repair of double strand breaks (DSBs). We have performed semi-empirical free-energy calculations and QM/MM calculations to study their non-covalent interactions with ATP and ADP. Such studies provide insight into the mechanisms of ATP/ADP \(\rightarrow\) RecA energy transfer and, therefore, about specific functional uses of incoming energy for DNA repairing mechanisms. We present a detailed analysis of the non-covalent interactions which minimize the interaction Gibbs free energies leading to the most stable non-covalent binding sites. Van der Waal, hydrogen bonding and electrostatic interactions has been quantified which provides a detailed insight into the mechanisms of ATP-RecA interaction. Further, possible chemical interactions and functional roles of RecA proteins are explored based on the previously mentioned studies. Acknowledgements: Funded, in part, by DTRA award 106339 (JHR). Dr. Mark C. Palenik and Mrs. Lora Beard are gratefully acknowledged

1Supported in part by DTRA award 106339
1:27PM B48.00010 Photo-Activated Localization Microscopy of Single Carbohydrate Binding Modules on Cellulose Nanofibers. AMY HOR, DARYL DAGEL, QUOCANH LUU, MADHUSUDAN SAVAIAKAR, South Dakota School of Mines and Technology, SHI-YOU DING, Michigan State University, STEVE SMITH, South Dakota School of Mines and Technology — Photo-Activated Localization Microscopy (PALM) is used to conduct an in vivo study of the binding affinity of polysaccharide-specific Carbohydrate Binding Modules (CBMs) to insoluble cellulose substrates. Two families of CBMs, namely TrCBM1 and CiCBM3, were modified to incorporate photo-activatable mCherry fluorescent protein (PAmCherry), and exposed to highly crystalline Valonia cellulose nano-fibers. The resulting PALM images show CBMs binding along the nano-fibril long axis in a punctuated linear array, localized with an average, 10 nm precision. Statistical analysis of the binding events results in nearest neighbor distribution peaks but differences in the overall binding density. The form is attributed to steric hindrance among the CBMs on the nano-fibril whereas the latter is attributed to differences in the CBMs’ binding strength. These results are compared to similar distributions derived from TEM measurements of dried samples of CiCBM3-CdS quantum dot bioconjugates and AFM images of CiCBM3-GFP bound to similar Valonia nano-fibers.

1:39PM B48.00011 Force spectroscopy of biomolecular folding and binding: theory meets experiment. OLGA DUDKO, University of California, San Diego — Conformational transitions in biological macromolecules usually serve as the mechanism that brings biomolecules into their working shape and enables their biological function. Single-molecule force spectroscopy probes conformational transitions by applying force to individual macromolecules and recording their response, or “mechanical fingerprints,” in the form of force-extension curves. However, can we decode these fingerprints so that they reveal the kinetic barriers and the associated timescales of a biological process? I will present an analytical theory of the mechanical fingerprints of macromolecules. The theory is suitable for decoding such fingerprints to extract the barriers and timescales. The application of the theory will be illustrated through recent studies on protein-DNA interactions and the receptor-ligand complexes involved in blood clot formation.


11:15AM B50.00001 Spontaneous emergence of autocatalytic information-coding polymers. ALEXEI TKACHENKO, SERGEI MASLOV, Brookhaven National Laboratory — Self-replicating systems based on information-coding polymers are of crucial importance in biology. They also recently emerged as a paradigm in design on nano- and micro-scales. We present a general theoretical and numerical analysis of the problem of spontaneous emergence of autocatalysis for heteropolymers capable of template-assisted ligation driven by cyclic changes in the environment. Our central result is the existence of the first order transition between the regime dominated by free monomers and that with a self-sustaining population of sufficiently long oligomers. We provide a simple mathematically tractable model that predicts the parameters for the onset of autocatalysis and the distribution of chain lengths, in terms of monomer concentration, and two fundamental rate constants. Another key result is the emergence of the kinetically-limited optimal overlap length between a template and its two substrates. Template-assisted ligation allows for heritable transmission of information encoded in oligomer sequences thus opening up the possibility of long-term memory and evolvability of such systems.

Research was carried out in part at the Center for Functional Nanomaterials at Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886. Work at Biosciences Department was supported by US Department of Energy Office of Biological Research Grant PM-031.

11:27AM B50.00002 Evidence against a mean field description of short-range spin glasses revealed through thermal boundary conditions. JONATHAN MACHTA, WENLONG WANG, University of Massachusetts Amherst, HELMUT KATZGRABER, Texas A&M University — A theoretical description of the low-temperature phase of short-range spin glasses has remained elusive for decades. It is not known if there is a single pair of pure states as predicted by the droplet model, or infinitely many pure states, as predicted by mean field theory. Here we study the three-dimensional Edwards-Anderson Ising spin glass in thermal boundary conditions using population annealing Monte Carlo. In thermal boundary conditions all eight combinations of periodic vs antiperiodic boundary conditions in the three spatial directions appear in the ensemble with their respective Boltzmann weights, thus minimizing finite-size corrections due to domain walls. From the relative weighting of the eight boundary conditions for each disorder instance a sample stiffness is defined, and its typical value is shown to grow with system size according to a stiffness exponent. An extrapolation to the large-system-size limit is consistent with a single pair of pure states in every volume but incompatible with the mean field, replica symmetry breaking picture.

11:39AM B50.00003 Probing temperature chaos through thermal boundary conditions. WENLONG WANG, JONATHAN MACHTA, University of Massachusetts Amherst, HELMUT KATZGRABER, Texas A&M University — Using population annealing Monte Carlo, we numerically study temperature chaos in the three-dimensional Edwards-Anderson Ising spin glass using thermal boundary conditions. In thermal boundary conditions all eight combinations of periodic vs antiperiodic boundary conditions in the three spatial directions appear in the ensemble with their respective Boltzmann weights, thus minimizing finite-size corrections due to domain walls. By studying salient features in the specific heat we show evidence of temperature chaos. Our results suggest that these bumps are mainly caused by system-size excitations where the free energy of two boundary conditions cross. Furthermore, we study the scaling of both entropy and energy at boundary condition crossings and find that the scaling of the entropy is very different from the scaling obtained by a simple change of boundary conditions. We attribute this difference to the stronger finite-size effects induced via a simple change of boundary conditions all eight combinations of periodic vs antiperiodic boundary conditions in the three spatial directions appear in the ensemble with their respective Boltzmann weights, thus minimizing finite-size corrections due to domain walls. By studying salient features in the specific heat we show evidence of temperature chaos. Our results suggest that these bumps are mainly caused by system-size excitations where the free energy of two boundary conditions cross. Furthermore, we study the scaling of both entropy and energy at boundary condition crossings and find that the scaling of the entropy is very different from the scaling obtained by a simple change of boundary conditions. We attribute this difference to the stronger finite-size effects induced via a simple change of boundary conditions. Finally, we show that temperature chaos occurs more frequently at higher temperatures within the spin-glass phase and for larger system sizes, while the normalized distribution function with respect to temperature is about the same for different system sizes.

1:15PM B50.00004 Effective Hamiltonians of 2D Spin Glass Clusters. COLIN CLEMENT, Cornell University, DANILIO LIARTE, University of Sao Paulo, ALAN MIDDLETON, Syracuse University, JAMES SETHNA, Cornell University — We have a method for directly identifying the clusters which are thought to dominate the dynamics of spin glasses. We also have a method for generating an effective Hamiltonian treating each cluster as an individual spin. We used these methods on a 2D Ising spin glass with Gaussian bonds. We study these systems by generating samples and correlation functions using a combination of Monte Carlo and high-performance numerically exact Pfaffian methods. With effective cluster Hamiltonians we can calculate the free energy asymmetry of the original clusters and perform a scaling analysis. The scaling exponents found are consistent with Domain-Wall Renormalization Group methods, and probe all length scales. We can also study the flow of these effective Hamiltonians by clustering the clustered spins, and we find that our hard spin Hamiltonians at high temperature retain accurate low-temperature fluctuations when compared to their parent models.

The work is supported from NSF (Grant No. DMR-1208046).
12:03PM B50.00005 Overfrustrated and Underfrustrated Spin-Glasses in d=3 and d=2: Evolution of Phase Diagrams and Chaos Including Spin-Glass Order in d=2, EFE ILKER, Sabanci University, A. NIHAT BERKER, Sabanci University and MIT — In spin-glass (SG) systems, frustration can be adjusted continuously and considerably, without changing the antiferromagnetic (AF) bond probability p, by using locally correlated quenched randomness, both on hypercubic and hierarchical lattices [1]. With removal of 51% frustration, a SG phase occurs in d=2. With addition of 33% frustration, the SG phase disappears in d=3. In general, frustration lowers the SG ordering temperature. At low temperatures, increased frustration favors the spin-glass phase (before it disappears) over ferromagnetic (F) and AF phases. When any amount of frustration is introduced, chaotic rescaling of local interactions occurs in the SG phase. Chaos increases with increasing frustration. The distinct Lyapunov exponents of all chaotic phases and phase boundaries are calculated. From entropy and specific-heat curves in d = 3, it is seen that frustration lowers in temperature the onsets of long- and short-range orders in spin-glass phases, more effectively on the former. From entropy versus p, it is seen that ground-state and low-temperature entropy already mostly sets in within the F and AF phases, before the SG phase is reached.


12:15PM B50.00006 The cavity method for phase transitions in sparse reconstruction algorithms, MOHAMMAD RAMEZANALLI, Rutgers University, PARTHA MITRA, Cold Spring Harbor Laboratory, ANIRVAN SENGUPTA, Rutgers University — Compressed sensing methods are capable of reconstructing high-dimensional sparse signals using a limited amount of measurements under certain conditions. The boundaries of good performance of compressed sensing methods are associated with certain phase transitions when the number of variables go to infinity. Many compressed sensing methods are formulated as optimization problems. Usual statistical physics approach to this problem involves inventing a finite temperature version of the problem, analyzing the mean field theory via replica trick, and, then taking the zero temperature limit. Although this method has been very successful in reproducing the observations, the replica trick and the non-trivial zero temperature limit obscure the essential reasons for failure of a compressed sensing algorithm. In this work, we employ the cavity method to give an alternative derivation of the phase transitions, working solely with the zero-temperature limit and providing insight into the origin of different terms in the mean field self-consistency equations. The cavity method naturally invokes a susceptibility which is central to understanding different phases in this system, and could be generalized to a much broader class of compressed sensing problems.

12:27PM B50.00007 Multiply charged monopoles in cubic dimer model , SREEJITH GANESH JAYA, Max Planck Institute for Physics of Complex Systems, STEPHEN POWELL, The University of Nottingham — The classical cubic dimer model is a 3D statistical mechanical system whose degrees of freedom are dimers that occupy the edges between nearest neighbour vertices of a cubic lattice. Dimer occupations are subject to the local constraint that every vertex is associated with exactly one dimer. In the presence of an aligning interaction, it is known that the system exhibits an unconventional continuous thermal phase transition from a symmetry broken columnar phase to a Coulomb-phase. The transition is in the NCCP1 universality class, which also describes the Neel-VBS transition in the JQ model and the $S = \frac{1}{2}$ Heisenberg model with suppression of hedgehog defects. Using Monte-Carlo simulations of a pair of defects in a background of fluctuating dimers, we calculate the scaling exponents for fugacities of monopole defects of charge $Q = 2$ and $3$ at this critical point. Our estimates suggest that $Q = 3$ monopoles are relevant and could therefore drive the JQ model away from the NCCP1 critical point on a hexagonal lattice.

12:39PM B50.00008 A matrix product state method for solving combinatorial optimization problems1, S.S. PELTON, University of Central Florida, C. CHAMON, Boston University, E.R. MUCCIOLLO, University of Central Florida — We present a method based on a matrix product state representation to solve combinatorial optimization problems. All constraints are met by mapping Boolean gates into projection operators and applying operators sequentially. The method provides exact solutions with high success probability, even in the case of frustrated systems. The computational cost of the method is controlled by the maximum relative entropy of the system. Results of numerical simulations for several types of problems will be shown and discussed.

1 NSF grants CCF-1116590 and CCF-1117241


1:03PM B50.00010 Large-Scale Quantization and consequences in statistical mechanics, GEORGE LIVADIOTIS, Southwest Research Institute, USA — Recent developments revealed the existence of a new quantization constant $\hbar_\ast$, similar to the Planck constant $\hbar$, but $10^{12}$ orders of magnitude larger. Planck’s constant constitutes the smallest possible phase-space parcel for collisionless particle systems characterized by collective behavior and local correlations. The majority of space plasmas throughout the heliosphere are such systems, but any other type of systems exhibiting collective behavior and correlations between their particles can be characterized by the large-scale quantization. Here, we discuss the consequences of this alternative phase-space scale to statistical mechanics. The generalization of the old-known Sackur-Tetrode entropic formulation for systems with local correlation is such an example.

1:15PM B50.00011 Modeling the thermal conductivity and shear viscosity of mixtures of methane and n-decane under high pressure and high temperature conditions using molecular simulations, JOHN SHELTON, Carnegie Mellon Univ — Atomistic molecular dynamics simulations were carried out at equilibrium to calculate the shear viscosity and thermal conductivity of various mixtures of methane and n-decane within the range of ambient to extreme temperature and pressure conditions (i.e. up to 500 degree F and 35,000 psi). Both a computationally efficient united-atom force field and an all-atom force field were employed in this investigation. A quantitative comparison of the results was performed against experimental values and values predicted from a high temperature - high pressure perturbed chain - statistically associated fluid theory (HPHT PC-SAFT) model. Analysis of the intermolecular structure of the fluid as well as its dynamical characteristics were performed.
While recent self-propelled particle models generically predict a glass/jamming transition that is driven by packing density, our work suggests that biological tissues can accommodate these disparate requirements because the tissues are close to glass or jamming transition. Initially rearrange and move over relatively large distances, like a liquid. Subsequently, these same tissues must undergo buckling and support shear stresses, like a solid.

1:30PM B50.00013 Unleashing the Power of Microcanonical Inflection-Point Analysis: The Principle of Minimal Sensitivity

Using selected-bond removal networks, we demonstrate that one can drive the overall system to different regimes of behavior. Consequently one can exploit disorder to achieve unique, varied, textured and tunable global response.

1:51PM B50.00014 Optimisation by hierarchical search

We investigate adsorption properties of a simple-cubic lattice polymer model. The pseudophase diagram based on microcanonical inflection-point analysis is constructed. This example confirms the general potential of microcanonical statistical analysis for studies of pseudophase transitions for systems of finite size.


Independence of bond-level response means that one can drive the overall system to different regimes of behavior. Consequently one can exploit disorder to achieve unique, varied, textured and tunable global response.

11:15AM B51.00002 A theoretical framework for jamming in confluent biological tissues

A theoretical framework for jamming in confluent biological tissues, M. LISA MANNING, Syracuse University — For important biological functions such as wound healing, embryonic development, and cancer tumorogenesis, cells must initially rearrange and move over relatively large distances, like a liquid. Subsequently, these same tissues must undergo buckling and support shear stresses, like a solid. Our work suggests that biological tissues can accommodate these disparate requirements because the tissues are close to glass or jamming transition. While recent self-propelled particle models generically predict a glass/jamming transition that is driven by packing density, they happen at some critical \( \varphi = \frac{c}{c} \) and depend only on single cell properties such as cell-cell adhesion, cortical tension and cell elasticity. This model additionally predicts that an experimentally observable parameter, the ratio between a cell's perimeter and the square root of its cross-sectional area, attains a specific critical value at the jamming transition. We show that this prediction is precisely realized in primary epithelial cultures from human patients, with implications for asthma pathology.

12:27PM B51.00003 Arboreal solutions: diodes, pumps, and diggers inspired by trees

Arboreal solutions: diodes, pumps, and diggers inspired by trees, ANETTE HOSONI, Massachusetts Institute of Technology — Many natural systems have evolved to perform certain tasks – climbing, sensing, swimming – as perfectly as possible within the limits set by the laws of physics. This observation can be used both to guide engineering design, and to gain insights into the form and function of biological systems. In this talk we will consider both of these themes in the context of trees. Beginning with the roots, we examine the role of flexibility in moving through granular substrates. Next we discuss fluid transport in tall plants and finally we apply our findings to the design of engineered solid state pumps and diodes.

This work was partially funded by DARPA’s Maximum Mobility and Manipulation (M3) Program.
1:03PM B51.00004 Mechanical Instabilities at Finite Temperature. XIAOMING MAO, University of Michigan — The “softness” of soft materials oftentimes originates from their proximity to mechanical instabilities. Recent advances in soft matter research have revealed multiple classes of mechanical instabilities, featuring different scalings, different patterns of emergent rigid structure, and even different orders of rigidity transitions. These interesting behaviors have been observed in a wide range of systems, from granular packings to biological tissues and self-assembled structures. In this talk, we review this rich spectrum of behavior and discuss dramatic effects of thermal fluctuations near mechanical instabilities. We discuss a few ordered and disordered lattice models that represent different classes of mechanical instabilities, and show using analytic theories how thermal fluctuations lead to interesting finite-temperature phase diagrams in each case. In particular, (i) using a square lattice model that exhibits a mechanical instability towards exponentially many degenerate ground states, we show that fluctuations can drive the mechanical instability to a first-order transition, owing to divergent fluctuations near the isostatic point; and (ii) using two classes of disordered lattices, we show how under-coordinated random networks can be stabilized by fluctuations and discuss various regimes of unusual entropic rigidity, sharing similarities with jammed packings at finite temperature.

1:39PM B51.00005 Soft interfaces: complex, dynamic, reacting and evolving. TODD SQUIRES, UCSB Chemical Engineering — Various surface-active species ranging from small, amphiphilic molecules to proteins to colloidal particles—adsorb to fluid interfaces, enabling multiphase materials like foams and emulsions. Biophysical structures like cell membranes and lung surfactant monolayers, and a host of novel two-dimensional materials more generally. Moreover, many such interfaces exhibit rich structural and dynamical properties, including the two-dimensional (surface) analogs of three-dimensional rheology, including viscoelasticity, shear thickening and thinning, and yield stresses. We have developed active interfacial micro rheology techniques that simultaneously track the evolution of the microstructure of these complex interfaces, enabling morphology to be directly related to rheology. We will highlight particularly interesting two-dimensional materials, and will also discuss interfaces that evolve as surfactants adsorb (as occurs, e.g., in micro emulsions, or protein solutions) or as reagents react (e.g., during interfacial polymerization reactions). In addition to probing the heterogeneous and mechanical properties of such evolving interfaces, we have developed techniques to visualize the evolution of bulk concentration fields as such reactions proceed, yielding new capabilities to probe reacting and evolving interfaces.


11:15AM B52.00001 Yb$_2$Pt$_2$Pb: Emergent Criticality on the Frustrated Shastry-Sutherland Lattice'. MEIGAN ARONSON, Stony Brook University/Brookhaven National Lab — Metallic Yb$_2$Pt$_2$Pb forms in the U$_3$Pt$_5$S$_3$ structure, with layers of Yb ions forming the orthogonal dimers of the Shastry-Sutherland lattice (SSL). The Yb$^{3+}$ moments are strongly Ising-like, with an energetically isolated doublet ground state. Fits to the temperature dependent susceptibility confirm that dimerization occurs, and that the B=0 energy separation of the singlet ground state and the triplet excited state $\Delta \sim 4.5$ K. Yb$_2$Pt$_2$Pb orders antiferromagnetically at 2.06 K, with a striped modulation of the Yb moments in the SSL plane, with two wave vectors $q_{AF} = (0.2, 0.2, 0)$ rlu. The Yb moments are oriented perpendicular to the (1,1,0) dimer bond directions, and the dimers form the rungs of two orthogonal spin ladders along the c-axis. A non-dispersing and inelastic excitation with energy $\sim 0.4$ meV is found for wave vectors in the SSL plane, in good agreement with the singlet-triplet gap $\Delta$ inferred from susceptibility measurements. The dispersion of the excitations along $\{00l\}$ closely resembles that of a spinon continuum, such as those found in spin chain compounds, with an effective c-axis exchange of $\sim 0.12$ meV. Yb$_2$Pt$_2$Pb is a unique system, where strong quantum fluctuations related to the spin-ladder or SSL characters of this compound may lead to unusual correlations in this excellent metallic host.

11:51AM B52.00002 Magnetic Frustration in the Shastry-Sutherland Kondo lattice and the Global Phase Diagram of Heavy Fermion Metals. JEDEDIAH PIXLEY, Condensed Matter Theory Center, Department of Physics, University of Maryland — Over the past decade there has been significant theoretical and experimental progress in our understanding of antiferromagnetic quantum critical heavy fermion metals [1]. Recent years have seen a surge of studies on heavy fermion compounds with local moments that reside on geometrically frustrated lattices, which may host entirely new types of quantum critical points [2]. With a particular emphasis on Yb$_2$Pt$_2$Pb [3] and related 221 systems [4,5], we consider the Shastry-Sutherland Kondo lattice [6]. We determine the zero temperature phase diagram as a function of magnetic frustration and Kondo coupling. We study the transition between the valence bond solid phase of the Shastry-Sutherland lattice and a heavy fermi liquid, and find a phase diagram remarkably similar to the theoretically proposed global phase diagram of heavy fermion metals. We discuss the implications of our results for other geometrically frustrated heavy fermion metals.

12:27PM B52.00003 Fragile antiferromagnetism in the heavy-fermion compound YbBiPt. ALAN I. GOLDMAN, Ames Laboratory and Iowa State University — The discovery of YbBiPt [1] generated strong interest due to its extraordinary Sommerfeld coefficient ($\sim 8 J/molK^2$) and the fact that all of its relevant energy include the Kondo temperature, Weiss temperature, crystal field splitting, and a proposed antiferromagnetic (AFM) ordering below $T_N \approx 0.4$ K are small and comparable, suggesting a complex interplay of competing interactions at low temperature. Much of the recent attention on YbBiPt has focused on the possibility of a magnetic-field-tuned AFM quantum critical point occurring at a low critical magnetic field of $\mu_0 H_c \approx 0.4$ T [2]. Although thermodynamic and transport measurements in ambient fields suggested that YbBiPt manifests AFM order below $T_N$, scattering measurements over the past 22 years failed to identify magnetic ordering in powder or single-crystal samples. In this talk, I will present recent elastic and inelastic neutron scattering experiments on single crystals of YbBiPt that demonstrated clear scattering signatures of unusual AFM order at low temperature [3]. The ambient field elastic scattering consists of two components: a narrower component that appears below $T_N \approx 0.4$ K, which can be identified with features observed in the bulk transport measurements; and a broad scattering component that persists up to $T^* \approx 0.7$ K corresponding to AFM correlations extending over $\sim 200$ rlu. The Yb moments are strongly Ising-like, with an energetically isolated doublet ground state. Fits to the temperature dependent susceptibility confirm that dimerization occurs, and that the B=0 energy separation of the singlet ground state and the triplet excited state $\Delta \sim 4.5$ K. Yb$_2$Pt$_2$Pb orders antiferromagnetically at 2.06 K, with a striped modulation of the Yb moments in the SSL plane, with two wave vectors $q_{AF} = (0.2, 0.2, 0)$ rlu. The Yb moments are oriented perpendicular to the (1,1,0) dimer bond directions, and the dimers form the rungs of two orthogonal spin ladders along the c-axis. A non-dispersing and inelastic excitation with energy $\sim 0.4$ meV is found for wave vectors in the SSL plane, in good agreement with the singlet-triplet gap $\Delta$ inferred from susceptibility measurements. The dispersion of the excitations along $\{00l\}$ closely resembles that of a spinon continuum, such as those found in spin chain compounds, with an effective c-axis exchange of $\sim 0.12$ meV. Yb$_2$Pt$_2$Pb is a unique system, where strong quantum fluctuations related to the spin-ladder or SSL characters of this compound may lead to unusual correlations in this excellent metallic host.

1This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. Ames Laboratory is operated for the U.S. DOE by Iowa State University under contract # DE-AC02-07CH1135
1:03PM B52.00004 Strange metal without magnetic instability in $\beta$–YbAlB$_4$, SATORU NAKATSUJI, ISSP, University of Tokyo — Many prototypical quantum critical materials found within the class of 4$f$ heavy fermion compounds are known to have an almost integral valence and appear at the border of magnetism. An exception to this rule was recently discovered in $\beta$–YbAlB$_4$, which exhibits quantum criticality despite strong mixed valency.$^{[4]}$ Ultrasonic single crystals of this material exhibit intrinsically singular thermodynamic and transport behaviors, which are extremely sensitive to a magnetic field.$^{[5]}$ In particular, $T/B$ scaling of the magnetization has been observed over four decades of $T/B$, projected to extend down to fields as small as 0.1 mT. In this talk, we will discuss our results on the zero field criticality by the $T/B$ scaling in a broad regime of $T$ and $B$, and through an extensive series of pressure measurements.$^{[6]}$ We will show that the intrinsic quantum criticality of YbAlB$_4$ occupies an extended region of pressure, indicating a formation of a phase. Furthermore, we will present that the strange metal region is clearly surrounded and separated from a high-pressure magnetic instability by a finite pressure range of Fermi liquid behavior.

This work is based on the collaboration with Yosuke Matsumoto, Takahiro Tomita, Kentaro Kuga, Yoshiya Uwatoko, Yasuyuki Shimura, Piers Coleman, Andriy H. Nevidomskyy, E. O’Farrell, T. Sakakibara, Y. Karaki, S. Suzuki, H. Cao, D. MacLaughin, M. Okawa, S. Shin

5$^{[5]}$ M. Sutherland et al., arXiv:1407.6142.

1:39PM B52.00005 Kondo effect and quantum criticality in Ce-based pnictides, YONKANG LUO, Los Alamos National Laboratory — The pnictides have not only triggered enthusiasm in searches for high-$T_c$ superconductors, but also paved a new way for investigating the Kondo effect and quantum criticality. In this talk, I will start with the phase diagram of CeFeAs$_1-x$P$_x$O which hosts two possible quantum critical points (QCPs) [1]. Due to the entanglement of 3d and 4f magnetism, CeFeAsO is not a good candidate for investigating quantum criticality, therefore we turn to CeAs. The Ce-sublattice shows two successive AFM transitions at $T_{\text{N1}} = 9.3$ K and $T_{\text{N2}} = 7.3$ K, while the Ni-sublattice is nonmagnetic [2]. Under pressure, both AFM transitions are suppressed, and a QCP is obtained at $p_c = 6.5$ kbar. Similar phenomenon was also observed by P/As-substitution, which leads to a critical doping at $x_c = 0.4$. The quantum fluctuations near these QCPs are discussed, and the possibility of a Kondo-destruction type QCP is addressed [3]. Finally, I will briefly talk about the pressure effect on the 122 cousin, CeNi$_2$As$_2$ [4], which seems to provide a rare paradigm of quantum criticality in the low carrier density limit.

In collaboration with: Z. Xu, J. Dai, G. Cao, L. Pourovskii, Q. Si, N. P. Ong, and J. D. Thompson et al.

the superconducting states in this material, and their perturbation by various nanoscale disorders within the FeSe film and its substrate.

**MOODERA, Massachusetts Institute of Technology, JENNIFER E. HOFFMAN, Harvard University — FeSe possesses the simplest stoichiometry within the**

**DENNIS HUANG, Harvard University, TATIANA A. WEBB, University of British Columbia, CAN-LI SONG, Harvard University, CUI-ZU CHANG, JAGADEESH**

**L. COHEN, STEVEN G. LOUIE, UC Berkeley, Lawrence Berkeley National Laboratory — We show that the electron-phonon coupling in an FeSe monolayer on**

**α**

**by symmetry in the non-magnetic phase. The spectral function for the electron-phonon coupling (\(T_c \approx 20\) K, \(T_c^{\max} \approx 20\) K, \(T_c^{\min} \approx 18.0\) K), which is about 30% higher than that found in the bulk materials and superior high field performance over the low temperature superconductors. [Nature Commun. 4, 1347 (2013)]. Recently, we were successful in further enhancement of \(J_c\) without \(T_c\) degradation by ion irradiation, especially, at high temperature and high magnetic field. The low-energy proton irradiation produces a \(J_c\) enhancement of one order of magnitude over the field of 6T//\(c\) at 12 K. Extensive TEM studies of the irradiated FST films have been carried out, which revealed an intriguing defect morphology provided by the irradiation. We will discuss the relationship between the superconducting properties and the created defects of the iron-chalcogenide films.

**2:30PM D0.00001 Influence of ion irradiation on iron-chalcogenide superconducting films**

**TOSHINORI OZAKI, WEIDONG SI, CHENG ZHANG, LIJUN WU, QIANG LI, Brookhaven National Laboratory — Iron-chalcogenide superconductors have**

**rather simple crystal structure and no charge reservoir. They also exhibit remarkable properties including small anisotropy, high upper critical fields, a significant pressure effect on superconductivity. We have grown iron-chalcogenide FeSe0.5Te0.5 (FST) superconducting films on various substrate by pulsed laser deposition**

**[Rep. Prog. Phys. 74, 124510 (2011)]. The FST films on CeO2 buffer layer exhibit enhanced \(T_c\) (\(T_c^{\max} > 20\) K, \(T_c^{\min} = 18.0\) K), which is about 30% higher than that found in the bulk materials and superior high field performance over the low temperature superconductors. [Nature Commun. 4, 1347 (2013)]. Recently, we were successful in further enhancement of \(J_c\) without \(T_c\) degradation by ion irradiation, especially, at high temperature and high magnetic field. The low-energy proton irradiation produces a \(J_c\) enhancement of one order of magnitude over the field of 6T//\(c\) at 12 K. Extensive TEM studies of the irradiated FST films have been carried out, which revealed an intriguing defect morphology provided by the irradiation. We will discuss the relationship between the superconducting properties and the created defects of the iron-chalcogenide films.

**2:42PM D0.00002 Strong electron-phonon interaction in an FeSe monolayer**

**SINISA COH, MARVIN L. COHEN, STEVEN G. LOUIE, UC Berkeley, Lawrence Berkeley National Laboratory — We show that the electron-phonon coupling in an FeSe monolayer on a \(\text{SrTiO}_3\) substrate is significantly larger than in earlier theoretical estimates. The role of the \(\text{SrTiO}_3\) substrate is two-fold. First, the interaction of the FeSe and \(\text{TiO}_2\) terminated face of \(\text{SrTiO}_3\) prevents the FeSe monolayer from undergoing a shearing-type (orthorhombic) structural phase transition. Second, the substrate allows an anti-ferromagnetic ground state of FeSe which opens certain electron-phonon coupling channels within the monolayer that are prevented by symmetry in the non-magnetic phase. The spectral function for the electron-phonon coupling (\(\alpha^2 F\)) in our calculations agrees well with inelastic tunneling data.**

**1This work was supported by NSF Grant No. DMR10-1006184 and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by the DOE at Lawrence Berkeley National Laboratory’s NERSC facility.**

**2:54PM D0.00003 STM investigation of nanoscale inhomogeneity in single-layer FeSe/\(\text{SrTiO}_3\)**

**DENNIS HUANG, Harvard University, TATIANA A. WEBB, University of British Columbia, CAN-LI SONG, Harvard University, CUI-ZU CHANG, JAGADEESH MOODERA, Massachusetts Institute of Technology, JENNIFER E. HOFFMAN, Harvard University — FeSe possesses the simplest stoichiometry within the family of iron-based high-\(T_c\) superconductors. The ability to grow high quality films layer-by-layer using molecular beam epitaxy (MBE) yields opportunities to engineer high-\(T_c\) superconducting heterostructures with novel behaviors. In particular, single-layer FeSe deposited on \(\text{SrTiO}_3\) exhibits an order of magnitude increase in \(T_c\) from its bulk value, possibly due to strain, charge doping or enhanced electron-phonon coupling from the substrate. We use a combined scanning tunneling microscope (STM) and MBE system to examine single-layer FeSe/\(\text{SrTiO}_3\) at the atomic scale. Using real-space spectroscopic imaging, we investigate the superconducting states in this material, and their perturbation by various nanoscale disorders within the FeSe film and its substrate.**

**3Work supported by the US National Science Foundation grant DMR-0847433 and the STC Center for Integrated Quantum Materials under NSF grant DMR-1231319.**
3:06PM D0.00004 Fermi surface topology and gap anisotropy in monolayer FeSe thin film

YAN ZHANG, SIMES, LBNL; JAMES LEE, ROBERT MOORE, WEI LI, MING YI, SIMES, Stanford Unv.; MAKOTO HASHIMOTO, DONGHUI LU, SSRL, SLAC, ZAHID HUSSAIN, LBNL; TOM DEVEREAUX, SIMES, Stanford Unv.; DUNG-HAI LEE, UC Berkeley, ZHI-XUN SHEN, SIMES, Stanford Unv.

The discovery of superconductivity in monolayer FeSe thin film has generated great interests. The superconducting transition temperature (Tc) was reported to be over 65 K, which holds the record in iron-based superconductors. More intriguingly, the superconductivity was found only in one monolayer (1ML) film, while the films thicker than 1ML are non-superconducting. Utilizing the angle-resolved photoemission spectroscopy (ARPES), we studied the Fermi surface topology and superconducting gap anisotropy in 1ML FeSe. We resolved two ellipse-like electron pockets at the zone corner overlapping with each other. No hybridization between these two electron pockets was observed, which indicates that the glide mirror symmetry breaking due to the substrate is extremely weak in 1ML FeSe. Multi-gap behavior and gap anisotropy were further observed on the electron pockets. The superconducting gap minimums locate along the M-X direction for both inner and outer electron pockets. The observed Fermi surface topology and gap distribution provide a good starting point for constructing theoretical models and put strong constrains on determining the pairing symmetry in 1ML FeSe.

3:18PM D0.00005 STM investigation of FeSe/SrTiO3 band structure1

TATIANA A. WEBB, University of British Columbia, DENNIS HUANG, CAN-LI SONG, Harvard University, CUI-ZU CHANG, JAGADEESH MOODERA, Massachusetts Institute of Technology, JENNIFER E. HACKMAN, Harvard University — Growing a single unit cell of FeSe on a SrTiO3 substrate (1 u.c. FeSe/STO) enhances the superconducting transition temperature (Tc) by an order of magnitude. While the dramatic effect of the interface is evident, a mechanism is not. ARPES studies have revealed that the band structure differs significantly from bulk FeSe and the majority of other Fe-based superconductors, most notably in lacking a hole pocket at the Fermi level. ARPES, however, is limited to probing the filled electron states. STM/STS has access to the band structure, both above and below the Fermi level, with spatial resolution, and the data encodes electronic properties including orbital character and interactions. We present an STM/STS study of 1 u.c. FeSe/STO grown by molecular beam epitaxy (MBE), focusing on the empty-state band structure of this new high Tc superconductor.

1Work supported by the US National Science Foundation grant DMR-0847433, and STC Center for Integrated Quantum Materials under NSF grant DMR-1231519.

3:30PM D0.00006 Investigation of superconductivity in single layer FeSe on SrTiO3 (001) by quasi-particle interference and impurity states 

TONG ZHANG, QIN FAN, WENHAO ZHANG, XI LIU, MIAO XIA, HONGYAN CHEN, RUI PENG, HAICHAO XU, BINPING XIE, DONGLAI FENG, Fudan University — Recently, single layer FeSe films on SrTiO3 (001) were discovered to have much enhanced superconductivity [1]. Here by using scanning tunneling microscopy/spectroscopy, we investigated the superconductivity of single layer FeSe through quasi-particle interference (QPI), magnetic vortex mapping and impurity induced bound states. The films were grown by MBE and transfer to STM in-situ. The magnetic vortex lattice was observed in dI/dV mappings in the field. QPI mappings show that intra-band and inter-band scattering of superconducting quasi-particles have significant anisotropy. Single atom impurities were introduced on the surface by in-situ deposition. We found that nonmagnetic impurities (Zn, Ag, K) do not induce bound states in the superconducting gap, but the magnetic ones (Cr, Mn) do. Upon these observations, the pairing symmetry of single layer FeSe will be discussed.


3:42PM D0.00007 Interface enhanced superconductivity in one unit-cell FeSe films grown on SrTiO3 

XUCUN MA, Department of Physics, Tsinghua University — Heterostructure based interface engineering has been proved an effective method for finding new superconducting systems and raising superconducting transition temperature (Tc). Recently discovered high temperature superconductivity in one unit-cell (UC) FeSe films on SrTiO3 (STO) substrate grown by molecular beam epitaxy has attracted intensive attention. In sharp contrast to FeSe films on graphite where a 2.2 meV superconducting gap is observed on thick films and no superconducting gap on 1-UC FeSe films grown by MBE, we discovered a large superconducting gap in 1-UC FeSe films grown on STO substrate. Another interesting point of this system is its simple band structure consists of only electron Fermi pockets at M points, which is different from that of bulk FeSe. In this talk, a comprehensive study of 1-UC FeSe films by in situ scanning tunneling microscopy/spectroscopy (STM/STS) and angle-resolved photoemission spectroscopy (ARPES) and ex situ transport measurements are presented to discuss the possible superconducting mechanism in this well-defined heterostructure.

Collaborators: Qi-Kun Xue, Lili Wang, Yuau Wang (Tsinghua University); Xingjiang Zhou (Institute of Physics, CAS); Jian Wang (Peking University)

4:18PM D0.00008 Phase separation or not in KxFe2−xSe2 (KFs) 

DESPINA LOUCA, JUNJIE YANG, University of Virginia — The coexistence of insulating and superconducting phases in the KxFe2−xSe2 family of Fe-based superconductors is investigated using neutron scattering on samples grown under different conditions. In this family, three scenarios have so far been proposed regarding the superconducting phase. In the first, a superconducting minority phase with the 122 composition is separated from the insulating and majority 245 phase. Under this scenario several phase diagrams have been developed in which the superconducting phase is sandwiched between semiconducting and insulating, antiferromagnetic phases. In the second, the superconducting phases exists in an inhomogeneous structure, hence no phase separation. And in the third, a purely superconducting phase of the alkali intercalated FeSe can be made with the 122 structure that has no other phases. By probing the local structure, we previously observed that superconductivity emerges in a locally distorted Fe sublattice that accommodates two kinds of bonding environments, forming a double-band distribution that changes with the concentration of K. In addition, the Fe bond distribution changes with the annealing treatment. Implications to the coexistence of the two phases will be discussed.

4:30PM D0.00009 Suppression of Phase Separation and Enhanced Superconducting Transition Temperature of FeSe1−xTe x Thin Films1

FUYUKI NABESIMA, YUICHI SAWADA, YOSHINORI IMAI, ATSUTAKA MAEDA, The University of Tokyo — To clarify the mechanism of superconductivity of Fe-based superconductors, it is crucial to investigate superconductivity of FeSe1−xTeX, which has the simplest crystal structure. There is, however, a serious obstacle to the understanding of its superconductivity; phase separation by spinodal decomposition occurs in the region of 0.1 < x < 0.4 and thus a whole phase diagram has not been available. A useful method to fabricate metastable materials is thin-film deposition because of its thermodynamically non-equilibrium growth. In the presentation we will report the first demonstration of the suppression of the phase separation of FeSe1−xTeX thin films on CaF2 substrates[1]. Surprisingly the optimal composition to achieve the highest superconducting transition temperature, Tc, was found in this phase separation region; Tc reaches ~23 K. A whole phase diagram we will present provides a new perspective for the superconductivity of this material. [1] F. Nabeshima et al., Appl. Phys. Lett. 103 (2013) 172602.

1Partially supported by Strategic International Collaborative Research Program (SICORP) of Japan Science and Technology Agency.
4:42PM D0.00010 Fermi surface deformation in a simple iron-based superconductor, FeSe$^1$

AMALIA COLDEA, MATTHEW WATSON, University of Oxford, UK, TIMUR KIM, Diamond Light Source, UK, AMIR HAGHIGHIRAD, University of Oxford, UK, ALIX MCCOLLAM, High Field Magnet Laboratory, Nijmegen, The Netherlands, MORITZ HOERSCH, Diamond Light Source, UK, ANDREW SCHOFIELD, University of Birmingham — One of the outstanding problems in the field superconductivity is the identification of the normal state out of which superconductivity emerges. FeSe is one of the simplest and most intriguing iron-based superconductors, since in its bulk form it undergoes a structural transition before it becomes superconducting, whereas its single-layer form is believed to be a high-temperature superconductor. The nature of the structural transition, occurring in the absence of static magnetism, is rather unusual and how the electronic structure is stabilized by breaking of the rotational symmetry is the key to understand the superconductivity in bulk FeSe. Here we report angle-resolved photoemission spectroscopy measurements on FeSe that gives direct access to the band structure and orbital-dependent effects. We complement our studies on bulk FeSe with low-temperature angular-dependent quantum oscillation measurements using applied magnetic fields that are sufficiently strong to suppress superconductivity and reach the normal state. These studies reveal a strong deformation of Fermi surface through the structural transition driven by electronic correlations and orbital-dependent effects.

$^1$This work was supported by EPSRC, UK (EP/I004475/1), Diamond Light Source, UK and HFML, Nijmegen.

4:54PM D0.00011 Electronically-driven orthorhombic distortion in FeSe$^1$

MATTHEW WATSON, NATHANIEL DAVIES, AMIR HAGHIGHIRAD, ARJUN NARAYANAN, Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford OX1 3PU, TIMUR KIM, MORITZ HOERSCH, Diamond Light Source, Harwell Campus, Didcot, OX11 0DE, SAMUEL BLAKE, AMALIA COLDEA, Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford Oxford OX1 3PU — FeSe is structurally the simplest of Fe-based superconductors, and exhibits a tetragonal-to-orthorhombic structural transition at $\sim$ 90 K, but no long-range magnetism at any temperature. We report measurements of the resistivity anisotropy in FeSe above $T_s$ finding a large and divergent response to an applied strain, with a comparable magnitude and temperature-dependence to measurements in Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$, but opposite sign. We compare this data with literature reports on NMR and our own ARPES data, which taken together indicate that the structural transition is electronically-driven with orbital degrees of freedom playing a central role.

$^1$This work was supported by EPSRC, UK (EP/I004475/1) and Diamond Light Source.

5:06PM D0.00012 The superconductivity in single-layer FeTe$_{1-x}$Se$_x$ films on SrTiO$_3$.

LILI WANG, XUCUN MA, QIKUN XUE, Tsinghua University, XUE TEAM — For bulk FeSe, the highest transition temperature $T_c = 9$ K has been observed for the composition with stoichiometry Fe$_{1.1}$Se$_{1.1}$. The tetragonal-orthorhombic structural transition observed in FeSe is suppressed with Te substitution and the superconducting transition temperature reaches a maximum of $T_c = 15.2$ K at about 50% Te substitution. For single-layer FeSe films on SrTiO$_3$, in situ scanning tunneling microscopy and angle resolved photoemission spectroscopy have revealed a superconducting gap as large as 20 meV, and $\textit{ex situ}$ transport measurements have confirmed the interface enhanced superconductivity with $T_c$ above 55 K. Here we report a detailed $\textit{in situ}$ scanning tunneling microscopy and transport study of the single-layer FeTe$_{1-x}$Se$_x$ films on SrTiO$_3$. We found that Te substitution in the single-layer FeSe films doesn’t induce further increase of the transition temperature $T_c$, which is in contrast to the results for the corresponding bulk materials. This implies that the SrTiO$_3$ substrates play important role in the interfacial superconductivity.


5:18PM D0.00013 Theoretical studies of the effects of orbital ordering on spin fluctuations and superconductivity in FeSe.

SHANTANU MUKHERJEE, ANDREAS KREISEL, Niels Bohr Institute, University of Copenhagen, PETER J. HIRSCHFELD, Department Of Physics, University of Florida, BRIAN M. ANDERSEN, Niels Bohr Institute, University of Copenhagen — FeSe is currently one of the most hotly debated iron-based systems due in part to its very high $T_c$, when monolayers are placed on STO substrates, and in part due to the fact that the material exhibits a structural distortion near $T_S$ $\sim$ 90K without any concomitant magnetic order. In addition, undoped bulk FeSe samples, which become superconducting below $T_c$ $\sim$ 8K, display evidence of orbital ordering setting in near $T_S$. We discuss the normal and superconducting properties of FeSe using a ten orbital tight-binding model, and include the effect of ferro-orbital ordering. The model reproduces the essential features of FeSe band structure seen in ARPES [1] and quantum oscillation experiments [3]. Using this model, the spin lattice relaxation rate is calculated and the results are compared with recent NMR experiments [2]. We next discuss the consequences of a spin fluctuation mediated superconducting pairing in FeSe and the resulting gap structure. Finally, the local density of states derived from our calculations is compared to STM experiments [4].

4 C. L. Song et al., Science 332, 1410 (2010).

Monday, March 2, 2015 2:30PM - 5:30PM —
Session D1 DMP: Focus Session: Graphene - Mechanics and Strain

001A - Phillip First, Georgia Institute of Technology

2:30PM D1.00001 Strain-Engineering of Giant Pseudo-Magnetic Fields in Graphene/Boron Nitride (BN) Periodic Nanostructures$^1$

CHEN-CHIH HSU, JIAQING WANG, MARCUS TEAGUE, CHIEN-CHANG CHEN, NAI-CHANG YEH, Caltech — Ideal graphene is strain-free whereas non-trivial strain can induce pseudo-magnetic fields as predicted theoretically and manifested experimentally. Here we employ nearly strain-free single-domain graphene, grown by plasma-enhanced chemical vapor deposition (PECVD) at low temperatures, to induce controlled strain by placing the PECVD-graphene on substrates containing engineered nanostructures. We fabricate periodic pyramid nanostructures (typically 100 $\sim$ 200 nm laterally and 10 $\sim$ 60 nm in height) on Si substrates by focused ion beam, and determine the topography of these nanostructures using atomic force microscopy and scanning electron microscopy after we transferred monolayer h-BN followed by PECVD-graphene onto these substrates. We find both layers conform well to the nanostructures so that we can control the size, arrangement, separation, and shape of the nanostructures to generate desirable pseudo-magnetic fields. We also employ molecular dynamics simulation to determine the displacement of carbon atoms under a given nanostructure. The pseudo-magnetic field thus obtained is $\sim$150T in the center, relatively homogeneous over 50% of the area, and drops off precipitously near the edge. These findings are extended to arrays of nanostructures and compared with topographic and spectroscopic studies by STM.

$^1$Supported by NSF.
ZHIGONG SONG, ZHIPING XU, Tsinghua Univ — Defects in solids commonly limit mechanical performance of materials by reducing their rigidity and strength. In this talk, we report measurements of adhesion properties of large-area graphene transferred onto silicon oxide. Measurement of interfacial properties is crucial for practical and reliable applications of graphene. In this talk, we report measurements of adhesion properties of large-area graphene transferred onto silicon oxide. Using a high sensitive nanoindentation tool, we observed nonlinear adhesive interactions of graphene with an indenter. The nanoindentation measurements also provided interesting local behaviors of graphene related to wettability. The experimental results were analyzed with numerical simulation for further understanding.

1 Financial support was provided, in part, by the Office of Naval Research under grant N00014-10-1-0181, the National Science Foundation under grant DMR-0855358.
4:18PM D1.00010 Basal-plane dislocations in bilayer graphene - Peculiarities in a quasi-2D material¹. BENJAMIN BUTZ, Center for Nanoanalysis and Electron Microscopy (CENEM), University Erlangen-Nuremberg — Dislocations represent one of the most fascinating and fundamental concepts in materials science. First and foremost, they are the main carriers of plastic deformation in crystalline materials. Furthermore, they can strongly alter the local electronic or optical properties of semiconductors and ionic crystals. In layered crystals like graphene, dislocation movement is restricted to the basal plane. Thus, those basal-plane dislocations cannot escape their confinement in between only two atomic layers of the material. So-called bilayer graphene is the thinnest imaginable quasi-2D crystal to explore the nature and behavior of dislocations under such extreme boundary conditions. Robust graphene membranes derived from epitaxial graphene on SiC provide an ideal platform for their investigation. The presentation will give an insight in the direct observation of basal-plane partial dislocations by transmission electron microscopy and their detailed investigation by diffraction contrast analysis and atomistic simulations. The investigation reveals striking size effects. First, the absence of stacking fault energy, a unique property of bilayer graphene, leads to a characteristic dislocation pattern, which corresponds to an alternating AB ↔ BA change of the stacking order. Most importantly, our experiments in combination with atomistic simulations reveal a pronounced buckling of the bilayer graphene membrane, which directly results from accommodation of strain. In fact, the buckling completely changes the strain state of the bilayer graphene and is of key importance for its electronic/spin transport properties. Due to the high degree of disorder in our quasi-2D material it is one of the very few examples for a perfect linear magnetoresistance, i.e. the linear dependency of the in-plane electrical resistance on a magnetic field applied perpendicular to the graphene sheet up to field strengths of more than 6 T.

¹This research is financed by the German Research Foundation through the SFB 953 “Synthetic Carbon Allotropes.”

4:54PM D1.00011 Strain and defect induced enhancement of Young’s modulus of graphene. GUILLERMO LOPEZ-POLIN, CRISTINA GOMEZ-NAVARRO, MIRIAM JAAFAF, JULIO GOMEZ-HERRERO, Universidad Autonoma de Madrid, VINCENZO PARENTE, RAFAEL ROLDAN, Instituto de Ciencia de Materiales de Madrid, MIKHAIL KATSNELSON, Radboud University, FRANCESC PEREZ MURANO, Instituto de Microelectronica de Barcelona, FRANCISCO GUINEA, Instituto de Ciencia de Materiales de Madrid — Graphene, due to its extremely high in plane stiffness and low bending rigidity, presents important out of plane thermal fluctuations crucial for the understanding of its mechanical properties. In this work we measure Young’s modulus of graphene with induced vacancy density using AFM nanoindentations. Unlike predicted, we find that the stiffness of graphene increases with defect content until a vacancy density of 0.2 percent, where it doubles its initial value. For higher defect density the elastic modulus exhibits a decreasing tendency. We attribute the initial increase in stiffness to the quenching of the out of plane oscillations of graphene due to defects [1]. In order to validate this interpretation we also study the dependence of the elastic modulus with strain. We observe an increase of the Young’s modulus at pre-strains higher than 0.5 percent where it again doubles its initial value.


5:06PM D1.00012 Irradiation-Induced Superplasticity of Graphene and Carbon Nanotubes. ZHUHUA ZHANG, YU LIN, Department of Materials Science and Nanoeengineering, and the Smalley Institute for Nanoscale Science and Technology, Rice University, Houston, TX 77005, FENG DING, Institute of Textiles and Clothing, Hong Kong Polytechnic University, Kowloon, Hong Kong, Peoples Republic of China, BORIS I. YAKOBSON, Department of Materials Science and Nanoeengineering, and the Smalley Institute for Nanoscale Science — The superplasticity of carbon nanotubes has been related to the dynamics of pentagon-heptagon (57) dislocations, but the mechanism remains elusive in light of prohibitively high barrier (~ 7 eV) of dislocation migration [1,2]. Here, we reveal the key role of electron irradiation in facilitating the dislocation migration and promoting nanotube plasticity. Atomistic simulations show that irradiation-induced adatoms and monovacancies diffuse towards the sessile 57 dislocations and switch them into a mobile radical state with a migration barrier as low as 1.6 eV, thereby significantly enhancing the plastic flow. The radical dislocations also act as defect scavengers to prevent lattice disorder in the tube wall, in agreement with experimental phenomena. Further, a formula is derived to quantify the plasticity in terms of irradiation intensity, aimed to guide the irradiation engineering of plasticity of carbon nanomaterials.


5:18PM D1.00013 ABSTRACT WITHDRAWN –

Monday, March 2, 2015 2:30PM - 5:30PM – Session D2 DMP: Focus Session: Beyond Graphene - Optics in 2D Semiconductors I 001B - Farhan Rana, Cornell University

2:30PM D2.00001 Dependence of Monolayer WS2-Substrate Interaction on Substrate Type and Bonding Investigated by High-temperature Raman and Photoluminescence , LIQIN SU, Univ of NC - Charlotte, YIFEI YU, LINYOU CAO, North Carolina State University, YONG ZHANG, Univ of NC - Charlotte — We report the temperature and excitation wavelength dependence of the electronic and vibration properties of epitaxially grown WS2 monolayers on different substrates, SiO2 and sapphire, using photoluminescence (PL) and Raman spectroscopy with temperatures up to 500 °C. Similar to our previous study on MoS2 (Su et al., Nanoscale 6, 4920, 2014), the WS2 monolayers are shown to also exhibit strong interaction with substrates, manifesting as that their electronic and optical properties depend sensitively on the substrate type and film-substrate bonding. Raman frequency shifts for E1g(Γ) and A1g(Γ) modes and PL energy shifts are measured from room temperature up to 500 °C. Raman spectra shows strong substrate dependence, and the thermal quenching of the PL intensity in the high temperature region reveal nonradiative channels with large activation energies in the order of 0.5 eV. This study suggests the critical need to assess the potential impact of the substrate on the intrinsic properties of such 2-D materials and the opportunities for tailoring their properties by selecting different substrates.

2:42PM D2.00002 Single Quantum Emitters in Monolayer Tungsten Diselenide. GENEVIEVE CLARK, JOHN SCHABILEY, University of Washington, YU-MING HE, YU HE, M. C. CHEN, Y. J. WEI, X. DING, QIANG ZHANG, JIAN-WEI PAN, University of Washington - Single quantum emitters (SQEs) are central emerging photonemission technologies. While they have been realized in variety of solid state systems, all solid-state quantum emitters to date are embedded in a three dimensional bulk matrix. We present a new type of single quantum emitter in a two-dimensional system, in the form of neutral excitons localized to defects within atomically thin tungsten diselenide monolayers. These localized excitons show strong photoluminescence with 130 μeV emission lines from two non-degenerate, cross-polarized transitions. Their narrow line width is characteristic of localized exciton emission, and is several orders of magnitude narrower than seen from excitons delocalized in a monolayer. Second-order correlation measurements show strong photon anti-bunching, establishing that these localized excitons are single photon emitters. Magneto-optical measurements reveal an exciton g-factor of 8.7, significantly larger than that of delocalized excitons. SQE’s in monolayer WS2 may offer practical advantages such as efficient photon extraction and scalability, and in-situ control of local environment.

— Charlotte, YIFEI YU, LINYOU CAO, North Carolina State University, YONG ZHANG, Univ of NC - Charlotte — We report the temperature and excitation, LIQIN SU, Univ of NC - Charlotte, YIFEI YU, LINYOU CAO, North Carolina State University, YONG ZHANG, Univ of NC - Charlotte — We report the temperature and excitation,
2:54PM D2.00003 Quantum dots in graphene-like materials, THAKSHILA HERATH, VADYM APALIKOV, Georgia State University — We study numerically the electron states in silicenene and germainene quantum dots within the effective low energy model of silicene and germanene. The quantum dots are realized through spatial variation of perpendicular electric field, i.e., bias voltage. The energy spectra of such quantum dots are obtained for different parameters of the dots, which are the size of the dot and the strength of external electric field. For cylindrically symmetric spatial profile of electric field, the electron states of the dot are characterized by z-component of the angular momentum. Due to strong spin-orbit interactions in such buckled graphene-like materials, the states in the quantum dots have unique spin texture, which is more pronounced for germanene quantum dots. The dependence of spin polarization of electron states in the quantum dots on the strength of electric field is also obtained.

3:06PM D2.00004 Ultrafast laser spectroscopy of two-dimensional materials and their heterostructures, HUI ZHAO, University of Kansas — Monolayer transition metal dichalcogenides are new two-dimensional materials beyond graphene. Recently, extensive studies have revealed several unique properties of these materials and their potential applications in electronic and renewable-energy technologies. Furthermore, it is possible to use these atomic layers as building blocks to fabricate new van der Waals heterostructures with emergent properties. In this talk, I will report our recent ultrafast laser studies of several types of two-dimensional transition metal dichalcogenides and their heterostructures. First, we studied several nonlinear optical processes, such as second harmonic generation, which allows detection of the crystal orientation and symmetry of MoS$_2$ monolayers, and two-photon absorption, which was used to measure the bandgap and exciton binding energy of WSe$_2$ monolayers. Second, we used a transient absorption microscopy technique with high spatial resolution to study exciton dynamics in these materials, and measured their exciton lifetime, diffusion coefficient, and ballistic transport. Third, by performing transient absorption measurements with polarization resolution, we studied spin and valley dynamics of excitons in monolayer MoSe$_2$ and deduced a spin relaxation time of about 9 ps at room temperature. Finally, we used the transient absorption technique with layer selectivity to study heterostructures of graphene-WS$_2$, MoS$_2$-MoSe$_2$, and WSe$_2$-MoSe$_2$. We observed ultrafast and efficient charge and exciton transfer across the van der Waals interface in all these structures. The formation of spatially indirect excitons in the transition-metal-dichalcogenide heterostructures was also studied. Furthermore, we found that the optical properties of WS$_2$ can be effectively tuned by carriers in graphene in the graphene-WS$_2$ heterostructure.

3:42PM D2.0005 Pressure-Dependent Optical and Vibrational Properties of Monolayer Molybdenum Disulfide, AVINASH NAYAK, UT Austin, TRIBHUWAN PANDEY, Materials Research Center, Indian Institute of Science, Bengaluru, 560-012, India, DAMIEN VOIRY, Department of Materials Science and Engineering, Rutgers University, JIN LIU, Department of Geological Sciences, The University Of Texas at Austin, SAMUEL MORAN, ANKIT SHARMA, CHENG TAN, UT Austin, CHANG-HSIAO CHEN, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, 10617, Taiwan, LAIN-JONG LI, Physical Science and Engineering Division, King Abdullah University of Science & Technology (KAUST), Thuwal 23955, Saudi Arabia, MANISH CHHOWALLA, Department of Materials Science and Engineering, Rutgers University, JUNG-FU LIN, Department of Geological Sciences, The University Of Texas at Austin, ABHISHEK SINGH, Materials Research Center, Indian Institute of Science, Bengaluru, 560-012, India, DEJI AKINWANDE, UT Austin, DEJI AKINWANDE TEAM, ABHISHEK SINGH TEAM, LANCE LI COLLABORATION, MANISH CHHOWALLA COLLABORATION, HPSTAR COLLABORATION, — We study numerically the electron states in silicene and germanene quantum dots within the effective low energy model of silicene and germanene. When subjected to biaxial elastic strain, monolayer MoS$_2$ can embed wide band gap variations overlapping the visible spectrum, with calculations showing the modified electronic potential emanating from point-induced tensile strain perturbations mimicking the Coulomb potential in a mesoscopic atom. We have realized and confirmed this “artificial atom” concept via capillary-pressure-induced nanoindentation of monolayer MoS$_2$ from a tailored nanostructure. We demonstrate that a synthetic lattice of these building blocks forms an optoelectronic crystal capable of broadband light absorption and efficient funneling of photogenerated excitons to points of maximum strain at the atom centers. Such 2D semiconductors with spatially textured band gaps represent a new class of materials which may find applications in next-generation optoelectronics or photovoltaics.

3:54PM D2.00006 Optoelectronic Crystal of Artificial Atoms in Strain-Textured MoS$_2$, ALEX W. CONTRYMAN, HONG LI, ALEX H. FRAGAPANE, Stanford University, XIAOFENG QIAN, SINA MOEINI ARDAKANI, Massachusetts Institute of Technology, YONGJI GONG, XINGLI WANG, Rice University, JEFFREY M. WEISSE, CHI HWAN LEE, JIHENG ZHAO, Stanford University, PULICUEL M. AJAYAN, Rice University, JU LI, Massachusetts Institute of Technology, XIAOLIN ZHENG, HARI C. MANOHARAN, Stanford University — The atomically thin semiconductor MoS$_2$ possesses exceptional strength and a strain-tunable band gap. When subjected to biaxial elastic strain, monolayer MoS$_2$ can embed wide band gap variations overlapping the visible spectrum, with calculations showing the modified electronic potential emanating from point-induced tensile strain perturbations mimicking the Coulomb potential in a mesoscopic atom. We have realized and confirmed this “artificial atom” concept via capillary-pressure-induced nanoindentation of monolayer MoS$_2$ from a tailored nanostructure. We demonstrate that a synthetic lattice of these building blocks forms an optoelectronic crystal capable of broadband light absorption and efficient funneling of photogenerated excitons to points of maximum strain at the atom centers. Such 2D semiconductors with spatially textured band gaps represent a new class of materials which may find applications in next-generation optoelectronics or photovoltaics.

4:06PM D2.00007 Electronic and optical properties of single-layer, double-layer, and bulk SnSe and GeSe, EMMANOUIL KIOUPAKIS, GUANGSHA SHI, Materials Science and Engineering, University of Michigan — We used density functional and many-body perturbation theory to calculate the quasiparticle band structures and optical properties of single-layer, double-layer, and bulk SnSe and GeSe. The calculated direct and indirect band gaps of the bulk materials are in good agreement with experiment. While the electronic band gaps increase by up to 600 meV in the single-layer, double-layer, and bulk SnSe, the transition energy of the n = 1 exciton does not change as a function of thickness. The same trend was also discovered in GeSe. The fundamental band gaps were found to be direct in SnSe and GeSe monolayers. We calculated the absorption spectra for both the bulk and 2-dimensional systems, and determined the light absorbance for light polarization along the in-plane armchair and zigzag directions. This research was supported by the National Science Foundation CAREER award through Grant No. DMR-1254314. Computational resources were provided by the DOE NERSC facility.

4:18PM D2.00008 Light-matter interactions of monolayer semiconductors integrated with photonic microcavities, Y.-J. CHEN, T. STANEV, G. WEI, N. P. STERN, Department of Physics and Astronomy, Northwestern University, J. D. CAIN, V. DRAVID, Materials Science and Engineering, Northwestern University — Enhanced light-matter interactions in optical microcavities can enable hybrid photon-exciton quasiparticle excitations when in a regime of strong light-matter coupling. Because of their direct bandgap, atomic-scale thickness, and strong spin-orbit coupling, monolayers of transition metal dichalcogenides (TMDs) allow for exciton-polaritons in a two-dimensional regime with rich correlations between spin, momentum, and light polarization. We demonstrate integrated TMD photonic devices with MoS$_2$ grown by vapor transport and sandwiched between dielectric Bragg mirrors. We discuss evidence for exciton-polaritons in monolayer TMDs at room temperature using angle-resolved cavity reflectivity spectroscopy. This interpretation is supported by the dependence on MoS$_2$ layer number. Calculations of light-matter coupling parameters in TMDs yield values consistent with recent observations. We discuss our approach to integrated 2D monolayer photonics in the context of the valley-sensitive bandstructure of excitons in TMDs.

1 This work was supported by the National Science Foundation CAREER award through Grant No. DMR-1254314. Computational resources were provided by the DOE NERSC facility.

4:30PM D2.00009 Optical Two Dimensional Fourier Transform Spectroscopy of Layered Metal Dichalcogenides¹, P. DEY, J. PAUL, C.E. STEVENS, Dept of Physics, University of South Florida, Z.D. KOVALYUK, Z.R. KUDRYNSKYI, The National Academy of Sciences of Ukraine, A.H. ROMERO, Dept of Physics, West Virginia University, A. CANTARERO, Material Science, University of Valencia, D.J. HILTON, Dept of Physics, University of Alabama at Birmingham, J. SHAN, Dept of Physics, Pennsylvania State University, D. KARAIKAJ, Dept of Physics, University of South Florida, Z.D.KOVALYUK AND Z.R.KUDRYNSKYI COLLABORATION, A.H.ROMERO COLLABORATION, A. CANTARERO COLLABORATION, D.J.HILTON COLLABORATION, J. SHAN COLLABORATION — Nonlinear two-dimensional Fourier transform (2DFT) measurements were used to study the mechanism of excitonic dephasing and probe the electronic structure of the excitonic ground state in layered metal dichalcogenides. Temperature-dependent 2DFT measurements were performed to probe exciton-phonon interactions. Excitation density dependent 2DFT measurements reveal exciton-exciton and exciton-carrier scattering, and the lower limit for the homogeneous linewidth of excitons on positively and negatively doped samples.

¹U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0012635

4:42PM D2.00010 Layer-structured hexagonal boron nitride carbon semiconductor alloys for deep UV photonics¹, MD RAKIB UDDIN, Research Assistant, Nanophotonics Center, Texas Tech University, JING LI, Research Professor, Nanophotonics Center, Texas Tech University, JINGYU LIN, HONGXING JIANG, Professor, Electrical and Computer Engineering Department, Texas Tech University — Hexagonal boron nitride carbon alloys, \( h-(\text{BN})_{1-x} (\text{C}_2)_x \), are layer-structured semiconductor materials with a tunable bandgap energy from 0 eV (graphite) to 6.5 eV (h-BN). We report on synthesizing (BN)-rich \( h-(\text{BN})_{1-x} (\text{C}_2)_x \) semiconductor alloys using standard MOCVD growth technique on sapphire substrate. Bandgap energy variation with carbon concentration in the deep UV spectral range has been demonstrated through optical absorption measurements. Experimental results suggest that the critical carbon concentration \((x_c)\) to form the homogenous \( h-(\text{BN})_{1-x} (\text{C}_2)_x \) alloys is about 3.2% at a growth temperature of 1300 °C. It is expected that homogenous \( h-(\text{BN})_{1-x} (\text{C}_2)_x \) alloys with higher \( x \) can be achieved by increasing the growth temperature. This is a huge advantage over the InGaN alloy system in which higher growth temperatures cannot be utilized to close the miscibility gap. Together with our ability for producing high quality h-BN epilayers, \( h-(\text{BN})_x \) alloys and quantum wells open up new possibilities for realizing novel 2D optoelectronic devices with tunable physical properties.

¹National Science Foundation

4:54PM D2.00011 Electrically controlled fluorescence quenching of quantum dots on monolayer Molybdenum Disulfide – Part II, ANDREY KLOTS, DHIRAJ PRASAI, Department of Physics and Astronomy, Vanderbilt University, A.K.M. NEWAZ, Department of Physics and Astronomy, San Francisco State University, SCOTT NIEZGODA, NOAH ORFIELD, SANDRA ROSENTHAL, Department of Chemistry, Vanderbilt University, KANE JENNINGS, Chemical and Biomolecular engineering, Vanderbilt University, KIRILL BOLOTIN, Department of Physics and Astronomy, Vanderbilt University — In the second part of this talk, we investigate the mechanisms that enable energy exchange between semiconductor quantum dots (QDs) and two-dimensional (2D) materials. First, we study possible contributions due to multiple mechanisms such as charge transfer, metallic screening, mechanical strain, and Forster resonant energy transfer (FRET). By implementing different 2D materials (graphene, MoS\(_2\), hexagonal boron nitride), varying their thickness and QD emission wavelengths we demonstrate that QD fluorescence quenching is dominated by FRET. Next, we study the dependence of the FRET rate on electrostatic doping of 2D materials, focusing on the case of monolayer MoS\(_2\). We develop a simple model, which shows that that moderate (<10%) changes in MoS\(_2\) absorption induced by gating lead to much larger (∼50%) modulation of QD photoluminescence intensity. Finally, we demonstrate that FRET can be used as an efficient spectroscopic tool that proves states in 2D materials that are not accessible via conventional absorption spectroscopy.

5:06PM D2.00012 Electrically controlled fluorescence quenching of quantum dots on monolayer Molybdenum Disulfide – Part I, DHIRAJ PRASAI, ANDREY KLOTS, Department of Physics and Astronomy, Vanderbilt University, A.K.M. NEWAZ, Department of Physics and Astronomy, San Francisco State University, SCOTT NIEZGODA, NOAH ORFIELD, SANDRA ROSENTHAL, Department of Chemistry, Vanderbilt University, KANE JENNINGS, Chemical and Biomolecular engineering, Vanderbilt University, KIRILL BOLOTIN, Department of Physics and Astronomy, Vanderbilt University — We study hybrid electronic structures in which zero-dimensional semiconductor quantum dots (QDs) are coupled with two-dimensional monolayer molybdenum disulfide (MoS\(_2\)). To fabricate such devices, we mechanically transfer MoS\(_2\) onto a sub-monolayer of QDs assembled on a functionalized glass surface. We investigate quenching of the fluorescence of QDs which are selectively synthesized to have emission spectra which overlap with the excitonic absorption peak (2.1eV) in MoS\(_2\). Both photoluminescence intensity and lifetime for QDs on MoS\(_2\) decrease ∼ 5 times due to near-field energy transfer from QDs to MoS\(_2\). Furthermore, by electrostatically gating MoS\(_2\), we control the rate of energy transfer and modulate the photoluminescence intensity of QDs by ∼ 50%.

5:18PM D2.00013 Energy transfer between quantum dots and 2D materials: graphene versus MoS\(_2\), ARCHANA RAJA, JOHANNA ZULTAK, XIAOXIAO ZHANG, ANDRES MONTOYA-CASTILLO, ZILIANG YE, CYRIELLE ROQUELET, AREND VAN DER ZANDE, DANIEL CHENET, LOUIS BRUS, TONY HEINZ, Columbia University — Understanding charge and energy transfer processes at the interface of nanostructures is an important area of research, both from the fundamental and application points of view. Interactions between 0D semiconductor quantum dots and 2D van der Waals materials have been a subject of recent investigations [1,2]. Here, we report highly efficient near-field energy transfer from core-shell quantum dots to monolayer and few layer graphene, a semi-metal and MoS\(_2\), a semiconductor. We observe both quenching of single quantum dot photoluminescence (PL) and decreasing lifetime in time resolved PL. Our measurements show that increasing the number of layers in the acceptor van der Waals material results in contrasting trends in the rate of non-radiative energy transfer. The energy-transfer rate increases significantly with increasing layer thickness for graphene, but decreases with increasing thickness for MoS\(_2\) layers. Energy transfer rates on the order of 1-10ns\(^{-1}\) are determined. We interpret the results in terms of differences in the interplay between dielectric loss and screening.


Monday, March 2, 2015 2:30PM - 5:30PM
Session D4 APS: Undergraduate Research/Society of Physics Students II — Mayor Cockrell Room 004 - Cortney Bougher, American Physics Society
2:30PM D4.00001 Photoresponsive memory device based on Graphene/Boron Nitride heterostructure . SALMAN KAHN, JAIRO VELASCO JR, LONG JU, DILLON WONG, JUWON LEE, HSIN ZON TSAI, Department of Physics, University of California, Berkeley, TAKASHI TANIGUCHI, KENJI WATANABE, Advanced Materials Laboratory, National Institute for Materials Science, ALEX ZETTL, FENG WANG, MICHAEL CROMMIE, Department of Physics, University of California, Berkeley — Recent technological advancements have allowed the stacking of two dimensional layered material in order to create van der Waals heterostructures (VDH), enabling the design of novel properties by exploiting the proximal interaction between layers with different electronic properties. We report the creation of an optoelectronic memory device using a Graphene/Boron Nitride (hBN) heterostructure. Using the photo-induced doping phenomenon, we are able to spatially ‘write’ a doping profile on graphene and ‘read’ the profile through electrical transport and local probe techniques. We then utilize defect engineering to enhance the optoelectronic response of graphene and explore the effect of defects in hBN. Our work introduces a simple device architecture to create an optoelectronic memory device and contributes towards understanding the proximal effects of hBN on Graphene.

2:42PM D4.00002 High quality factor titanium nitride and aluminum resonators for increased superconducting qubit coherence 1. N. E. FRATTINI, A. DOVE, D. M. TOYLI, S. HACOHEN-GOURGY, A. EDDINS, I. SIDIQI, QNL, University of California, Berkeley — Superconducting qubits have successfully realized effective two–level quantum systems whose state can be read out by dispersive coupling to a linear resonator. Superconducting films which exhibit low loss in the microwave frequency regime at millikelvin temperatures and single photon excitation provide an essential ingredient in realizing high-coherence qubits and high-fidelity readout. To explore the magnitude of these losses and their correlation with fabrication recipes, we prepare and characterize both lumped element and distributed element resonators derived from titanium nitride on silicon and aluminum on sapphire. We study the role of substrate annealing, film growth conditions, and lithographic technique on resonator quality factor.

2:54PM D4.00003 The Characteristic Phase Transitions of Co-doped BaFe2As2 Synthesized via Flux Growth 1. C. H. SHEA, Ithaca College, Department of Physics and Astronomy, C. RONCAIOLI, C. ECKBERG, T. DRYE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, M. C. SULLIAVAN, Ithaca College, Department of Physics and Astronomy, J. PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland — Since the discovery of a new family of type II superconductors in 2008, the iron pnictides, researches have had suspicions that they might bear similar electronic properties to the well-known (but not easily realized) oxide superconductors. For this reason studies of this family of compounds has been of great interest to the materials science community. Our efforts have been aimed at single crystal growth and measurement of a particular member of this family, BaFe2As2. While this material is not superconducting at standard pressure, the partial substitution of cobalt on the iron site has been shown to suppress an anti-ferromagnetic phase transition occurring at lower temperatures allowing for the appearance of a superconducting phase. Transport and low field magnetization measurements taken on our samples show clean transitions, indicating Tc's of up to 24 K in optimally doped samples. We will discuss the growth methods and temperature dependent phase transitions of this material at different cobalt concentrations.

3:06PM D4.00004 ABSTRACT WITHDRAWN

3:18PM D4.00005 Measurements of Viscosity and Dynamics of Thin Films of Organic Glass TPD via Hole Growth Dewetting Studies 1. KAREEM WAHID, University of Texas Pan American, YUE ZHANG, MU LI, ZAHRAR AGHRAI, Department of Chemistry, University of Pennsylvania — In this study, we aim to measure the viscosity of thin glassy films of the small organic molecule N,N-Bis(3-methylphenyl)-N,N-diphenylbenzidine (TPD). Organic glasses such as TPD have various applications in organic light emitting diodes (OLED), and organic photovoltaics. An understanding of the origin for nano-scale properties (e.g. viscosity) would allow for better design of such devices in future applications. Viscosity is simple to measure in bulk systems but challenging at the nanometer scale. Dewetting experiments provide a simple and non-invasive method to measure viscosity in thin film systems. By following dewetting kinetics over time, we are able to identify material related viscous dissipation and substrate related frictional dissipation involved during dewetting. Both homogeneously and heterogeneously nucleated holes have been observed on TPD films of various thicknesses or various substrates. There is reasonable agreement between these observations and with full-slip dewetting models among heterogeneously nucleated holes. However, this is not observed in homogeneously nucleated holes. Careful substrate treatment and control of substrate properties influence the slip length and the dewetting dynamics.

3:30PM D4.00006 Monitoring Residual Solvent Additives and Their Effects in Solution Processed Solar Cells 1, DEREK M. FOGEL, Wake Forest University, JAMES I. BASHAM, NIST and Penn State University, SEBASTIAN ENGMANN, SUJITRA J. POOKPANRATANA, EMILY G. BITTLE, NIST, OANA D. JÜRCHESCU, Wake Forest University, DAVID J. GUNDLÄCH, NIST — High boiling point solvent additives are a widely adopted approach for increasing bulk heterojunction (BHJ) solar cell efficiency. However, experiments show residual solvent can persist for hours after film deposition, and certain common additives are unstable or reactive. We report here on the effects of residual 1,8-diiodooctane on the electrical performance of poly(3-hexylthiophene-2,5-diyl) (P3HT) phenyl-C71-butyric acid methyl ester (PC(71)BM) BHJ photovoltaic cells. We optimized our fabrication process for efficiency at an active layer thickness of 220 nm, and all devices were processed in parallel to minimize unintentional variations between test structures. The one variable in this study is the active layer post spin drying time. Immediately following the cathode deposition, we measured the current-voltage characteristics at one sun equivalent illumination intensity, and performed impedance spectroscopy to quantify charge density, lifetime, and recombination process. Spectroscopic ellipsometry, FTIR, and XPS are also used to monitor residual solvent and correlated with electrical performance. We find that residual additive degrades performance by increasing the series resistance and lowering efficiency, fill factor, and free carrier lifetime.

3:42PM D4.00007 Solution Processed Polymeric Semiconductors for Carbon Nanotube-Enabled, Vertical, Organic Field Effect Transistors 1. ALEXANDER SCHACHTNER2. Dept. of Physics, University of Oregon, NICHOLAS S. CUNNINGHAM, CHRISTOPHER C. SAMOUCHE, MAXIME C. LEMAITRE, ANDREW G. RINZLER, Dept. of Physics, University of Florida — Carbon nanotube-enabled, vertical, organic field effect transistors (CN-FETs) based on the small molecule diphenyl[2,3-b:2′,3′-f]thieno[3,2-b]thiophene (DTNT) have demonstrated high current, low-power operation suitable for driving active matrix organic light emitting diode (AMOLED) displays [1]. This performance is achieved without the need for costly high-resolution patterning, despite the low mobility of the organic semiconductor, by employing sub-micron channel widths, defined in the vertical devices by the thickness of the semiconducting layer. Replacing the thermally evaporated small molecule semiconductor with a solution-processed polymer would possibly further simplify the fabrication process and reduce manufacturing cost. Here we investigate several polymer systems as wide bandgap semiconducting channel layers for potentially air stable and transparent CN-FETs. The field effect mobility and optical transparency of the polymer layers are determined, and the performance and air stability of CN-FVET devices are measured. 1. M. A. McCarthy et al. Science 2011 332, 570

1A. S. gratefully acknowledges support from the National Science Foundation under DMR-1156737
2Work done at the Dept. of Physics, University of Florida
extend lanthanum dititanate’s (LTO), La$_2$Ti$_2$O$_7$, and dimensions in order to optimize the enhancement. Ultimately, we will fabricate devices and characterize the plasmonic properties with optical techniques, which could be useful in a wide range of applications. Finite element methods are used to approximate the electromagnetic responses, giving the ability to alter the designs and more localized plasmonically enhanced electric fields. These unique metal devices encompass tunable, enhanced plasmonic and optical properties that can overcome the resolution limits of traditional electron beam lithography and can also be used to increase resolution in photolithography fabrication as well.

determined enhancement factors and the plasmonic and optical properties of these structures. The nanomasking technique is a new process that is employed in the devices fabricated with a recently developed nanomasking technique that is based on the self-aligned process. Computational electromagnetic modeling has approximated using poor man’s scaling analysis. Here, we focus on using the more accurate numerical renormalization group method to calculate the location of quantum phase transitions around the Fermi energy, then quantum phase transitions will occur. The phase boundaries of the pseudogap Anderson impurity model have been previously approximated using poor man’s scaling analysis. Here, we focus on using the more accurate numerical renormalization group method to calculate the location of these boundaries. We then compare these numerical results with the predictions derived from the scaling approximations. The development of nanotechnology like quantum dots and STM have rekindled interest in the Kondo effect since it can now be studied within controlled settings.

5:06PM D4.00014 Measurement of Specific Heat of Pr$_{1-x}$Nd$_x$Os$_2$Sb$_{12}$ from 11K-300K$^1$ —  TAYLOR MCCULLOUGH-HUNTER, SHOJI HISHIDA, PEI-CHUN HO, Physics Department, California State University, Fresno, BRIAN MAPLE, Physics Department, University of California, San Diego, TATSUYA YANAGISAWA, Physics Department, Hokkaido University, Japan — The filled skutterudite compound Pr$_{1-x}$Nd$_x$Os$_2$Sb$_{12}$ exhibits heavy fermion behavior and unconventional superconductivity at low temperatures (T$_c$ = 1.85K). The exact causes of these behaviors are unknown. The compound Nd$_2$Os$_2$Sb$_{12}$ exhibits ferromagnetism at a Curie temperature near 1 K. Originally, Nd doped compounds of the form Pr$_{1-x}$Nd$_x$Os$_2$Sb$_{12}$ were developed to investigate the effect of ferromagnetism on the unconventional superconductivity and heavy fermion behavior of Pr$_2$Os$_2$Sb$_{12}$. The specific heat of Pr$_{1-x}$Nd$_x$Os$_2$Sb$_{12}$ (where x = 0.25, 0.5, 0.75, 0.8, and 1) is measured at 11K-300K to investigate the compounds' normal state properties. The specific heat is measured using relaxation calorimetry of finite heat pulse in a cryocooler system. Values of the electronic specific heat coefficient, $\gamma$, for these compounds are estimated to be 10-60 mJ/K$^2$.mol. This contrasts with previous low temperature measurements (<10K) of Nd$_2$Os$_2$Sb$_{12}$ with $\gamma$ approximately 520 mJ/K$^2$.mol.

$^1$Research at USF-Fresno is supported by NSF DMR-1104544; at UCSD by NSF DMR-1206533 and US DOE DE FGO2-04ER46105; and at Hokkaido Univ. by MEXT, Japan.

5:18PM D4.00015 Colossal Piezoresistance in strained La$_{0.67}$Sr$_{0.33}$MnO$_3$ thin films$^1$ — MARIA VI-ITANIEMI, IN HAE KWAK, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, FL 32611 — Piezoresistance is the change in electrical resistance as a function of strain. A known mechanism leading to piezoresistance is thermodynamic phase separation. It has been shown that the compound (La$_{1-x}$Pr$_x$)$_{1-x}$Ca$_x$MnO$_3$ (LPCMO) exhibits colossal piezoresistance (CPR) for a wide range of electronic phase separation. For use in many applications, such as sensors, materials must exhibit CPR near room temperature. A possible candidate compound is La$_{0.67}$Sr$_{0.33}$MnO$_3$ (LSMO) which has a Curie temperature of approximately 350 K. However, bulk LSMO single crystals do not show CPR since such samples are uniformly ferromagnetic and metallic with no phase separation. In this study, we examine the piezoresistance of ultrathin LSMO films grown on SrTiO$_3$ (STO) substrates using a three-point beam bending method to control the compressive and tensile strain. It has been suggested that the lattice mismatch strain due to the substrate induces phase separation in these thin films. We have observed CPR in such strained LSMO thin films even at room temperature.

$^1$NSF DMR-1410237

Monday, March 2, 2015 2:30PM - 5:30PM — Session D5 FIAP: Fractional Quantum Hall Effect III

2:30PM D5.00001 Position-Momentum Duality, Geometrical Description and Ideal Host Lattices for Fractional Chern Insulators — MARTIN CLAASSEN, Department of Applied Physics, Stanford University, CHING-HUA LEE, Department of Physics, Stanford University, RONNY THOMALE, Institute for Theoretical Physics, University of Wuerzburg, XIAO-LIANG QI, Department of Physics, Stanford University, THOMAS DEVEREAUX, SLAC National Accelerator Laboratory, Stanford Institute for Materials and Energy Sciences — The recent discovery of fractional quantum Hall (FQH) physics in flat-band Chern insulators without external magnetic field presents a profound theoretical challenge to understand the interplay of universal long-wavelength physics of the FQH effect and short-wavelength physics determined by the host lattice. Here, we present a first quantization description of fractional Chern insulators that is dual of the anisotropic FQH problem, with the roles of position and momentum interchanged. The fundamental guiding-center geometry of the problem emerges from the interplay of lattice and interaction metrics that act as momentum-space duals of Haldane’s geometrical description of the anisotropic FQH effect. We introduce a novel broad class of ideal C$_2$1 Chern insulator lattice models that are duals of the isotropic limit of the conventional FQH effect. These models afford a particularly elegant analytical framework and act as parent Hamiltonians for lattice FQH states with emergent guiding-center and SU(C) symmetry. Resulting microscopic insight into stabilization of FQH states on the lattice provides a foundation for future analyses of non-Abelian phases and fractional topological insulators.

2:42PM D5.00002 Projective construction of the $Z_k$ Read-Rezayi fractional quantum Hall states and their excitations on the torus geometry — CECILE REPPELLIN, Ecole Normale Superieure, France, TITUS NEUPERT, Princeton center for theoretical science, B. ANDREI BERNEVIG, Princeton University, NICOLAS REGNAULT, Ecole Normale Superieure, France, Princeton university — The torus is an ideal mathematical object for developing projective construction methods for fractional quantum Hall states and their excitations. We use the independence of these states on the choice of projective construction method as a tool to construct new models of fractional quantum Hall states.
3:06PM D5.00004 Magneto-transport characteristics of a 2D electron system driven to negative magneto-conductivity by microwave photoexcitation1. RAMESH MANI, Georgia State University, A. KRIISA, Emory University — Negative diagonal magneto-conductivity/resistivity is a spectacular and thought provoking property of driven, far-from-equilibrium, low dimensional electronic systems. The physical response of this exotic electronic state is not yet fully understood since it is rarely encountered in experiment. The microwave-radiation-induced zero-resistance state in the high mobility GaAs/AlGaAs 2D electron system is believed to be an example where negative magneto-conductivity/resistivity is responsible for the observed phenomena. Here, we examine the magneto-transport characteristics of this negative conductivity/resistivity state in the microwave photo-excited two-dimensional electron system (2DES) through a numerical solution of the associated boundary value problem. The results suggest, surprisingly, that a bare negative diagonal conductivity/resistivity state in the 2DES under photo-excitation should yield a positive diagonal resistance with a concomitant sign reversal in the Hall voltage.

1Transport measurements are supported by the DOE, Office of Basic Energy Sciences, Material Sciences and Engineering Division under DE-SC0001762. Additional support by the ARO under W911NF-07-01-015

3:18PM D5.00005 Non-Abelian two dimensional topological phases constructed from coupled wires and connections to exceptional lie algebras. MAYUKH KHAN, Department of Physics, University of Illinois at Urbana-Champaign, IL 61801, USA, JEFFREY TEO, Department of Physics, University of Virginia, Charlottesville, VA 22904 USA, TAYLOR HUGHES, Department of Physics, University of Illinois at Urbana-Champaign, IL 61801, USA — Non-abelian anyons exhibit exotic braiding statistics which can be utilized to realize a universal topological quantum computer. In this work we focus on Fibonacci anyons which occur in Z2 Read Rezayi fractional quantum hall states. Traditionally they have been constructed using su(2)/u(1) coset theories. We introduce conformal field theories (CFTs) of exceptional and non-simply laced Lie Algebras at level 1, for example G2, F4 which host Fibonacci anyons. We realize these CFT’s concretely on the 1d gapless edge of an anisotropic 2d system built out of coupled, interacting Luttinger wires. Interactions are introduced within a bundle of wires to fractionalize the original chiral bosons into different sectors. Next, we couple these sectors to get the desired topological phase in the bulk. The 2d bulk of the stack is gapped by backscattering terms between counterpropagating modes on different bundles. The emergence of this topological phase can be interpreted using techniques of anyon condensation. We also explicitly construct the Kac Moody algebra on the edge CFT using original bosonic degrees of freedom. We acknowledge support from NSF CAREER DMR-1351895 (TH) and Simons Foundation (JT).

3:30PM D5.00006 Variational study of bosonic phases in two dimensions: fractional Chern insulator, Mott insulator and superfluid. BRYAN CLARK, HASSAN SHAPOURIAN, University of Illinois at Urbana Champaign — We numerically study the model wave functions for a system of hard core bosons at half filling on a square lattice. The candidate wave functions are based on the projective construction approach [1] where a boson is decomposed into two (slave) fermions, each described by a Chern insulator model. Our results confirm that the wave functions demonstrate the following phases: the superfluid, the Mott insulator and the fractional Chern insulator. In addition, we find that the wave functions can be continuously tuned from one phase to another by varying the parameters of slave particles. We further propose a microscopic Hamiltonian with a rich phase diagram which supports all the aforementioned phases in different regimes of parameters. The critical behavior across the phase boundaries is investigated and the critical exponents are computed. [1] M. Barkseshi and J. McGreevy, Phys. Rev. B 89, 235116 (2014).

3:42PM D5.00007 Pairing in half-filled Landau level1. ZHIQIANG WANG, UCLA, IPSITA MANDAL, Perimeter Institute for Theoretical Physics, Canada, SUDIP CHAKRAVARTY, UCLA — Pairing of composite fermions in half-filled Landau level state is reexamined by solving the BCS gap equation with full frequency dependent current-current interactions. Our results show that there can be a continuous transition from the Halperin-Lee-Read state to a chiral odd angular momentum Cooper pair state for short-range contact interaction. This is at odds with the previously established conclusion of first order pairing transition, in which the low frequency effective interaction was assumed for the entire frequency range. We find that even if the low frequency effective interaction is repulsive, it is compensated by the high frequency regime, which is attractive. We construct the phase diagrams and show that l = 1 angular momentum channel is quite different from higher angular momentum channel l ≥ 3. Remarkably, the full frequency dependent analysis applied to the bilayer Hall system with a total filling fraction ν = 1/2 + 1/2 is quantitatively changed from the previously established results but not qualitatively.


1This work was supported by US NSF under the Grant DMR-1004520, the funds from the David S. Saxon Presidential Chair at UCLA (37952), and by the Institute for Basic Science in Korea through the Young Scientist grant (5199-2014003).

3:54PM D5.00008 What Determines the Fermi Wave Vector of Composite Fermions1. DOBROMIR KAMBUROV, Princeton Univ, YANG LIU, M.A. MUEED, MANSOUR SHAYEGAN, LOREN PFIEFFER, KENNETH WEST, KIRK BALDWIN, Princeton University — We report the observation of a pronounced asymmetry in the magnetic field positions of the commensurability resistance minima of fully spin-polarized composite fermions (CFs) with respect to the field at ν = 1/2 in two-dimensional (2D) electron and hole systems. The asymmetry is observed across a wide range of 2D densities and modulation periods. We present evidence the asymmetry quantitatively if we assume that the CFs are fully spin-polarized and their density is equal to the density of the minority carriers in the lowest, spin-resolved Landau level (LL), namely the density of electrons when ν < 1/2 and of holes when ν > 1/2. Our results provide direct evidence that CFs are formed by pairing up of the minority carriers in the lowest spin-resolved LL with flux quanta. They further indicate that the CF commensurability minima are not observed at ν and (1 − ν), as expected from a simple particle-hole symmetry principle, pointing to a subtle breaking of this symmetry.

1We acknowledge support through the DOE BES (DEFG02-00-ER45841), the Gordon and Betty Moore Foundation (Grant GBMF4420), Keck Foundation, NSF (ECCS-1001719, DMR-1305691, and MRSEC DMR-0819860). A portion of this work was performed at the NHMFL.

4:06PM D5.00009 Continuous preparation of a fractional Chern insulator. CHRISTOPHER LAUMANN, University of Washington, MAISSAM BARKESHLI, Microsoft Station Q, NORMAN YAO, University of California, Berkeley — We present evidence of a direct, continuous quantum phase transition between a Bose superfluid and the ν = 1/2 fractional Chern insulator in a microscopic lattice model. In the process, we develop a detailed field theoretic description of this transition in terms of the low energy vortex dynamics. The theory explicitly accounts for the structure of lattice symmetries and predicts a Landau forbidden transition that is protected by inversion. That the transition is continuous enables the quasi-adiabatic preparation of the fractional Chern insulator in non-equilibrium, quantum optical systems.
4:18PM D5.00010 Optical Signatures of Competing Quantum Phases in the Second Landau Level1. ANTONIO LEVY, Columbia University Department of Physics, URSULA WURSTBAUER, Technische Universität München Department of Physics, ARON PINCZUK, Columbia University Department of Physics, JOHN WATSON, GEOFF GARDNER, MICHAEL MANFRA, Purdue University Department of Physics, KEN WEST, KIRK BALDWIN, LOREN PFEIFFER, Princeton University Department of Electrical Engineering — The fractional quantum Hall states and anisotropic phases of electrons in the N=1 Landau Level (LL) have drawn considerable experimental focus in recent years[1-3]. We report evidence that the competition and coexistence of these phases is probed directly by optical recombination from the partially populated N=1 LL at dilution refrigerator temperatures. Spectral bands that display striking dependence on perpendicular magnetic field in the full range 3−8 T are interpreted as linked to anisotropic phases. Optical recombination thus enables the monitoring of the evolution competing phases as the N=1 LL filling is changed. Remarkable changes in the optical recombination reveal that coexistence of distinct quantum phases has a marked dependence on filling of the N=1 LL. The signatures of anisotropic phases remain strong at filling factors of the FQHE. This is consistent with recent reports on anisotropic IQHE states in the second Landau level[1-3]. References: [1] J. Xia et al, Phys. Rev. Lett. 105, 176807 (2010). [2] J. Xia, J.P. Eisenstein, L.N. Pfeiffer, and K. West, K.W. Nature Phys. 7, 845–848 (2011). [3] Y. Liu, et al, Phys. Rev. B 88, 035307 (2013).

3Supported by award NSF-DMR-1306976.

4:30PM D5.00011 DMRG Study of a $\nu = 1/3 + 1/3$ Bilayer Fractional Hall System, SCOTT GERAEDTS, California Institute of Technology, MICHAEL ZALETEL, Microsoft Station Q, ZLATKO PAPIĆ, Perimeter Institute, ROGER MONG, University of Pittsburgh — DMRG Study of a $\nu = 1/3 + 1/3$ Bilayer Fractional Hall System Bilayer quantum Hall systems provide new experimental parameters that generate a rich phase diagram proposed to contain a new non-Abelian phase. We use the density matrix renormalization group (DMRG) and exact diagonalization to study a bilayer quantum Hall system with filling fraction 1/3 per layer. Using this method, we can study the phase diagram in terms of parameters such as interlayer separation, interlayer tunnelling, layer width, and density imbalance between the layers. We identify the possible phases based on their entanglement properties and determine the order of phase transitions. Prospects for stabilizing new non-Abelian phases with small perturbations to the Coulomb interaction will be discussed.

4:42PM D5.00012 Microwave spectroscopic observation of multiple phase transitions in the bilayer electron solid in wide quantum wells, ANTHONY HATKE, LLOYD ENGEL, NHMFL, YANG LIU, MANSOUR SHAYEGAN, LOREN PFEIFFER, KEN WEST, KIRK BALDWIN, Princeton University — The termination of the low Landau filling factor ($\nu$) fractional quantum Hall series for a single layer two dimensional system results in the formation of a pinned Wigner solid for $\nu < 1/5$ [1]. In a wide quantum wells the system can support a bilayer state in which interlayer and intralayer interactions become comparable, which is measured in traditional transport as an insulating state for $\nu < 1/2$ [2]. We perform microwave spectroscopic studies of this bilayer state and observe that this insulator exhibits a resonance, a signature of a solid phase. Additionally, we find that as we increase the density of the well at fixed $\nu$ this bilayer solid exhibits multiple sharp reductions in the resonance amplitude vs $\nu$. This behavior is characteristic of multiple phase transitions, which remain hidden from dc transport measurements.


5:00PM D5.00014 Collapse of the $\nu = 1$ quantum Hall effect near a Landau level crossing1. SUKRET HASDEMIR, YANG LIU, M.A. MUEED, LOREN PFEIFFER, KEN WEST, KIRK BALDWIN, MANSOUR SHAYEGAN, Princeton University — We report magneto-resistance measurements of 2D hole systems (density $2.1 \times 10^{11}$ cm$^{-2}$) confined to a 40-nm-wide GaAs quantum well as a function of tilted magnetic fields. We observe a strong $\nu = 1$ quantum Hall effect (QHE) at zero parallel field ($B_{||}$). The $\nu = 1$ QHE disappears at $B_{||} \approx 4.8$ T, where we expect a crossing between the lowest two Landau levels. Near this crossing, the energy gap for the $\nu = 1$ QHE collapses from 6 K to zero in a very small $B_{||}$ range of 0.3 T. The $\nu = 1$ QHE comes back at $B_{||} \approx 8.1$ T and eventually disappears at $B_{||} > 17$ T where the system becomes bilayer-like. The sudden collapse of the $\nu = 1$ QHE and the fact that it comes back after a large $B_{||}$ range of 3.3 T is intriguing and suggests a pinning of the Landau levels near the crossing.

1We acknowledge support through the NSF (DMR-1305691, DMR-1310199 and MRSEC DMR-0819860), the DOE BES (DE-FG02-00-ER45841), the Gordon and Betty Moore Foundation (Grant GBMF4420), and the Kwon Foundation.

5:18PM D5.00015 Exact diagonalization study of $\nu = 1/3 + 1/3$ bilayer quantum Hall in search of Fibonacci anyons1. EUN-AH KIM, ABOLHASSAN VAEZI, KYUNGMIN LEE, Cornell University — Non-abelian states with Fibonacci anyons that can support universal topological quantum computation have been elusive. Recently it has been proposed that a remarkably simple setting of Abelian quantum Hall bilayer could support an exotic state with Fibonacci anyons (Vaezi and Barkeshli, arXiv:1403.3383). Here we explore $\nu = 1/3 + 1/3$ bilayer quantum Hall system considering different possibilities for interaction between bilayers using exact diagonalization. We find a sizable region in phase space potentially exhibiting topological degeneracy expected of Fibonacci anyon states.

1This work has been supported by NSF CAREER with grant number DMR-0955822

Monday, March 2, 2015 2:30PM - 5:30PM – Session D6 DMP DCOMP: Focus Session: Domain Walls, Surfaces, Interfaces 006A - Xiaqing Pan, University of Michigan
2:30PM D6.00001 Universal intrinsic origin for ferroelectric domain wall motion¹, SHI LIU, ILYA GRINBERG, ANDREW RAPPE, The Makeni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania — The existence of domain walls in ferroelectric materials can have a profound influence on the properties of ferroelectrics [1]. We explored the dynamics of the 90° domain walls in PbTiO$_3$ with molecular dynamics simulations [2] under a wide range of temperatures and electric fields. We found an intrinsic “creep-depinning” transition for the temperature- and field-dependence of the wall velocity, resulted from the nucleation-and-growth mechanism. By mapping non-180° domain walls to a 180° domain wall, we proposed an analytical model that is able to quantify the dynamics of all types of domain walls in various ferroelectrics, enabling rapid estimation of the domain wall velocity with first-principles inputs. This work offers a unified picture for domain wall motion and an efficient framework for computational optimization of ferroelectrics.


¹NSF ONR DOE HPCMO NERSC

2:42PM D6.00002 Anomalous Dielectric Loss at Ferroelectric Domain Walls Revealed by Microwave Impedance Microscopy, XIAOYU WU, YUAN REN, Department of Physics, University of Texas at Austin, RONGWEI HU, SANG-WOOK CHEONG, Department of Physics and Astronomy, Rutgers University, KEJI LAI, Department of Physics, University of Texas at Austin — Domain walls (DWs) in multiferroic materials, within which the ferroic order parameter changes its orientation, may possess emergent properties that are absent in the bulk domains. Combining the standard piezo-force microscopy (PFM), conductive atomic-force microscopy (C-AFM), and a novel microwave impedance microscopy (MIT), we observed strong dielectric loss at the domain walls and vortex cores on the (001) charge neutral surface of hexagonal manganite in the bulk domains. We explored the dynamics of the 90° microdomains (MIM) technique, we observed strong dielectric loss at the domain walls and vortex cores on the (001) charge neutral surface of hexagonal manganite YMnO$_3$. The DW contrast was detected for a broad frequency range between 100MHz and 3GHz. The equivalent DW conductivity inferred from the MIM images is estimated to be five orders of magnitude higher than that of the bulk YMnO$_3$, which cannot be explained within the existing theoretical framework. By applying a DC bias on the MIM probe, we have also observed the transition from DW contrast to domain contrast in the impedance images. The MIM technique provides a unique opportunity to probe the nanoscale electronic anomalies in various topological defects, which will be crucial for future device applications of multiferroics.

2:54PM D6.00003 All-Epitaxial Ferroelectric Tunnel Junctions with Ultrathin BaTiO$_3$, DANIEL SANDO, SEUNGRAN LEE, YEONG JAE SHIN, Center for Correlated Electron Systems, IBS, Seoul National University, MYEONG RAE CHO, YUN PARK, Department of Physics and Astronomy, Seoul National University, TAE WON NOH, Center for Correlated Electron Systems, IBS, Seoul National University — Ferroelectric tunnel junctions (FTJs) are a promising route toward the development of high density, nonvolatile memories with non-destructive readout [1]. The principle of operation is polarization-dependent tunneling electroresistance (TER). The direction of polarization in the ferroelectric layer defines high and low resistance states. So far, the most impressive results regarding TER ON/OFF ratios have been either without a top electrode, or using a top electrode of a non-oxide metal. However, defects in the ferroelectric [2] or interfacial layer can reduce performance. To overcome these limitations, we have fabricated fully-strained epitaxial FTJs using perovskite oxides for all layers. L$_{3a}$Sr$_{0.7}$Fe$_{1.3}$MnO$_3$/BaTiO$_3$/SrRuO$_3$/SrTiO$_3$. The heterostructures are grown by pulsed laser deposition at high substrate temperatures of 900°C. The electrodes are patterned using e-beam lithography. Piezoresistance and microwave impedance microscopy shows that ferroelectricity is maintained for a barrier thickness as low as 3 unit cells. We present our results on TER performance and the dependence of switching properties on the BaTiO$_3$ thickness. [1] V. Garcia, et al. Nature 460, 81-84 (2009). [2] M. Dawber, K. M. Rabe, J. F. Scott, Rev. Mod. Phys. 77, 1083 (2005).

3:06PM D6.00004 Direct visualization of magnetoelectric domains in hexagonal manganites¹, WEIDA WU, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, 08854, USA — Multiferroics are materials with coexisting magnetic and ferroelectric orders, where the cross-coupling between two ferroic orders can result in strong magnetoelectric effects [1-4]. Therefore, it is of both fundamental and technological interest to visualize cross-coupled magnetoelectric domains and domain walls in multiferroics. Recently, introducing top electrodes of six interlocked structural antiphase and ferroelectric domains merging into a vortex core were revealed in multiferroic hexagonal R$^e$Mn$_3$O$_7$ (RE=rare earths) [5, 6]. Many emergent phenomena, such as enhanced conduction and unusual piezoelectric response, were observed in charged ferroelectric domain walls protected by these topological defects [7-9]. More interestingly, alternating uncompensated magnetic moments were discovered at coupled structural antiphase and ferroelectric domain walls in hexagonal manganites using cryogenic magnetic force microscopy (MFM) [10], which demonstrates the cross-coupling between ferroelectric and magnetic orders. Using a newly-developed Magnetoelectric Force Microscopy (MeFM), which combines MFM with in-situ modulating high electric fields, we directly visualize the magnetoelectric response of the multiferroic domains in hexagonal manganites. The development of MeFM opens up explorations of emergent phenomena in multifunctional materials with multiple coupled orders [11, 12].


³The work is supported by DOE BES under Award # DE-SC0008147.

3:42PM D6.00005 Dynamical magnetoelectric effects associated with ferroelectric domain walls¹, SERGEY PROSANDEEV, Univ of Arkansas-Fayetteville, ANDREI MALASHEVICH, Yale University, New Haven, IGOR RAEVSKI, Southern Federal University, Rostov-na-Donu, LAURENT BELLAICHE, Univ of Arkansas-Fayetteville — Molecular dynamics simulations using a first-principles-derived effective Hamiltonian are conducted on lead zirconium titanate ultrathin films possessing nanoscale ferroelectric domains and being under GHz electric field. Pulses of magnetization are predicted to occur in this system, when sudden changes of magnetization result from switching of ferroelectric domains. A simple equation relating the magnetization and product between the electrical polarization and its time derivative is further derived from a simple model (via the relation between the magnetization and time derivative of the so-called electrical toroidal moment). This equation naturally explains our numerical findings, as well as previously observed magnetoelectric effects in moving ferroelectric domain walls/phase boundaries in ferroelectrics and magnetoelectrics.

¹ONR Grants N00014-11-1-0384 and N00014-12-1-1034. 14-02-90438 Ucr,a of the RFBR.
3:54PM D6.00006 First-principles study of the effect of oxygen vacancies around the 180° ferroelectric domain walls of tetragonal PbTiO$_3$. HOE-CHEOL SONG, HYE JUNG KIM, YOUNG-HAN SHIN*, University of Ulsan. People have extensively studied the dynamics of ferroelectric materials to apply them to nonvolatile memory devices. One of the issues in ferroelectric random access memory is the fatigue effect, which results from the presence of oxygen vacancy. Many cycles of polarization switching increase the density of oxygen vacancy around ferroelectric domain walls, and it makes the ferroelectric energy barrier higher to slow down the switching rate. In this presentation, we examine the domain dynamics around the 180° ferroelectric domain walls of tetragonal PbTiO$_3$ with and without the oxygen vacancy by using the first-principles calculations. We estimate the energy barriers of several possible reaction paths with the nudged elastic band method. Compared to the oxygen vacancy far away from domain walls, the oxygen vacancy around ferroelectric domain walls tends to be thermodynamically stable with lower energy barriers. Finally, we expect that by controlling of oxygen vacancy density around the ferroelectric domain wall could be the solution for solving fatigue problem in ferroelectric materials.

4:06PM D6.00007 Pinning of Ferroelectric Domain Walls in Nanostructured CoFe$_2$O$_3$-BiFe$_3$O$_4$ Composite, KEREN FREEDY, RYAN COMES, University of Virginia. Department of Materials Science and Engineering, Charlottesville, VA, KERRY SIEBEN, National Institute of Standards and Technology, Center for Nanoscale Science and Technology, Gaithersburg, MD, JIWEI LU, University of Virginia, Department of Materials Science and Engineering, Charlottesville, VA, STUART WOLF, University of Virginia, Department of Materials Science and Engineering, Department of Physics, Charlottesville, VA — Ferroelectric domain walls in BiFe$_3$O$_4$ thin films have attracted interest due to the observation of enhanced electronic transport at the domain walls in an otherwise insulating material. To understand the properties of domain walls in nanostructured thin films having matrix-pillar morphology, thin films of CoFe$_2$O$_3$ (CFO)-BiFe$_3$O$_4$ were grown epitaxially by pulsed electron deposition on SrTiO$_3$ (STO) substrates. Piezoresistance, force microscopy (PFM) measurements indicate that the vertically-oriented CFO nanopillars act as pinning sites for the in-plane domain walls. The pinning effect is most likely due to misfit dislocations at the matrix/pillar interface which have been identified in transmission electron microscopy images. The ability to produce ordered nanocomposites by directed self-assembly offers potential for more extensive investigation of domain wall behavior.

4:18PM D6.00008 Ferroelectric Striped Nanodomains in PbTiO$_3$/SrTiO$_3$ Superlattice Islands, QINGTENG ZHANG, JOONKYU PARK, Univ of Wisconsin, Madison, ROSS HARDER, JORG M. MASER, Argonne National Laboratory, MOHAMMED YUSUF, MATTHEW DAWBER, Stony Brook University, PAUL G. EVANS, Univ of Wisconsin, Madison — The ferroelectric remnant polarization of isolated, unscreened ferroelectric layers in ultrathin films or ferroelectric/dielectric superlattices spontaneously forms striped domains to minimize the total electrostatic energy. The X-ray scattering patterns of domains in a PbTiO$_3$/SrTiO$_3$ ferroelectric/dielectric superlattice indicate that the striped domains have a highly disordered arrangement with an average period of approximately 8 nm. Isolated superlattice islands have been fabricated with lengths of 2 μm and widths ranging from 150 nm to 800 nm using focused ion beam (FIB) patterning. Coherent x-ray scattering patterns show that the striped domain pattern is preserved in the nanopatterned islands. Neither the width nor the in-plane coherence length of the domains have shown any meaningful dependence on the width of the island. In addition, the correlation of the coherent scattering patterns indicates that the temporal fluctuation of the domain patterns is different from what has been previously observed in the unpatterned areas. We expect that such difference be due to the mechanical boundary introduced by the FIB etching.

4:30PM D6.00009 Electrical and Magnetic Properties of PbTiO$_3$/SrRuO$_3$ superlattices, HSJING-HUNG HSING, SARA CALLORI, JUDITH GABEL, SIMON DIVILOV, PIRANAVAN KUMARAVADIVEL, XU DU, MARIVI FERNÁNDEZ-SERRA, MATTHEW DAWBER., Stony Brook University — Theoretical calculations on PbTiO$_3$/SrRuO$_3$ (PTO/SRO) superlattices suggest that the SRO layer should retain metallic character, even when their thickness is only a single unit cell. They further suggest that when the SRO layer is 2 unit cells or thicker there is coupling between spin and the electric polarization. Here we report on the electrical transport properties of PTO/SRO superlattices, which were fabricated using off-axis RF magnetron sputtering. In the out of plane direction, the samples demonstrate ferroelectricity and tunneling current characteristics that confirm the metallicity of the SrRuO$_3$ layers. We also studied the impact of the compositionally broken inversion symmetry and magnetic field on the capacitance-voltage characteristic of our superlattices. Changes in the dielectric constant were induced by the application of magnetic field at low temperatures.

5:45PM D6.00011 Fluctuating defects in the incipient relaxor K$_{x}$Li$_{1-x}$TaO$_3$ (x = 0.02), PETER GEHRING, NIST · Natl Inst of Stds & Tech, CHRIS STOCK, University of Edinburgh, GUANGYONG BU, Brookhaven National Lab, DANIEL LAMAGO, Karlsruher Inst fur Technologie, DMITRY REZNICH, University of Colorado, MARGARITA RUSSINA, Helmholtz Zentrum Berlin, JINSHENG WEN, Nanjing University, LYNN BOATNER, Oak Ridge National Lab — We have measured the structural correlations associated with the apparent relaxor transition near 70 K in K$_{0.98}$Li$_{0.02}$TaO$_3$ (KLT(0.02)) with neutrons. No elastic diffuse scattering or soft mode anomaly is observed, a situation that diverges from that in other relaxors like PMN. The structural correlations in KLT(0.02) are dynamic at all temperatures with timescales of ~THz. The fluctuations are overdamped, non-propagating, spatially uncorrelated, and absent in the parent material KTaO$_3$. The temperature dependence correlates with the dielectric response, implying that the fluctuations are associated with local, ferroelectric regions induced by the Li-doping. The ferroelectric transition induced by the introduction of sufficient Li cations is thus characterized by quasistatic fluctuations, which is a stark contrast to the soft-harmonic-mode-driven transition observed in perovskite ferroelectrics like PbTiO$_3$. The glass-like structural correlations in KLT(0.02) are much faster than those in random-field, lead-based relaxors, which occur on the ~GHz timescale, and they are better correlated spatially. Our results support the view that random fields give rise to the relaxor phenomena, and that the glassy dynamics observed here represent a nascent response.

5:06PM D6.00012 Polar State in Freestanding Strontium Titanate Nanoparticles, TREVOR TYSION, TIAN YU, New Jersey Institute of Technology, MARK CROFT, Rutgers University, MEGAN SCOFIELD, DARIE BOBB-SEMPLE, State University of New York at Stony Brook, JING TAO, Brookhaven National Laboratory, CHERNO JAYS, DANIEL FISCHER, National Institute of Standards and Technology, STANISLAUS WONG, State University of New York at Stony Brook — Monodispersed strontium titanate nanoparticles were prepared and studied in detail. It is found that ~10 nm as-prepared stoichiometric nanoparticles are in a polar structural state (with possibly ferroelectric properties) over a broad temperature range. A tetragonal structure, with possible reduction of the electronic hybridization is found as the particle size is reduced. In the 10 nm particles, no change in the local Ti off-centering is seen between 20 and 300 K. This work is supported by DOE Grant DE-FG02-07ER46402.
Monday, March 2, 2015 2:30PM - 5:30PM –
Session D7 DMP DCMP: Focus Session: Synthesis & Characterization of Topological Insulators

006B - Anthony Richardella, Pennsylvania State University

2:30PM D7.00001 Single crystal growth and characterization of Na$_3$Bi and Bi$_2$Te$_2$Se topological materials$^1$. SATYA K. KUSHWAHA, JASON W. KRIZAN, R.J. CAVA, Princeton University — In recent years, the discoveries of topological insulators (TI) and three-dimensional (3D) Dirac semimetals (TDS) have been of significant interest in condensed matter science. To study these materials experimentally, it is of great importance to grow them in the form of high quality single crystals. Na$_3$Bi is recently discovered TDS and Bi$_2$Te$_2$Se$_2$ (BTS) is one of the interesting TI materials. Na$_3$Bi is extremely air sensitive and shows nontrivial crystallization behavior. BTS crystals usually grow with various point defects and typically exhibit metallic behavior. Here we will report the crystal growth of high quality Na$_3$Bi and insulating BTS single crystals. The characterization of their electronic properties by our collaborators in physics at Princeton and Brookhaven National Laboratory will be briefly described.

$^1$The growth of single crystals of TIs and TDS is supported at Princeton by grants from the ARO MURI and DARPA.

2:42PM D7.00002 Intrinsic conduction through topological surface states of insulating Bi$_2$Te$_3$ epitaxial thin films$^1$. KATHARINA HOEFER, CHRISTOPH BECKER, DIANA RATA, Max Planck Institute for Chemical Physics of Solids, Dresden, JESSE SWANSON$^2$, University of British Columbia, Vancouver, PETER THALMEIER, LIU HAO T.JEUNG, Max Planck Institute for Chemical Physics of Solids, Dresden — Topological insulators represent a novel state of matter with surface charge carriers having a massless Dirac dispersion and locked helical spin polarization. Many exciting experiments have been proposed by theory, yet, their execution have been hampered by the extrinsic conductivity associated with the unavoidable presence of defects in Bi$_2$Te$_3$ and Bi$_2$Se$_3$ (BTS) is one of the interesting TI materials. Na$_3$Bi is extremely air sensitive and shows nontrivial crystallization behavior. BTS crystals usually grow with various point defects and typically exhibit metallic behavior. Here we will report the crystal growth of high quality Na$_3$Bi and insulating BTS single crystals. The characterization of their electronic properties by our collaborators in physics at Princeton and Brookhaven National Laboratory will be briefly described.

$^1$K. Hoefer et al. PNAS, 2014, 111(42), 14979-14984
$^2$J. Swanson was supported by the Max-Planck – UBC centre for Quantum Materials

2:54PM D7.00003 Stability investigation on the non-basal surfaces of topological insulator Bi$_2$Te$_3$: a first-principles study$^1$. NA WANG, Tsinghua Univ, YIYANG SUN, Rensselaer Polytechnic Institute, YUANG ZHANG, Vanderbilt University, DAMIEN WEST, Rensselaer Polytechnic Institute, WENHUI DUA, Tsinghua Univ, SHENGBAI ZHANG, Rensselaer Polytechnic Institute — The basal (0001) surface of Bi$_2$Te$_3$ is the most stable surface and has been predominantly observed in experiment and studied in great details. The stability of other surfaces has been rarely discussed so far despite the fact that vicinal surfaces are always present at the crystal edges. In this work, we systematically study the thermodynamic stability of the vicinal surfaces of Bi$_2$Te$_3$ based on first-principles calculations. In particular, it is found that the (0015) surface has a surface energy of only about two times larger than that of the (0001) surface. Due to the particularly low surface energy, the sidewalks of free-standing Bi$_2$Te$_3$ crystals are predicted to be the (0015) surface, which is not perpendicular to the basal (0001) surface. The Wulff construction based on our calculated surface energies is consistent with experiment. However, in the presence of substrates, e.g., in molecular beam epitaxial growth, the shape of a crystal flake is further affected by the interface energy. In this case, the sidewalks could be (0110), (011 10) or (0114) depending on the binding strength between the flake and the substrate.

3:06PM D7.00004 Measuring Surface and Bulk Conductance of a Topological Insulator Using Top and Bottom Contacts$^1$. YUN SUK EO, STEVEN WOLGAST, CAGLIYAN KURDAK, Randall Laboratory of Physics, University of Michigan - Ann Arbor — In most 3D topological insulators, the existence of bulk conduction makes electrical transport measurements of the surface conduction very challenging. Standard transport measurements that are performed only on one side of a bulk crystal are not capable of distinguishing surface conduction from bulk conduction. Recently, configurations that measure top and bottom surfaces together have enabled researchers to distinguish surface conduction from bulk conduction in the mixed-valence compound SnB$_6$F$_6$. Inspired by these measurements, we analyze different types of top/bottom transport geometries such as a Corbino disc patterned on the top surface/a metal disc patterned on the bottom surface, a four-probe measurement on the top/entirely metalized on the bottom, etc. by numerical simulations. Although each configuration has certain limitations, the surface and bulk conductance can be found respectively from our results.

$^1$This project was funded by NSF grant #DMR-1006500 and DMR-1441965.
$^3$D. Kim et al., Scientific Reports 3, 3150 (2013)
various orientations of the magnetic field \((B)\). Interestingly, it was found that the \(B\) showed a clear oscillation signal under the in-plane \(B\). In addition, the observed oscillation was quite periodic in \(1/B\) implying that the Landau quantization plays a role. As the orientation of \(B\) was rotated toward the direction perpendicular to the plane, the oscillation signal disappeared and the resistance showed a very sharp decrease at low magnetic fields, which was consistent with the weak antilocalization (WAL) behavior. Those new findings are believed to be related to the nature of \(Bi\textsubscript{2}Te\textsubscript{3}\) films as a topological insulator (TI) and to unveil the unexplored aspects of TIs waiting for an explanation.

3:30PM D7.0006  Study of long-time aging effect on low carrier MBE-grown Bi2Se3 with various capping layers . MARYAM SALEHI, MATTHEW BRAHLEK, NIKESH KOIRALA, SEONGSHIK OH, Rutgers university — Although there have been a lot of advances in the growth engineering and characterization of the topological insulators (TI) since their discovery, one of the remaining challenges is to stabilize them against degrading due to aging over time. Stabilizing the properties of TIs under the ambient conditions is of great interest, and indeed is a crucial step towards building stable TI-integrated electronic devices. One of the immediate and effective solutions to the aging problem is to find an efficient, and compatible capping layer. In this work we focus on how properties of \(Bi\textsubscript{2}Se\textsubscript{3}\) as a prototypical TI can be stabilized in air. We were able to achieve high quality \(Bi\textsubscript{2}Se\textsubscript{3}\) thin films with low carriers concentration and high mobility using Molecular Beam Epitaxy (MBE). Aging study of samples with such low carriers will be more reliable compared to other MBE grown samples with higher carriers concentration. In this work, long-term study (over 200 days) of aging effect on the transport properties of thin films with no capping layer, and ones with various in-situ (in the MBE chamber) and ex-situ deposited capping layers will be presented. Finally, by comparing the results between different capping layers, the most effective capping layer will be reported.

3:42PM D7.0007  Investigation of the transport properties of \(Bi\textsubscript{2}Se\textsubscript{3}\) films grown on various substrates . YANG, Dept. of Physics, National Taiwan Univ., Taipei 10617, Taiwan, Y.H. LIN, K.H. CHEN, B.Y. YANG, Dept. of Physics, National Taiwan University, Taipei 10617, Taiwan, M. HONG, Graduate Institute of Applied Physics, National Taiwan University, Taipei 10617, Taiwan, J. KWO, Dept. of Physics, National Tsing Hua Univ., Hsinchu 30013, Taiwan — Topological insulators, a new state of quantum matter, displayed a variety of physical phenomena. We have obtained high quality TI films of \(Bi\textsubscript{2}Se\textsubscript{3}\), \(Bi\textsubscript{2}Te\textsubscript{3}\), and \(Sb\textsubscript{2}Te\textsubscript{3}\) grown on various substrates with streaky RHEED patterns and large domains 1-2um in size. However, the Fermi level of \(Bi\textsubscript{2}Se\textsubscript{3}\) tends to locate in the bulk conduction band due to the high density of intrinsic defects in TIs. To fine tune the Fermi level to be within the band gap, \(Bi\textsubscript{2}Se\textsubscript{3}\) films were grown on amorphous oxide layers such as \(SiO\textsubscript{2}\), \(Y\textsubscript{2}O\textsubscript{3}\), and \(Al\textsubscript{2}O\textsubscript{3}\) thick deposited on GaAs and Si substrates in back gate structure for the electrical field effect. Compare to \(Bi\textsubscript{2}Se\textsubscript{3}\) thin films on crystalline substrates such as sapphire, samples grown on amorphous oxides such as \(Al\textsubscript{2}O\textsubscript{3}\) showed lower carrier concentration for the film thickness less than 10 QL, and the resistivity showed an insulating behavior at T below 50K. Other transport properties such as mobility, WAL effects are underway.

3:54PM D7.0008  Demonstration of large field effect in topological insulator films via a high-\(\kappa\) back gate . YANG, H.Y. LIN, Dept. of Physics, Natl Tsing Hua Univ., Hsinchu 30013, Taiwan, Y.H. LIN, K.H. CHEN, B.Y. YANG, Graduate Institute of Applied Physics and Dept. of Physics, Natl Tsing Hua Univ., Taipei 10617, Taiwan, K.H.M. CHEN, J.Z. PENG, Dept. of Physics, Natl Tsing Hua Univ., Hsinchu 30013, Taiwan, S.F. LEE, Institute of Physics, Academia Sinica, Taipei 11529, Taiwan, M. HONG, Graduate Institute of Applied Physics and Dept. of Physics, Natl Tsing Hua Univ., Hsinchu 30013, Taiwan — In topological insulators (TI) the spins are locked to opposite momentum direction when the Fermi level passes through Dirac point of its helical surface states, and the electrical field effect is a very promising way to manipulate TI spins for spintronic devices. We have fabricated the back gate structure by growing TI films on high-\(\kappa\) oxide layers including amorphous oxides of \(SiO\textsubscript{2}\), \(Y\textsubscript{2}O\textsubscript{3}\), and \(Al\textsubscript{2}O\textsubscript{3}\) deposited on conducting substrates for applying the field effect with smaller operating voltage compared to SiC back gate. We have performed the surface conduction measurements of thin films with different thicknesses of FIM/TI, SC/TI structures intended for various studies. For \(Bi\textsubscript{2}Se\textsubscript{3}\) grown on these amorphous oxide thin films, streaky RHEED patterns indicated the film is highly crystalline. Weak antilocalization effect was observed to verify the time-reversal symmetry protected transport property. Very large field effect was demonstrated; for example, in the 6QL samples we are able to modulate as much as \(2E\textsubscript{13}\) cm\(^{-2}\) holes in applying negative gate bias. Field effect of Sb doped \(Bi\textsubscript{2}Te\textsubscript{3}\) to realize sign reversal of carrier concentration will also be presented.

4:06PM D7.0009  Shubnikov-de Haas Oscillations from topological surface states of metallic \(Bi\textsubscript{2}Se\textsubscript{3}\) on \(Te\textsubscript{0.9}\). KESHAV SHRESTHA, TcSUH and Department of Physics, University of Houston, 3201 Cullen Blvd., Houston, Texas 77204, USA, VERA MARIANOVA, Institute of Optical Materials and Technology, Bulgarian Academy of Sciences, Acad. G. Bonchev Str. 109, Sofia 1113, Bulgaria, BERND LORENZ, PAUL C.W. CHU\textsuperscript{2}, TcSUH and Department of Physics, University of Houston, 3201 Cullen Blvd., Houston, Texas 77204, USA — We have studied the quantum oscillations in the conductivity of metallic, \(p\)-type \(Bi\textsubscript{2}Se\textsubscript{3}\) at 10\textsuperscript{-18} cm\(^{-2}\) holes in applying negative gate bias. Field effect of Sb doped \(Bi\textsubscript{2}Te\textsubscript{3}\) to realize sign reversal of carrier concentration will also be presented.

\textsuperscript{1}This work is supported in part by the US Air Force Office of Scientific Research, the Robert A. Welch Foundation (E-1297), the T.L.L. Temple Foundation, the J. J. and R. Moores Endowment, and the State of Texas through the TCSUH and at LBNL by the DoE.

\textsuperscript{2}LBNL, 1 Cyclotron Road, Berkeley, California 94720, USA

4:18PM D7.00010  Synthesis and low-temperature transport measurement of pure and In-doped SnTe nanoplate . JIE SHEN, YUJUN XIE, JUDY J. CHA, Yale Univ — SnTe is a topological crystalline insulator that possesses different surface states on the \{100\}, \{110\}, and \{111\}surfaces. Thus, to access surface states selectively, it is critical to control the morphology of SnTe. Moreover, indium doping in SnTe induces superconductivity, making it a candidate for a topological superconductor. Here, we grow pure and In-doped SnTe nanoplates, whose top and bottom surfaces are either \{100\} or \{111\}, via vapor-liquid-solid and vapor-solid growth mechanisms. For pure SnTe nanoplate, we observe a structural phase transition from rock salt to rhombohedral structure in samples with low carrier density and electron-electron interactions in samples with high carrier density. In addition, by studying nanoplates with indium-doping concentrations ranging from 0% to 10%, we show that nanoplates become more diffuse in bulk and such that the surface states appear at higher concentrations of indium. This is supported by a three-dimensional weak antilocalization in low magnetic fields and a two-dimensional(2D) linear magnetoresistance(LMR) in high magnetic fields. This 2D LMR comes from the Dirac-dispersive surface state, in agreement with Abrikosov’s quantum limit model.
4:30PM D7.00011 Defect induced negative magnetoresistance and surface state immunity in topological insulator BiSbTeSe
2. KARAN BANERJEE, JAESUNG SON, PRAVEEN DEORANI, Nati Univ of Singapore, PENG REN, Nanyang Technological University, LAN WANG, RMIT University, HYUNSOO YANG, Nati Univ of Singapore — The absence of backscattering due to time reversal symmetry is one of the hallmark features of a topological insulator. However, the introduction of defects can result in diminishing the transport properties of topological insulators. In this work, we introduce defects into the topological insulator BiSbTeSe
2 by subjecting it to ion milling and study the effect of disorder on the transport properties. We find that a negative contribution arises in the magnetoresistance of BiSbTeSe
2 at low temperatures. However, the surface state remains remarkably robust to the introduction of disorder. We demonstrate that the negative magnetoresistance originates from an increase in the density of defect states created by the introduction of disorder. We also find the bulk contribution to remain negligible even after subjecting to ion milling.

4:42PM D7.00012 ABSTRACT WITHDRAWN —

4:54PM D7.00013 Surface conduction in encapsulated topological gated structures
1. YURY DESHEKO, INNA KORZHOVSKA, LUKAS ZHAO, The City College of New York, GHIDEWON AREFE, Columbia University, MARCIN KONCZYKOWSKI, Ecole Polytechnique, France, LIA KRUSIN-ELBAUM, The City College of New York — In three-dimensional (3D) topological insulators (TIs), the surface Dirac fermions intermix with the conducting bulk, thereby complicating access to the low-energy surface charge transport or magnetic response. The subsurface 2D states of bulk origin are vulnerable to bandbending due to surface adatoms, a band modification thought to be responsible for the ‘aging’ effect. To minimize this effect, we have developed an inert environment mechanical exfoliation technique to fabricate transistor-like gated structures in which prototypical binary TIs as well as ultra-low bulk carrier density ternaries (such as Bi
2
2
and Te
2
2
and Sb
2
2
and Se
2
2
) were encapsulated by thin h-BN layers, with electrical contacts made using exfoliated graphene. The effects of electrostatic tuning by the gate bias voltage on surface conductivity as a function of thickness of the TI layers and the variation with disorder will be presented.

1Supported by NSF-DMR-1312483, and DOD-W911NF-13-1-0159

5:06PM D7.00014 Van der Waals epitaxy of Bismuth Telluro-Sulfide nanosheats and magneto-transport in devices. TANUJ TRIVEDI, SUSHANT SONDE, SANJAY K. BANERJEE, Microelectronics Research Center, The University of Texas at Austin — Growing interest in probing topological surface states from transport experiments has led to the recent development of ternary and quaternary compounds of Bismuth chalcogenides. The search for complex 3D topological insulator compounds is motivated by the need for reduced bulk conduction and easier access to the Dirac point of the surface states, as compared to in the binary phases Bi
x
2
x
3
(X=Te,Se). To this end, we have grown nanosheats of Bismuth Telluro-Sulfide directly on different substrates with van der Waals epitaxy. The growth method utilizes novel solid-state, non-elemental precursors of Bismuth, Tellurium and Sulfur. Nanosheet growth is observed on different substrates, such as amorphous SiO
x
(2.5<10nm) and mica, and grow layer-by-layer in varying thicknesses (3 nm to >100 nm) and sizes (up to few microns). Stoichiometric analysis of the nanosheats is close to previously reported crystal growth of tetradymites, and the crystalline nature is confirmed with Raman and XRD measurements. We have fabricated devices on as-grown nanosheets of varying thicknesses, with nonmagnetic metal contacts. Preliminary magneto-transport experiments are promising, motivating further in-depth transport analysis for probing topological surface states.

5:18PM D7.00015 Molecular Beam Epitaxy of Ultra-Thin Sb Films for Surface Transport Studies
3. KAUSHINI WICKRAMASINGHE, CHOMANI GASPE, SHAYNE CAIRNS, NOLAN TEASDALE, TETSUYA MISHIMA, JOEL KEAY, MATTHEW JOHNSON, SHEENA MURPHY, MICHAEL SANTOS, University of Oklahoma, Homer L. Dodge Department of Physics and Astronomy — Our growth study of ultra-thin Sb films is motivated by theoretical studies that predict a topoelectronic phase transition as a function of Sb film thickness due to quantum confinement and surface coupling effects. In thick films, transport measurements will be dominated by bulk conduction because the band structure of bulk elemental Sb is semi-metallic. Our goal is to enable transport measurements of topological surface states by suppressing the bulk conductivity through quantum confinement in thin Sb layers. Good control over the growth conditions allowed us to vary the thickness of the Sb films ranges from 0.7 nm to 6 nm with good repeatability. Electrical transport measurements indicate that surface states are responsible for about 25% of the conductivity at 20K in a 3.7 nm thick Sb layer where the bulk conductivity is suppressed by about a factor of 2. We will discuss the structural properties of the Sb films using different electron microscopy techniques.

3This material is based upon work supported by the NSF under Grant No. DMR-1207537

Monday, March 2, 2015 2:30PM - 5:18PM — Session D8 DCMP: Complex Films & Surfaces: Oxides, Alloys, and Semiconductors 006C -

2:30PM D8.00001 Investigation of Thin Layered Cobalt Oxide Nano-Islands on Gold. MICHAL BAJDICH, SLAC - STANFORD, ALEX S. WALTON, JAKOB FESTER, iNANO, Aarhus University, MOHAMMAD A. ARMAN, JACEK OSIECKI, JAN KNUDSEN, Lund University, ALEKSANDRA VOJVODIC, SLAC - STANFORD, JEPPE V. LAURITSEN, iNANO, Aarhus University — Layered cobalt oxides have been shown to be highly active catalysts for the oxygen evolution reaction (OER), but the synergistic effect of contact with gold is yet to be fully understood. The synthesis of three distinct types of thin-layered cobalt oxide nano-islands supported on a single crystal gold (111) substrate is confirmed by combination of STM and XAS methods. In this work, we present DFT+U theoretical investigation of above nano-islands using several previously known structural models. Our calculations confirm stability of two low-oxygen pressure phases: (a) rock-salt Co-O bilayer and (b) wurzite Co-O quadrayer and single high-oxygen pressure phase: (c) O-Co-O trilayer. The optimized geometries agree with STM structures and calculated oxidation states confirm the conversion from Co2+ to Co3+ found experimentally in XAS. The O-Co-O trilayer islands have the structure of a single layer of CoOOH proposed to be the true active phase for OER catalyst. For that reason, the effect of water on the Pourbaix stabilities of basal planes and edge sites is fully investigated. Lastly, we also present the corresponding OER theoretical overpotentials.
2:2PM D8.00002 Effects of hydroxylated $\gamma$-Al₂O₃ support and H adsorbate on the Geometry and Electronic Structure of Pt Nanoparticles¹, GHAZAL SHAFAI, University of Central Florida, Orlando, FL, 32816, SAMPYO HONG, University of Central Florida, Orlando, FL, 32816 — We have studied the effects of hydroxylated $\gamma$-Al₂O₃(110) support and H adsorbate on the geometry and electronic structures of Pt$_n$ (n=22,44) nanoparticles (NP) using DFT. We find that Pt$_{22}$ interacts more strongly with a less hydrated support, while Pt$_{44}$ more with a hydroxylated one. We also find a structural transition of the Pt$_{22}$ (and not Pt$_{44}$) from a bliparal to a 3D-like shape as a function of hydroxilation. H induces a much larger shift in the unoccupied d-band center than does the support. Also, these shifts are well correlated with metal-support interaction. The increased hydroxylation on $\gamma$-Al₂O₃(110) causes weaker metal-support interaction. As a result, the d-band width of a Pt NP decreases causing the center of the unoccupied d band to shift to lower energy (red shift). In the light of these results, we will discuss the features of XANES spectra obtained for $\gamma$-Al₂O₃(110) supported Pt nanoparticles [1].

¹Work supported in part by NSF under grant CHE-1310327.

2:54PM D8.00003 A new model for $\sqrt{3} \times \sqrt{3} \times R9^\circ$ reconstruction of $\alpha$-Al₂O₃ (001), HAWOONG HONG, Argonne National Laboratory, AARON GRAY, TAI-C. CHIANG, University of Illinois, Urbana-Champaign — Research in oxides surface suffers reproducibility problems on its structure. However, $\sqrt{3} \times \sqrt{3} \times R9^\circ$ reconstructed $\alpha$-Al₂O₃ (001) surface has been generated repeatedly by many different groups. This sapphire surface structure was known to be quite inert even to air exposure. The detailed structures have been studied with LEED, x-ray diffraction and AFM. The recent experimental studies conclude that the few topmost layers are composed of aluminum atoms and have metallic properties [1, 2]. Then a question arises why this surface seems to be inert to air exposure. Metallic aluminum is prone to oxidation according to theoretical investigation. Here we propose a new model for the $\sqrt{3} \times \sqrt{3} \times R9^\circ$ reconstruction involving oxidized top layers. For the direct structural information in the surface-normal direction, specular and non-specular crystal truncation rods were measured with x-ray diffraction. Only successful, if not perfect, fitting occurs with a dense top layer, which is reminiscent of oxidized aluminum (111) surface [3].


2:06PM D8.00004 Preparation of atomically flat TiO$_2$ (001) surfaces¹, YANG WANG, Oak Ridge National Lab, HANNO H. WEITERING, University of Tennessee, Knoxville, PAUL C. SNIJJDERS, Oak Ridge National Lab — Transition metal oxides with the rutile structure (MO$_2$, M = e.g. Ti, V, or Nb) have highly directional partially occupied t$_{2g}$ orbitals. Some of these orbitals form quasi-1D electronic bands along the rutile c-axis, and Peierls-like ordering phenomena have been observed in VO$_2$ and NbO$_2$. Tailoring the electronic properties of these materials via quantum confinement requires epitaxial growth on suitable substrates such as low index TiO$_2$ surfaces. Because of the high surface energy of rutile TiO$_2$(001), the standard approach of sputtering and annealing usually introduces faceting. Here we demonstrate a facile method to create atomically flat, non-faceted TiO$_2$(001) surfaces. Using scanning tunneling microscopy we observe terraces with a width of approximately 150 nm. Step heights of approximately 0.3 nm are observed, consistent with the c lattice parameter of rutile TiO$_2$. Low energy electron diffraction patterns reveal sharp diffraction spots with an in-plane lattice constant of 0.358 nm which is consistent with a (1x1) ordering of the (001) plane. These TiO$_2$(001) single crystal surfaces can serve as an ideal substrate for further growth of rutile heterostructures.

¹Work supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

3:18PM D8.00005 Physical Character and Morphology of Platinum Nanocrystals on Strontium Titanate, JOSHUA GILD, MICHAEL PIERCE, Rochester Institute of Technology, VLADIMIR KOMANICKY, University of Pavol Jozef Safarik, ANDI BARBOUR, HOYDOO YOU, Argonne National Lab — The physical characteristics of platinum nanocrystals on single crystal strontium titanate, SrTiO$_3$, can effect the chemical properties of this important model catalyst. The morphology, epitaxy, distribution, and size of the Pt nano-crystals can all be controlled through different growth and processing mechanisms. Nanometer scale platinum thin films are deposited on strontium titanate at ambient temperatures then annealed at range of temperatures and in various oxidizing environments. The process of how these conditions influence the formation of uniformly epitaxial platinum crystals on the sample surface has been investigated using basic materials characterization techniques. Single crystal x-ray diffraction is the primary tool for these experiments, coupled with atomic force microscopy for morphology and x-ray and electron spectroscopy to determine chemical bonding between the particles and gases introduced into the system. These substrate supported nanoparticle samples will then be utilized in experiments to test their catalytic activity compared to an amorphous platinum film.

3:30PM D8.00006 Imaging of Pt Nanocrystals on SrTiO$_3$ Substrate: Coherent X-ray Diffraction and Scanning Microscopy Studies, TRAVIS DOUGLAS, JOSHUA GILD, MICHAEL PIERCE, Rochester Institute of Technology, VLADIMIR KOMANICKY, Faculty of Science, Safarik University, ANDI BARBOUR, HOYDOO YOU, Argonne National Laboratory — Imaging of nano-scale structures, particularly those in real-world environments, presents a significant challenge. X-ray Coherent Diffractive Imaging (CDI) provides one avenue of accessing the structural information of a nano-scaled sample in a harsh environment. However, while this problem has been solved for Au and Pb nano-crystals in clean, vacuum environments, much work remains before it can be rapidly employed in other systems. Our efforts center on determining the real-space structure of Pt nanocrystals grown on SrTiO$_3$ substrates using a combination of CDI and atomic force scanning microscopy (AFM). X-ray speckle patterns have been obtained using coherent diffraction of these crystals which can be transformed back to real space coordinates to calculate the crystal structure using CDI algorithms. Microscopy provides complementary information allowing us to simulate the speckled diffraction patterns from real-space images of the actual particles. This dual approach of using both real and reciprocal space information to solve the structures should lead to a practical set of algorithms and procedures whereupon the samples can be imaged quickly in the environments and conditions of interest.
3:42PM D8.00007 Probing the role of Ga in amorphous conducting oxides through local structure studies, STEPHANIE MOFFIT, QIMIN ZHU, QING MA, DONALD BUCHHOLZ, ROBERT CHANG, THOMAS MASON, TOBIN MARKS, MICHAEL BEDZYK, Northwestern University — The study of amorphous (a-) conducting oxides is an emerging field. The lack of grain boundaries, smooth surfaces, and low temperature deposition position these materials as ideal candidates for large area applications and flexible electronics. Most impressively, these materials maintain high electron mobility in the amorphous state. These benefits have led the recent commercialization of a-IGZO (Ga and Zn doped indium oxide) as a replacement for a-Si as the channel layer of thin film transistors in display technology. Despite this success, fundamental understanding of structure-property relationships is still lacking and must be improved to guide further development of amorphous conducting oxides. X-ray absorption spectroscopy (XAS) is one of the few tools that can be used to probe the structure of amorphous materials. Amorphous indium oxide doped with Ga (a-IGO) is a model system to help develop the role of dopants in amorphous oxides. An in depth XAS study was carried out to determine inter-atomic distances, coordination numbers, and structural disorder parameters as a function of Ga doping level. The correlation between XAS-derived structural properties and the dopant-dependent evolution of both electrical properties and thermal stability of a-IGO will be discussed.

1This work is supported by the NSF MRSEC program No. DMR1121262

3:54PM D8.00008 Optical constants and transient absorption of solution-deposited RuO2 thin films, JEFFREY OWURTSKY, RYAN COMPTON, JAMES LONG, CHRISTOPHER CREVIN, KONRAD BUSSMANN, ADAM DUNKELBERGER, BRYAN SPANN, IRINA PALIN, DEBRA ROLISON, PAUL CUNNINGHAM, JOSEPH MELINGER, PAUL DESARIO, Naval Research Lab, DAN WEIDINGER, Schaffer Corp., EDWIN HEILWEIL, National Institute of Standards & Technology — Optical and electrical conductivity properties are determined for the promising, broadband transparent conductor material, solution-deposited RuO_2 nanostructured films. The 10-30 nm thick films or nanoskins are less conductive but more optically transmissive than polycrystalline, sputtered RuO_2 films which are inherently metallic. The optical constants (0.6 to 4.5 eV) determined by ellipsometry show that c_1 is positive for the nanoskins in the spectral region investigated so they are not plasmonic. Transient picosecond absorption with visible (400 nm) pump and various probe wavelengths (visible and THz) are performed for nanoskins calcined to different temperatures. When heated to 200°C the absorption increases in the visible and THz. After heating to 300°C, the films become more polycrystalline and there is evidence for the appearance of a new absorption. Decreased absorptions or bleaches are observed in the THz and for longer visible wavelengths (> 750 nm). The absorption is ascribed to a damped plasmon band of the crystalline nanoparticles formed in the film upon heating.

4:06PM D8.00009 Effect of Ions and pH on the H-bond Network at the Quartz(101)-Water Interface, MARK DELLOSTRITTO, JAMES KUBICKI, JORGE SOFO, The Pennsylvania State University — Reactions in aqueous systems are common, and yet can be difficult to study, as the structure and dynamics of the H-bond network can dominate the rates of reactions by determining the access reactants have to each other. This is thought to be the case at the quartz-water interface, where the addition of ions to solution or an increase in pH can increase the dissolution rate by an order of magnitude without any change in the activation energy. This suggests that the dissolution reaction is unchanged and the ions modify the structure of water at the interface such that the reaction occurs at a greater frequency. To investigate this effect, we performed ab-initio molecular dynamics (AIMD) simulations of the quartz(101)-water interface in several different ionic solutions under different pH and temperature conditions. We found that both anions and cations in a near-surface configuration tend to increase the order of interfacial water, although at neutral pH this competes with a decrease in the H-bond lifetime induced by the presence of an anion-pair cation. We also found that neither the H or O atoms of H_2O or OH^- have greater access to the surface with the introduction of ions, but there is a greater incidence of intrasurface H-bonding in all systems studied. This suggests that intrasurface proton transfer could be an important component of the dissolution reaction, while nucleophilic attack of Si by H_2O is unlikely to occur at the interface studied.

Work supported by the Division of Chemical Sciences, Geosciences and Biosciences, Office of Basic Energy Sciences, U.S. Department of Energy

4:18PM D8.00010 N vacancy, self-interstitial diffusion, and Frenkel-pair formation/dissociation in TiN studied by ab-initio and classical molecular dynamics, DAVIDE G. SANGIOVANNI, BJØRN ALLING, LARS HULTMAN, IGOR A. ABRIKOSOV, Department of Physics (IFM), Linköping University, Sweden — We use ab-initio and classical molecular dynamics (AIMD, CMD) to simulate diffusion of N vacancy and N self-interstitial point-defects in B1 TiN. The physical properties of TiN, important material system for thin film and coatings applications, are largely dictated by concentration and mobility of point defects. We determine N dilute-point-defect diffusion pathways, activation energies, attempt frequencies, and diffusion coefficients as a function of temperature. In addition, MD simulations reveal an unanticipated atomistic process, which controls the spontaneous formation of N-self-interstitial/N-vacancy pairs (Frenkel pairs) in defect-free TiN. This entails that a N lattice atom leaves its bulk position and bonds to a neighboring N lattice atom. In most cases, Frenkel-pair N and N^V reconstruct within a fraction of ns; 50% of these processes result in the exchange of two nitrogen lattice atoms. Occasionally, however, Frenkel-pair N-interstitial atoms permanently escape from the anion vacancy site, thus producing unpaired N^3 and N^1 point defects.

1The Knut and Alice Wallenberg foundation (Isotope Project, 2011.0094), the Swedish Research Council (VR) Linköping Linnaeus Initiative LiLi-NFM (grant 2008-0652), and the Swedish Government Strategic Research (grant MatLiU 2009-00971).

4:30PM D8.00011 Structural analysis of ferromagnetic Ni-Mn-Sn thin films fabricated by co-sputter deposition, SEMA GUVENC, MEHMET YUMAK, Bogazici University, Dept. of Physics, 34342, Istanbul, Turkey, A. QUINTANA, SEMA GUVENC, MEHMET YUMAK, Bogazici University, Dept. of Physics, 34342, Istanbul, Turkey, A. QUINTANA. The Knut and Alice Wallenberg foundation (Isotope Project, 2011.0094), the Swedish Research Council (VR) Linköping Linnaeus Initiative LiLi-NFM (grant 2008-0652), and the Swedish Government Strategic Research (grant MatLiU 2009-00971).

4:30PM D8.00011 Structural analysis of ferromagnetic Ni-Mn-Sn thin films fabricated by co-sputter deposition, JORGE SOFO, SEMA GUVENC, MEHMET YUMAK, Bogazici University, Dept. of Physics, 34342, Istanbul, Turkey, A. QUINTANA. The Knut and Alice Wallenberg foundation (Isotope Project, 2011.0094), the Swedish Research Council (VR) Linköping Linnaeus Initiative LiLi-NFM (grant 2008-0652), and the Swedish Government Strategic Research (grant MatLiU 2009-00971).
4:42PM D8.00012 Surface nanocrystalline and hardening effects of Ti–Al–V alloy by electrospinning ultrasonic shock1, XIAOXIN YE, GUOYI TANG, Tsinghua University — The effect of electrospinning ultrasonic shock (EUS) on the surface hardening and microstructure of Ti6Al4V alloy was studied. It was found that electrospinning improved the microhardness dramatically both in the influential depth and maximum value, compared with the only ultrasonic- shocked sample. It’s indicated that refined surface layer with nanocrystalline and improved microhardness were obtained on account of surface severe plastic deformation, dynamic recrystallization (DRX) and phase change, which was implemented at relative low temperature and high strain rate/capacity due to the coupling of the thermal and athermal effects of EUS. It’s different from conventional experiments and theory. It’s discussed that the positive contributions of EPT in the thermodynamics and kinetics of microstructure and properties change were attributed to the reduction of nucleation energy barrier and acceleration of atomic diffusion. Therefore, it’s supposed that EUS is an energy-saving and high-efficiency method of surface treatment technique with the help of high-energy electropoles, which is promising in cost reduction of the surface engineering and energy management.

1The work is supported by National Natural Science Foundation of China (No. 50571048) and Shenzhen science and technology research funding project of China (No. SGLH2012100814750946)

4:54PM D8.00013 Shedding Light on the Emission Mechanisms of In_{0.54}Ga_{0.46}N Disks in GaN Nanowires Using C.W. Non-Linear Spectroscopy1, CAMERON NELSON, ALBERT LIU, SANIYA DESHPANDE, SHAHAF JAHANGIR, PALLAB BHATTACHARYA, DUNCAN STEEL, University of Michigan, Ann Arbor: EECS Department — Linear and non-linear spectroscopy has been performed on an ensemble of 3 nm thick In_{0.54}Ga_{0.46}N disks grown in self-assembled GaN nanowires (∼30 nm diameter). PLE measurements near resonant with the PL show a mostly broad, featureless spectrum with a linear increase in absorption as a function of energy, similar to InGaN/GaN quantum wells. Unlike InGaN quantum wells, the centroid of the PL spectrum shows a negligible intensity-dependent shift in PL emission wavelength. Further, the non-linear optical spectrum is dominated by excitonic resonances with line widths ~20-30 meV in the same region as the PLE data. Distinguishable peaks in the PL spectrum overlap with the non-linear resonances. Continuous-wave nearly degenerate pump-probe absorption measurements show no evidence of spectral hole burning within the resonances; however there is evidence of population pulsations in the 3rd order signal. This data shows evidence consistent with regular excitonic saturation and two beam coupling similar to that expected in discrete (e.g. 2 or 3 level systems). The excitonic behavior is also consistent with anti-bunching seen in g2 measurements from single dots.

1This work was supported by NSF-CPHOM at the University of Michigan.

5:06PM D8.00014 Chemical Reactions and Atomic Removal Dynamics during Gallium Nitride Chemical Mechanical Polishing Process: Quantum Chemical Molecular Dynamics Simulations1, KENTARO KAWAGUCHI, YUJI HIGUCHI, NOBUKI OZAWA, MOMOJI KUBO, Fracture and Reliability Research Institute Graduate School of Engineering, Tohoku University — The chemical mechanical polishing (CMP) is promising for efficient polishing of the GaN substrate, and it is essential for manufacturing of GaN devices. However, the detailed CMP mechanisms are unclear, and then the design of efficient and precise CMP process is difficult. We performed polishing simulations of a GaN substrate by a SiO₂ abrasive grain in a solution including OH radicals in order to reveal effects of OH radicals on the polishing process. The OH radicals in the solution are adsorbed on the GaN surface and occupy the hollow sites on the surface. Then, a surface-adsorbed O atom is generated by the chemical reaction between the surface-adsorbed OH species and a OH radical in the solution. In the friction interface between the GaN substrate and the abrasive grain, the surface-adsorbed O atom is mechanically pushed into the GaN substrate by the abrasive grain. This O atom intrusion induces the dissociation of Ga-N bonds of the GaN substrate. Moreover, volatile N₂ molecules and soluble Ga(OH)₂ molecules are generated due to the dissociation of Ga-N bonds. Then, we suggested that the GaN CMP process efficiently proceeds by the mechanically induced chemical reactions: a surface-adsorbed O atom is generated and pushed into the GaN bulk by the abrasive grain.

Monday, March 2, 2015 2:30PM - 5:30PM
Session D9 DCMP: Superconduction in Cuprates: Photoemission 006D - Donghui Lu, Stanford University

2:30PM D9.00001 An Angle Resolved Thermodynamics Study of Cuprate Superconductors, XIAOAING ZHOU, HAOXIANG LI, STEPHEN PARHAM, JUSTIN VAUGH, University of Colorado at Boulder, JOHN SCHNEELOCH, RUIDAN ZHONG, Brookhaven National Lab, ENDA GU, University of Colorado at Boulder, HELMUTH BERGER, Département de Physique, Ecole Polytechnique Fédérale de Lausanne, KUNIHICO OKA, University of Colorado at Boulder, HIROSHI EISAKI, Nanoelectronics Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), GERALD ARNOLD, DANIEL DESSAU, University of Colorado at Boulder — The thermodynamics properties of a system contain vital information on its electronic states, the contribution of which in typical bulk measurements is averaged and integrated over momentum and energy space. Therefore, it’s supposed that EUS is an energy-saving and high-efficiency method of surface treatment technique with the help of high-energy electropoles, which is promising in cost reduction of the surface engineering and energy management. It’s discussed that the positive contributions of EPT in the thermodynamics and kinetics of microstructure and properties change were attributed to the reduction of nucleation energy barrier and acceleration of atomic diffusion. Therefore, it’s supposed that EUS is an energy-saving and high-efficiency method of surface treatment technique with the help of high-energy electropoles, which is promising in cost reduction of the surface engineering and energy management.

2:42PM D9.00002 Extraction of normal and pairing self-energies and Eliashberg functions of high temperature superconductor Bi2212 from Laser-based ARPES experiment1, JIN MO BOK, National Laboratory for Superconductivity, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Science, SEUNG HWAN HONG, JONG JU BAE, HAN-YONG CHOI, Department of Physics and Institute for Basic Science Research, SungKyunKwan University, CHANDRA M. VARMA, Department of Physics and Astronomy, University of California, Riverside, WENTAO ZHANG, JUNFENG HE, YUXIAO ZHANG, LI YU, X.J. ZHOU, National Laboratory for Superconductivity, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Science — The angle-resolved photoemission (ARPES) measurements provide momentum and frequency dependence of the electronic structure that enables quantitative analysis using single particle Green’s function. This is particularly important for studying the cuprate superconductors that are known to have anisotropic electronic structure and anisotropic d-wave superconducting gap. Here we report the extraction of the normal and pairing self-energies from high resolution Laser-based ARPES data of the underdoped and overdoped Bi2212. We also obtain the Eliashberg functions, η₂ and η₆, by inverting Eliashberg equations using maximum entropy method. Implications of these results for understanding the superconductivity mechanism will be discussed.

1NSFC (Grant No. 11190022) and the MOST of China (Program No: 2011CB921703 and 2011CB605903)
extend these studies for the first time to a Bi2212 sample in the superconducting state, and disentangle the shift in chemical potential from surface voltage.

Intriguing results on several materials showing how laser pulses can manipulate their chemical potential on ultrafast timescales, and it’s been suggested that high-temperature superconductors, including the quasiparticle relaxation, cooper pair recombination, and many-body interactions. There have also been several conceptual differences between the two lifetimes.

In order to reduce the correlation length we substituted Cu$^{2+}$ ($S=1/2$) by Zn$^{2+}$ ($S=0$). The modification of the AF correlation length as a function of Zn concentration and temperature was derived using NMR and a direct correspondence between the amplitude of the spectral weight beyond the AF zone boundary and the correlation length was established. Remarkably, even at correlation lengths as short as 3 lattice constants we still observe a significant spectral weight in the back-bended band. These findings prove that the ARPES technique is very sensitive to short-range correlations and provide a hint for the understanding of ARPES results in the underdoped regime of high temperature superconductors.

We employ femtosecond time- and angle-resolved photoelectron spectroscopy to study optimally doped Bi-2212 ($T_c = 96$ K). In the low excitation limit, the energy-resolved population lifetime displays abrupt changes near 60-80 meV both below and above $T_c$. Moreover, the lifetime near this characteristic energy is independent of excitation density. These behaviors are consistent with theories based on electron-phonon interactions, which connect the population lifetimes to the single-particle lifetimes measured by equilibrium photoemission. However, the absolute values of these two quantities are different by one to two orders of magnitude. We further demonstrate that this discrepancy is independent of experimental techniques and materials, and point out the fundamental conceptual differences between the two lifetimes.

The relationship between the pseudogap and superconducting gap in high temperature cuprate superconductors remains an outstanding issue. In this talk, we will present our high resolution laser-ARPES measurement on Bi2212CaCu2O8 superconductor. We will use the latest generation of ARPES system equipped with the VUV laser and the time-of-flight (TOF) electron energy analyzer. This enables us to have super-high energy resolution, high momentum resolution, simultaneous coverage of two-dimensional momentum space, high data acquisition efficiency and much reduced nonlinearity effect. From detailed temperature dependence near the nodal and antinodal regions, we will discuss on the relationship between the pseudogap and superconducting gap in the cuprate superconductors.

The extremely correlated Fermi liquid (ECFL) theory recently introduced by Shraer has renewed interest in quantitatively understanding ARPES line shapes. In this talk, we combine certain phenomenological considerations with the ECFL framework in order to describe the ARPES data. Our phenomenological models have the property of preserving the universal property of the original ECFL theory, while introducing phenomenological changes in a non-universal property. Our models describe, with unprecedented fidelity, the key aspects of the dichotomy between momentum distribution curves (MDCs) and energy distribution curves (EDCs) of high-$T_c$ ARPES data. Therefore, our study goes well beyond the prevailing studies that discuss only MDCs and EDCs.

This work was supported by Berkeley Lab’s program on Quantum Materials, funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract No. DE-AC02-05CH11231.
threshold for superconductivity has not yet been undertaken. Here we report the results of studying this regime.

quasiparticle dynamics in the very high and very low pump fluence regimes, but a systematic study of the changes in dynamics across the fluence vaporization to underlying mechanisms governing superconductivity, antiferromagnetism, charge ordering, and other types of competing orders. Time- and angle-resolved Technology, DUNG-HAI LEE, ALESSANDRA LANZARA, Materials Sciences Division, Lawrence Berkeley National Laboratory / Department of Physics, UC Berkeley, CHRIS JOZWIAK, Advanced Light Source, Lawrence Berkeley National Laboratory, TAKASHI NOJI, YOJI KOIKE, Department of Applied Physics, Tohoku University, HIROSHI EISAKI, Electronics and Photonics Research Institute, National Institute of Advanced Industrial Science and Technology, RUIDAN ZHONG, GENDA GU, Brookhaven National Laboratory, DANIEL DESSAU, University of Colorado at Boulder — The field of time-resolved ARPES (trARPES) has matured greatly in the last several years and has proven a useful tool in the study of cuprate superconductivity. However, previous experiments have been limited in the pump wavelength to energies of 1.5 eV (or more), far above the relevant energy scales for superconductivity. Here we use an OPA/DFG setup to create a mid-infrared pump, with tunable photon energies from 60-300 meV, allowing us to weakly perturb the superconductivity of optimally doped Bi$_2$Sr$_2$CaCu$_2$O$_{8+}$ under this excitation scheme.

We acknowledge funding from the Deutsche Forschungsgemeinschaft and the Center for Emergent Superconductivity, a BES EFRC.

Can La$_2$CuO$_4$ be made into an undoped metal / superconductor: insights from angle-resolved photoemission spectroscopy, HAOFEI WEI, Cornell University, CAROLINA ADAMO, Stanford University, DARRELL SCHLOR, KYLE SHEN, Cornell University — La$_2$CuO$_4$ is a well-known parent compound for the hole-doped cuprate superconductors. However, by shifting the apical oxygen away from the Cu-O plane, it can also be made into the parent for an electron-doped superconductor. La$_2$CuO$_4$ in this so-called T$'$ structure is metastable in bulk, but recent reports have succeeded in stabilizing thin films via molecular-beam epitaxy. These samples were reported to be metallic and even superconducting, in contrast to the Mott insulating state found in all other underdoped cuprate parent compounds. To determine whether it is truly a metal in its undoped state, we have for the first time directly measured the electronic structure of epitaxially grown thin films of nominally undoped T$'$-La$_2$CuO$_4$ using in-situ angle-resolved photoemission spectroscopy (ARPES). We observe dispersive bands which form a well-defined Fermi surface with intensity modulations consistent with scattering from an underlying SDW order, similar to those observed in doped n-type cuprates. We have also characterized the carrier density using Luttinger's rule, and will discuss what information our measurements provide on the role of oxygen non-stoichiometry in determining the properties of this system and on the potential for a metallic undoped cuprate.

Photodoping of Effects in Heavily Underdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ Revealed by Time and Angle Resolved Photoemission Spectroscopy

4:42PM D9.00012 Photodoping of Effects in Heavily Underdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ Revealed by Time and Angle Resolved Photoemission Spectroscopy

4:54PM D9.00013 Analyzing of Superconductivity from Fitting Result of the Diverging Effective Mass in YaBa$_2$Cu$_3$O$_{x+y}$, HYUN-TAK KIM, MIT Center in ETRI, South Korea — For cuprate superconductors, the mechanism of high-$T_c$ superconductivity is still an unclear and unsolved problem, because they are inhomogeneous. Here, we show analysis of superconductivity from the fitting result of the diverging-effective mass (DEM) extracted from the quantum-oscillation data in YaBa$_2$Cu$_3$O$_{6+y}$ [1]. The fitting was performed by extended Brinkman-Rice picture [2]. The fitting result presents the Fermi arc observed by angle-resolved-photoemission-spectroscopy data is presented. In particular, the growing Fermi arc from the nodal Fermi point to the isotropic Fermi surface with increasing $x$ and the nodal constant Fermi energy are revealed. Further, pairing symmetry of cuprate superconductors is analyzed as $\sigma$-wave. The quantum critical point is regarded as the nodal Fermi point: The intrinsic superconducting gap is formed at node. The mass diverges is an average effect and the true effective mass is constant.


Ultrafast Quasiparticle Relaxation Dynamics across the Superconducting Vaporization Threshold in Bi$_2$2212>

5:06PM D9.00014 Ultrafast Quasiparticle Relaxation Dynamics across the Superconducting Vaporization Threshold in Bi$_2$2212>

CHRISTOPHER SMALLWOOD, Materials Sciences Division, Lawrence Berkeley National Laboratory, WENTAO ZHANG, TRISTAN MILLER, GREG AFFELDT, KOSHI KURASHIMA, Materials Sciences Division, Lawrence Berkeley National Laboratory / Department of Physics, UC Berkeley, CHRIS JOZWIAK, Advanced Light Source, Lawrence Berkeley National Laboratory, TAKASHI NOJI, YOJI KOIKE, Department of Applied Physics, Tohoku University, HIROSHI EISAKI, Electronic and Photonics Research Institute, National Institute of Advanced Industrial Science and Technology, DUNG-HAI LEE, ALESSANDRA LANZARA, Materials Sciences Division, Lawrence Berkeley National Laboratory / Department of Physics, UC Berkeley — In cuprate superconductors, an important open question is the degree to which the timescales and pathways for quasiparticle relaxation relate to underlying mechanisms governing superconductivity, antiferromagnetism, charge ordering, and other types of competing orders. Time- and angle-resolved photoemission spectroscopy (time-resolved ARPES) is uniquely poised to address this question because of the technique’s exceptional ability to simultaneously probe the time-, energy-, and momentum-dependent properties of quasiparticles and band structure. Previous time-resolved ARPES studies have examined quasiparticle dynamics in the very high and very low pump fluence regimes, but a systematic study of the changes in dynamics across the fluence vaporization threshold for superconductivity has not yet been undertaken. Here we report the results of studying this regime.
RAM SHARMA, University of Illinois at Chicago, Chicago, IL — It has been revealed that the two high energy kinks in high $T_c$ superconductors (HTSC) in electron energy at $\sim 100$ meV and $\sim 160$ meV which were stated as found new [1], were discovered earlier [2] via dipolon theory [3,4] in explaining the photoemission line shape (sharp peak, dip and broad peak) and the low energy kink at $\sim 70$ meV. It was also mentioned [2] that the details for the high energy kinks would be reported elsewhere [5]. Thus Ref. 1 should be corrected by replacing “new” by “discovered earlier” in the text including the title. The dipolon theory is strong coupling field-theory including Mott renormalization, nonrigid electron bands, electron-hole attraction and all important and necessary electron correlations and not only explains but also predicts correctly the properties of HTSC [2-5].


Monday, March 2, 2015 2:30PM - 5:30PM — Session D10 DCMP: Optical and THz Properties of Topological Insulators 007A - Dennis Drew, University of Maryland

2:30PM D10.00001 Transient reflectance of photoexcited electrons and holes in cadmium arsenide$^1$, CHRIS WEBER, BRYAN BERGGREN, Department of Physics, Santa Clara University, ERNEST ARUSHANOV, Institute of Applied Physics, Academy of Sciences of Moldova, TAHEREH HOSSEINI, NIKOLAI KOULKIN, Departments of Electrical Engineering and Computer Science, University of Wisconsin-Milwaukee — We report ultrafast transient-grating measurements of crystals of the three-dimensional Dirac semimetal cadmium arsenide, Cd$_3$As$_2$, at both room temperature and 80 K. After photoexcitation with 1.5-eV photons, charge-carriers relax by two processes, one of sub-picosecond duration and the other of duration 3 ps. By measuring the complex phase of the change in reflectance, we determine that the faster signal corresponds to an increase in phase velocity, and the slower signal to a decrease in absorption, at the probe energy. We assign the fast signal to free-carrier absorption from photoexcited electron and hole populations, which relax by recombination, and the slower signal to phase-space filling by thermally excited electrons. The proposed processes closely mirror the response of graphene to photoexcitation. We also present evidence that both the electrons and the lattice are strongly heated.

$^1$This work was supported by the National Science Foundation Grant No. DMR-1105553

2:42PM D10.00002 Gated Terahertz Magneto-optical Measurements of 3D Dirac Semimetals$^1$, DON C. SCHMADEL, GREGORY S. JENKINS, ANDREI B. SUSHKOV, REMINGTON L. CAREY, H. DENNIS DREW, Dept of Physics & CNAM, Univ of Maryland-College Park, JASON W. KRIZAN, SATYA KUSHWAHA, QUINN GIBSON, ROBERT J. CAVA, Dept of Chemistry, Princeton Univ — We report gated terahertz magneto-optical measurements of the bulk and surface states of Na$_3$Bi and Cd$_3$As$_2$. The onset of interband transitions within the bulk 3D Dirac cone is observed. A gate is used to modulate surface carriers and bulk carriers near the surface resulting in differential optical signals. Gate-modulated cyclotron resonance and Fourier transform infrared spectroscopy characterize the bulk Dirac carriers along all three crystal axes as well as the Fermi-arc carriers, with Fermi Energy. The transport scattering and Fermi velocity anisotropy as well as potential fluctuations characterized near the Dirac point will be discussed.

$^1$UMD supported by NSF (DMR-1104433), Princeton supported by ARO MURI on topological insulators and NSF MRSEC.

2:54PM D10.00003 Theory of Kerr and Faraday rotation in Topological Weyl Semimetals$^1$, MEHDI KARGARIAN, MOHIT RANDERA, NANDINI TRIVEDI, Department of Physics, The Ohio State University, Columbus, OH 43210, USA — Topological Weyl semimetals are characterized by bulk Dirac nodes separated in momentum space by a distance $2b$ and lead to Fermi arcs in the surfaces electronic structure. We calculate the Faraday $\theta_F$ and Kerr $\theta_K$ angles for electromagnetic waves scattered from such a Weyl semimetal using the Kubo formalism. (1) For thin films with electromagnetic radiation incident on a surface without arcs, we show that $\theta_K = bd/\alpha \pi$ and $\theta_F = \alpha \pi/ bd$ where $\alpha$ is the fine structure constant, and the film thickness $d \ll \lambda$, the wavelength. We further show multiple reflections give rise to giant Kerr rotation, under certain conditions, for a film on a substrate. (2) In the case when the electromagnetic radiation is incident on the surface with arcs, the wave propagating inside the material acquires a longitudinal component $F$, $\theta \propto F$ and $\theta_L \propto F$. We discuss the implications of our results for thin films of pyrochlore iridates, and also for the recently discovered Dirac semimetals in a magnetic field.

$^1$We acknowledge the support of the CEM, an NSF MRSEC, under grant DMR-1420451.

3:06PM D10.00004 Temperature-driven band inversion in Pb$_{0.77}$Sn$_{0.23}$Se: Optical and Hall-effect studies, NAWEEN ANAND, Univ of Florida - Gainesville, FL, ZHIGUO CHEN, NHMFL Florida State University, Tallahassee, FL, SANAL BUADEV, Univ of Florida - Gainesville, FL, CARTIN, Ramapo college, Mahwah, NJ, KAMAL CHOUTHARY, Univ of Florida - Gainesville, FL, GENDU GU, Brookhaven National Lab, Upton, NY, S. SINNOTT, Univ of Florida - Gainesville, FL, ZHIQIANG LI, NHMFL Florida State University, Tallahassee, FL, A. HEBARD, D. TANNER, Univ of Florida - Gainesville, FL — Optical and Hall-effect measurements have been performed on single crystals of Pb$_{0.77}$Sn$_{0.23}$Se, a IV-VI mixed chalcogenide. The temperature dependent (10-300 K) reflectance was measured over 40-7000 cm$^{-1}$ (5-870 meV) with an extension to 15.50 cm$^{-1}$ (1.92 eV) at room temperature. The reflectance was fit to the Drude-Lorentz model using a single Drude component and several Lorentz oscillators. The optical properties at the measured temperatures were estimated via Kramers-Kronig analysis as well as by the Drude-Lorentz fit. The carriers were p-type with the carrier density determined by Hall measurements. A signature of valence intraband transition is found in the low-energy optical spectra. It is found that the valence-conduction band transition energy as well as the free carrier effective mass reach minimum values at 100 K, suggesting temperature-driven band inversion in the material. Some of the results from optical studies were compared with density function theory calculations.

3:18PM D10.00005 Single Photon Transport through an Atomic Chain Coupled to a One-dimensional Photonic Waveguide, ZEYANG LIAO, XIAODONG ZENG, M. SUHAIL ZUBAIRY, Texas A&M University — We study the dynamics of a single photon pulse travels through a single atomic chain coupled to a one-dimensional (1D) single mode photonic waveguide. We derive a time-dependent dynamical theory for this collective many-body system which allows us to study the real time evolution of the photon transport and the atomic excitations. Our result is consistent with previous calculations when there is only one atom. For an atomic chain, the collective interaction between the atoms mediated by the waveguide mode can significantly change the dynamics of the system. The reflectivity can be tuned by changing the ratio of coupling strength and the photon linewidth or by changing the number of atoms in the chain. The reflectivity of a single photon pulse with finite bandwidth can even approach 100%. The spectrum of the reflected and transmitted photon can also be significantly different from the single atom case. Many interesting physics can occur in this system such as the photonic bandgap effects, quantum entanglement generation, Fano-type interference, superradiant effects and nonlinear frequency conversion. For engineering, this system may be used as a single photon frequency filter, single photon modulation and photon storage.
3:30PM D10.00006 Electrostatic tuning of the surface states of irradiated topological insulators\textsuperscript{1} INNA KORZHNOVSKA, LUKAS ZHAO, YURY DESHKO, The City College of New York-CUNY, GIDEON AREFE, Columbia University, MARCIN KONCZYKOWSKY, Emanuele Polini, France- LIA KRUSIN-ELBAUM, The City College of New York-CUNY, COLUMBIA UNIVERSITY COLLABORATION — One of the main obstacles to accessing charge transport through Dirac surface states of topological insulators (TIs) is a significant conduction in the bulk. We have developed a new approach of reaching a stable charge neutrality point (CNP) using irradiation with 2.5 MeV energy electrons. By controlling the beam fluence and annealing protocol we can convert bulk conductivity from $p$- (hole-like) to $n$-type (electron-like) and back, crossing the Dirac point while preserving the robust topological signatures of surface channels. Electron beams act to compensate charged bulk defects and pull the Fermi level into the bulk gap – a process that decreases bulk conductivity by orders of magnitude to a minimum, $\sigma_{\text{Ti}},$ at CNP. We study the origins of minimum conductivity in electron-irradiated TIs in a transistor-like gated structures fabricated in inert environment by mechanical exfoliation with $\text{Bi}_2\text{Te}_3$ as a prototypical TI and h-BN as a gate dielectric. The effects of electrostatic tuning by the gate bias voltage on surface conductivity near CNP will be presented.

3:42PM D10.00007 Effects of the topological phase transition and band inversion on ultrafast dynamics in topological crystalline insulators\textsuperscript{1} Y.M. DAI, J. BOWLAN, A.J. TAYLOR, D.A. YAROTSKI, R.P. PRASANKUMAR, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos, NM 87545, R.D. ZHONG, G.D. GU, T. VALLA, C.C. HOMES, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973, T. YILMAZ, B. SINKOVIC, Department of Physics, University of Connecticut, Storrs, Connecticut 06269 — Topological crystalline insulators, characterized by a gapless metallic state on their high-symmetry surfaces that is protected by crystalline symmetry, are realized both theoretically and experimentally in the $\text{Pb}_1-x\text{Sn}_x\text{Te}$ and $\text{Pb}_1-x\text{Sn}_x\text{Se}$ compounds. In these materials, a topological phase transition and band inversion can be induced by doping, pressure or temperature. We use femtosecond optical pump-probe spectroscopy to study the evolution of the ultrafast dynamics as a function of both temperature and doping in the $\text{Pb}_1-x\text{Sn}_x$ Te system. The influence of these parameters on the topological phase transition and band inversion, as well as on quasiparticle dynamics, will be discussed.

3:54PM D10.00008 Cyclotron resonance of surface states in the bulk-insulating topological insulator $\text{Bi}_2\text{Se}_3$ by THz spectroscopy LIANG WU, The Johns Hopkins University, WANG-KONG TSE, Los Alamos National Laboratory, CHRISTOPHER MORRIS, The Johns Hopkins University, MATTHEW BRAHLEK, NIKESH KOIRALA, SEONGSHIK OH, Rutgers the State University of New Jersey, PETER ARMITAGE, The Johns Hopkins University, THE JOHNS HOPKINS UNIVERSITY TEAM, LOS ALAMOS NATIONAL LABORATORY TEAM, RUTGERS THE STATE UNIVERSITY OF NEW JERSEY TEAM — We have utilized magneto-optical time-domain terahertz spectroscopy to investigate the low frequency optical response of topological insulator films of $\text{Cu}_x\text{Bi}_2\text{Se}_3$ and $\text{Bi}_2\text{Se}_3$. Such experiments give sufficient information to measure the mobility and density of multiple conduction channels simultaneously. Sharp cyclotron resonances (CRs) were observed in both samples by Faraday rotation experiments. We find that the $\text{Cu}_x\text{Bi}_2\text{Se}_3$ films with certain Cu concentration are bulk insulators with only surface conduction channels. This is consistent with pure topological surface states conduction and an $E_F$ that is $\sim 150$ meV above Dirac point (around 70meV below conduction band minimum). Hence, a true topological insulator with insulating bulk is realized. In contrast, we find that $\text{Bi}_2\text{Se}_3$ with $E_F < -350$ meV above Dirac point has two channels; a dominant one that exhibits a CR in the Faraday rotation comes from surface states and a second channel which does not show a CR comes from bulk and/or 2DEG. Orbital effect on the electrodynamics of surface states and electron-phonon interaction are also discussed.

4:06PM D10.00009 Probing topological transitions in HgTe/CdTe quantum wells by magneto-optical measurements\textsuperscript{1} BENEDIKT SCHRÄF, ALEX MATOS-ABIAGIU, Department of Physics, SUNY at Buffalo, JAROSLAV FABIAN, Institute for Theoretical Physics, University of Regensburg, IGOR ZUTIC, Department of Physics, SUNY at Buffalo — In two-dimensional topological insulators, helical Quantum Spin Hall (QSH) states persist even at finite magnetic fields below a critical magnetic field $B_c$, above which only Quantum Hall (QH) states can be found [1]. Using linear response theory we theoretically investigate the magneto-optical properties of inverted HgTe/CdTe quantum wells, both for infinite two-dimensional and finite-strip geometries, and possible signatures of the transition between the QSH and QH regimes. In the absorption spectrum, several peaks arise due to non-equidistant quasiparticles levels in both regimes. However, in the QSH regime, we find an additional absorption peak at low energies in the finite-strip geometry. This peak arises due to the presence of edge states in this geometry and persists for any Fermi level in the QSH regime, while in the QH regime the peak vanishes if the Fermi level is situated in the bulk gap. Thus, by sweeping the gate voltage, it is potentially possible to distinguish between the QSH and QH regimes. Moreover, we investigate the effect of spin-orbit coupling and finite temperature on this measurement scheme.

1Supported by LANL LDRD and LANL-UCRF program.

4:18PM D10.00010 Coupling two lasers on a dielectric surface CRISTIAN BAHRIM, MD KHAIRUZZAMAN, MD MOZAMMAL RAJU, WEI-TAI HSU, Physics Department, Lamar University — We can modify the radiation perceived by a dielectric surface using a capacitor voltage set up across. The associated uniform electric field allows us to shift toward shorter wavelengths the optical response of the dielectric surface for a given monochromatic laser radiation incident on it. We use this capacitor configuration for coupling two laser beams incident simultaneously on the surface. The stronger coupling laser couples with the electric dipoles and impedes a probe laser to oscillate the same dipoles. The interaction between the two laser beams creates a destructive interference pattern in the Brewster angle region of the probe. Clear evidence of several minima of diffraction shows along the direction of reflection of the probe laser. This diffraction pattern indicates the ‘lock in’ of the probe laser on the surface. This new physics is related to an electromagnetic induced transparency (EIT)-type phenomenon with the major difference that in our case the coupling between two lasers is produced at the dielectric’s surface.

4:30PM D10.00011 Measurement of a topological edge invariant in a microwave network JASON C. PILLAY, WENCHAO HU, Nanyang Technological University, KAN WU, Shanghai Jiao Tong University, MICHAEL PASEK, PERRY PING SHUM, YIDONG CHONG, Nanyang Technological University — We report on the experimental measurement of topological edge invariants in an electromagnetic analog of a topological insulator, realized by a classical microwave network. This experiment serves as a classical electromagnetic realization of Laughlin’s “topological pumping” thought experiment for the quantum Hall effect. The experiment consists of determining the electromagnetic scattering matrix, based on the input and output wave amplitudes measured at the edges of the network via a network analyzer. The winding on the scattering matrix eigenvalues, resulting from a tunable phase shift built into the network, forms a topological invariant. We demonstrate the existence of a topologically trivial phase, where the winding is zero (no edge states), as well as a topologically nontrivial phase, where the winding is non-zero (topological edge states present). Unlike most other systems used to study topological insulator physics, the full complex scattering parameters can be measured in this setup. As in most microwave experiments, however, our system is susceptible to losses. We show that topological behavior can be meaningfully defined in the experiment despite the effects of loss.
4:42PM D10.00012 Experimental realization of microwave photonic topological insulators
JIANWEN DONG, Sun Yat-sen University — Topological properties play a fundamental role in many physical phenomena. While topology focus on electronic systems, there has been a recent emergence of interest in exploring topological orders with photons. Recent experiments have demonstrated substantial progress towards the implementation of Hamiltonians with topological robustness, from microwave to visible frequency domains. Here, we will show the demonstration on nontrivial photonic bandgaps, as well as the topologically protected edge states. We designed and fabricated a metacrystal comprising non-resonant meta-atoms sandwiched between two metallic plates. Spin Chern number of photonic crystals is calculated based on group theory and accurately predicts topological characters of edge states in different gaps. Topologically nontrivial gaps are achieved by mode exchange at high symmetric k-points. Nontrivial bandgap was confirmed by experimentally measured transmission spectra and calculated nonzero spin Chern number. Gapless spin-filtered edge states were demonstrated experimentally by measuring Ez fields and Hz fields, as well as their phase differences. Robustness of the edge states were also observed when an obstacle is introduced near the edge.

4:54PM D10.00013 Persistent Optical Gating of a Topological Insulator Heterostructure
ANDREW L. YEATS, Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637 & Dept. of Physics, University of California, Santa Barbara, CA 93106, YU PAN, ANTHONY RICHARDELLA, Dept. of Physics, Penn State University, University Park, PA 16802, PETER J. MINTUN, Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637, NITIN SAMARTH, Dept. of Physics, Penn State University, University Park, PA 16802, DAVID D. AWSCHALOM, Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637 & Dept. of Physics, University of California, Santa Barbara, CA 93106 — We demonstrate persistent, bidirectional control of the chemical potential in a (Bi,Sb)2Te3/SrTiO3 heterostructure through a two-color all-optical technique. By manipulating the space-charge distribution in a SrTiO3 substrate, we locally tune the field effect in a (Bi,Sb)2Te3 channel comparatively to electrostatic gating techniques but without additional materials or processing. The effect persists for thousands of seconds and functions from cryogenic to ambient temperatures. This enables us to write and re-write arbitrarily shaped p- and n-type regions, which we characterize electrically and image with scanning photocurrent microscopy. The ability to rapidly prototype mesoscopic electronic structures in a topological insulator may aid in the investigation of the spin-polarized surface and edge states unique to the topological insulating phase. The optical patterning technique may be adaptable to other material systems, which could form a basis for reconfigurable electronics.

5:06PM D10.00014 Circular Dichroism Observed by Photoemission from Ultrathin Bi2Te3 Films
CAI-ZHI XU, YANG LIU, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA, HYUK JONG KIM, Institute of Solid State Physics, The University of Tokyo, Kashiwa, Chiba 277-8581, Japan, LONG-XIANG ZHANG, TOM MILLER, TAI-CHANG CHIANG, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA — Circular dichroism (CD) observed by photoemission from the surface states of topological insulators has drawn much interest. It was initially attributed to the spin polarization or chiral orbital momentum of the initial states, but later proven to also involve the final states. The detailed mechanism remains controversial. To address this question, we have performed measurements of ultrathin films of the prototypical topological insulator Bi2Te3 over a wide range of film thickness and photon energy. The results show that the CD depends not only on the photon energy, but also on the film thickness in a nontrivial manner. A theoretical model has been developed that involves dipole transition, surface photoemission, and spin-orbit coupling. The computed results are in good agreement with the general trends of the data including sign reversals as a function of photon energy and film thickness. The complex behavior of the measured CD function is partially caused by modifications of both the initial and final states in the thin film geometry.

5:18PM D10.00015 Rashba effect and beating patterns in the THz magneto-photoresponse of a HgTe-based two-dimensional electron gas
MEHDI PAKMEHR, University at Buffalo, CHRISTOPH BRUENE, HARTMUT BUHMANN, LAURENS MOLENKAMP, University of Utrecht, BRUCE MCCOMBE, University at Buffalo — HgTe quantum wells with a gapped single Dirac cone electronic dispersion relation have been investigated by THz magneto-photoresponse (PR) and magneto-transport measurements. The HgTe has the conventional band alignment at well thickness of 6.1 nm, slightly smaller than the critical thickness for the topological phase transition. The effective gap is roughly 10 meV, and the large sheet density of electrons (n~≈1.5×1012 cm−2) results in a very large Fermi energy (EF~≈160 meV). We have found several interesting effects at these high densities. We focus here on an observed beating of quantum oscillations in the PR signal (at 1.83 THz) and compare it with direct measurements of oscillations in the longitudinal magneto-resistance (Rxx). The mechanism for the PR is cyclotron resonance absorption heating of the electrons (an electron bolometric effect). We attribute the beating to Rashba splitting of the spin states, which is barely observable in direct Rxx measurements even under strong gate-induced electric fields. We will discuss the origin of the enhanced visibility of the Rashba effect in the PR and the magnitude of the Rashba coefficient (αR) from these data.

5:29PM D10.00016 Experimental realization of microwave photonic topological insulators
JIANWEN DONG, Sun Yat-sen University — Topological properties play a fundamental role in many physical phenomena. While topology focus on electronic systems, there has been a recent emergence of interest in exploring topological orders with photons. Recent experiments have demonstrated substantial progress towards the implementation of Hamiltonians with topological robustness, from microwave to visible frequency domains. Here, we will show the demonstration on nontrivial photonic bandgaps, as well as the topologically protected edge states. We designed and fabricated a metacrystal comprising non-resonant meta-atoms sandwiched between two metallic plates. Spin Chern number of photonic crystals is calculated based on group theory and accurately predicts topological characters of edge states in different gaps. Topologically nontrivial gaps are achieved by mode exchange at high symmetric k-points. Nontrivial bandgap was confirmed by experimentally measured transmission spectra and calculated nonzero spin Chern number. Gapless spin-filtered edge states were demonstrated experimentally by measuring Ez fields and Hz fields, as well as their phase differences. Robustness of the edge states were also observed when an obstacle is introduced near the edge.

Monday, March 2, 2015 2:30PM - 5:30PM – Session D11 DMP: Coexisting Orders In Underdoped Cuprates
007B - Vivek Mishra, Argonne National Laboratory

2:30PM D11.00001 Combinatorial Deposition of La2−xBaxCuO4 Thin Films Across the x=1/8 Anomaly
JUSTIN LANE, ADAM WEIS, AZTON WELLS, University of Illinois at Urbana-Champaign, SO RA CHUNG, Belmont University, PATHIKUMAR SELLAPPAN, WALTRAUD KRIVEN, DALE VAN HARLINGEN, University of Illinois at Urbana-Champaign — La2−xBaxCuO4 (LBCO) has an unusual phase diagram that includes a charge stripe phase in proximity to suppressed superconductivity near x=1/8 doping. We will present recent improvements to LBCO thin films grown by pulsed laser deposition from high-quality metalorganic-synthesized ceramics. Using a combination of Ba-poor and Ba-rich deposition sources and a combinatorial pulsed laser deposition technique, we are able to tune doping of LBCO and measure the superconducting transition temperature as a function of doping. We correlate the spatial offset between deposition plume and substrate with the resultant sample’s dopant distribution. Characterization of these films by a high-throughput resistence technique and use of the samples in ongoing experiments will be discussed.

2:42PM D11.00002 ABSTRACT WITHDRAWN
2:54PM D11.00003 In-plane resistivity anisotropy in underdoped cuprates due to scattering by charge and spin fluctuations. MICHAEL SCHÜTT, RAFAEL M. FERNANDES, University of Minnesota — The existence of strong in-plane electronic anisotropies in underdoped cuprates has been reported by a variety of experimental probes, such as transport measurements, scanning tunneling microscopy, and x-ray and neutron scattering. Understanding the origin of these anisotropies and their interplay is fundamental to elucidate the role played by electronic nematicity in the phase diagram of the cuprates. Here we employ a Boltzmann equation approach to investigate the resistivity anisotropy due to scattering by anisotropic spin and charge fluctuations. We show that while spin fluctuations give rise to larger resistivity along the b direction, charge fluctuations promote larger resistivity along the a direction. Therefore, charge and spin fluctuations compete, these behaviors give rise to a particular dependence of the resistivity anisotropy with doping, which is consistent with transport experiments performed in YBa$_2$Cu$_3$O$_{6.5}$H$_x$. We discuss the important role played by the CuO chains in YBCO to select the observed type of nematic domains, and propose transport measurements in strained HgBa$_2$CuO$_4$ and Bi$_2$Sr$_2$CaCu$_2$O$_{y+δ}$ to shed light on the interplay between anisotropic fluctuations and anisotropic resistivity.

3:06PM D11.00004 Superconducting and charge order in 1/8 doped LBCO probed by proton-induced disorder. MAXIME LEROUX, VIVEK MISHRA, HELMUT CLAUS, ULRICH WELP, Materials Science Division, Argonne National Laboratory, ASGHAR KAYANI, Department of Physics, Western Michigan University, ZAHIRUL ISLAM, Advanced Photon Source, Argonne National Laboratory, GENDA GU, Department of Physics, Brookhaven National Laboratory, WAI-KWONG KWOK, Materials Science Division, Argonne National Laboratory — The question of how charge order coexists with superconductivity in underdoped cuprates is an important open question that has yet to be fully understood. Recently, the role played by the CuO chains in La$_2$CuO$_4$ has been probed and measured by neutron scattering and NMR, but the role played by the CuO chains in YBCO to select the observed type of nematic domains, and propose transport measurements in strained HgBa$_2$CuO$_4$ and Bi$_2$Sr$_2$CaCu$_2$O$_{y+δ}$ to shed light on the interplay between anisotropic fluctuations and anisotropic resistivity.

3:18PM D11.00005 $^{17}$O NMR Study of Under-doped Single Crystals of the High Temperature Superconducting Compound Hg1201. W.P. HALPERIN, JEONGSEOP A. LEE, YIZHOU XIN, Northwestern University, A.M. MOUNCE, Los Alamos National Laboratory, A.F. REYES, P.L. KUHNS, National High Magnetic Field Laboratory — We present measurements of $^{17}$O high field NMR on oxygen isotope exchanged under-doped single crystals of the single layer superconductor, HgBa$_2$CuO$_{4+y}$, a compound having a known tetragonal lattice. Our $^{17}$O data for two under-doped samples (T$_c$ of 87 K and 79 K) indicates that there are two inequivalent oxygen planar sites based on measurements of upper and lower quadrupolar satellites. Spectra were taken with 4 K $<$ T $<$ 400 K and 6 T $<$ H $<$ 30 T with a goniometer to precisely orient crystals relative to the magnetic field. We found an asymmetry in the line shape between the upper and lower satellites that cannot be accounted for by a model with a single planar oxygen site. Comparison will be made to earlier work on under-doped YBa$_2$Cu$_3$O$_{y+δ}$. [1] A.M. Mounce, et al., Phys. Rev. Lett. 111, 187003 (2013).

3:30PM D11.00006 Enhanced Fluctuation/Inhomogeneity Effects Near The Superconductor-Insulator Transition in Severely Underdoped 2D Films of Ca$_{0.3}$Y$_{0.7}$Ba$_2$Cu$_3$O$_{6.4}$+δ. THOMAS LEMBERGER, The Ohio State University — It has been shown that the superconductor-insulator transition in two-dimensional, severely underdoped films of Ca$_{0.3}$Y$_{0.7}$Ba$_2$Cu$_3$O$_{6.4}$+δ is accompanied by a linear scaling between the zero temperature superfluid density n$_s$(T = 0) and the temperature for the unbinding of thermally excited vortex pairs, T$_{BD}$. We present results from resistivity and magnetic screening studies on 2D Ca$_{0.3}$Y$_{0.7}$Ba$_2$Cu$_3$O$_{6.4}$+δ showing a linear relationship between the width of tails in the resistive transition and T$_{BD}$. These tails show a significant suppression of resistivity and can extend down for tens of Kelvin's before the films exhibit magnetic screening. We examine this relationship in light of a possible enhancement of inhomogeneous effects in the vicinity of the superconductor-insulator transition with underdoping.

3:42PM D11.00007 Simultaneous AFM-STM on BSCCO. DREW EDELBerg, MIHiR BHASKAR, PINSHANE HUANG, ABHAY PASUPATHY, Columbia University — Scanning tunneling microscopy is limited by its inability to resolve the difference between local electronic structure and surface topology since the tunneling current is a convolution of electronic density and tip height. Such a limitation is especially problematic in studying or order coexists with superconductivity in underdoped cuprates. Here we report that the T$_c$ of La$_{1.87}$Ba$_{0.125}$Cu$_2$O$_{6.5}$ (LBCO) increases by up to 50% after proton irradiation. At high enough energy, proton irradiation creates a uniform density of small nm-sized amorphous clusters and point defects, which results in a uniform and isotropic 3D distribution of defects [1]. However, it is well known that non-magnetic defects are pair-breaking for d-wave superconductivity, and should therefore reduce Tc. We speculate that proton-induced disorder directly affects the balance between competing density wave and superconducting ground states. [1] Jia, Y. et al. Appl. Phys. Lett. 103, 122601 (2013); M. A. Kirk, Cryogenics 33, 235 (1993); M. A. Kirk, Y. Yan, Micron 30, 507 (1999). This work is supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. D.O.E., Office of Science, Office of Basic Energy Sciences and by the D.O.E, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

3:54PM D11.00008 Nonlinear Hall effect and Shubnikov-de Haas quantum oscillations in thin films of the electron doped superconductor Pr$_2$CuO$_4$. NICHOLAS BREZNAy, Lawrence Berkeley National Lab, NITYAN NAIR, JAMES ANALYTIS, University of California Berkeley, ZENGWEI ZHU, KIMBERLY MODIC, ROSS MCDONALD, Los Alamos National Lab, YOSHIHARU KROCKENBERGER, NTT Basic Research Labs — Recent quantum oscillation studies in cuprate superconductors have allowed for considerable progress in understanding their Fermi surface topology. However, important questions remain about the influence of quantum criticality and competing orders, as well as the universality of these results; in particular quantum oscillation studies to date have largely been confined to a limited range of hole-doped bulk crystal systems. We have observed a field nonlinear Hall effect in superconducting thin films of the cuprate Pr$_2$CuO$_4$, and studied the temperature and magnetic field dependence of this behavior. The Hall effect data are consistent with a simple two-band transport model in this material, and we will interpret them in light of recently observed Shubnikov-de Haas quantum oscillations in these films.

4:06PM D11.00009 Near-Room Temperature Studies of the Pseudogap Phase of Underdoped Bi-2212. LING FU, AARON KRAFT, Clark University, GENDA GU, Brookhaven National Laboratory, MICHAEL BOYER, National High Magnetic Field Laboratory — We present measurements of the pseudogap state of underdoped Bi-2212 in the vicinity of T$_c$.
4:18PM D11.00010 Signatures of the Berezinskii–Kosterlitz–Thouless transition in highly underdoped La$_{2-x}$Sr$_x$CuO$_4$ 1, ZHENZHONG SHI, PAUL BAITY, XIAOYAN SHI, DRAGANA POPOVIĆ, Dept. of Phys. & Natl. High Magnetic Field Lab., Florida State Univ. — We investigated the nature of the thermally driven transition to a superconducting state on MBE-grown 100 nm thick La$_{2-x}$Sr$_x$CuO$_4$ films ($x = 0.07$ and 0.08) by studying a) superconducting fluctuations (SCFs), as determined from the magnetoresistance, b) voltage ($I-V$) characteristics, and c) fluctuations of conductance with time (noise). Noise was studied on confined width (20 μm) samples specifically designed for measurements in the eight-probe double-bridge configuration. We observe: a) the contribution of the SCFs to the conductivity increases monotonically with decreasing $T$ and diverges exponentially at $T_{BKT}$, where resistance also goes to zero; b) power-law behavior $V \propto T^\alpha(T)$ with $\alpha(T) \geq 3$ for $T < T_{BKT}$; and c) an orders-of-magnitude enhancement of the noise near $T_{BKT}$. Possible long-range correlations in the phase fluctuations near $T_{BKT}$ are also studied with higher-order spectrum analysis. Our observations suggest that the transition from superconductor to the normal state exhibits signatures of the Berezinskii–Kosterlitz–Thouless (BKT) transition.

1Supported by NSF DMR-1307075 and NHMFL via NSF DMR-1157490 and the State of Florida.

4:30PM D11.00011 Double criticality in the magnetic field driven transition of a high-TC superconductor 1, BRIGITTE LERIDON, LPEM/CNRS-ESPCIParisTech - UPMC, 10 rue Vauquelin - 75005 Paris - France, JOHAN VANACKEN, V.V. MOSCHHALKOV, INPAC-KULeuven, Celestijnenlaan 200 D, B-3001 Heverlee, Belgium, BAPTISTE VIGNOLLE, CNRS/LNCMI, 143 Avenue de Rangueil, 31040 Toulouse, France, RAJNI PORWAL, R.C. BUDHANI, NPL, CSIR, New Delhi 110012, and IIT Kanpur, Kanpur 208016, India — The magnetic-field driven transition of a set of high critical temperature $La_{2-x}Sr_xCuO_4$ superconducting thin films has been investigated using high pulsed magnetic fields. For the underdoped samples, the existence of two distinct critical regions in the superconductor/insulator transition has been evidenced for the first time. The first quantum critical region is observed at intermediate magnetic fields ($\approx 19T$) and temperatures and gives way at lower temperature to a quantum critical point at about twice critical magnetic field and resistance per square. The critical exponents inferred from scaling behaviour are markedly different for the two regions. We attribute this behaviour to the existence of a clean/dirty crossover due to the presence of electronic inhomogeneities.

This work has been supported by a SESAME grant from Region Ile-de-France. Part of the experiments at KULeuven have been founded by EuroMagNET II under the EU contract number 228043.

4:42PM D11.00012 Examining non-Fermi liquid behavior through magnetoresistance in nearly continuously doped La$_{(2-x)}$Sr$_x$CuO$_4$, ZAC STEGEN, ARKADY SHEKHTER, GREG BOEBINGER, Florida State University, FEDOR BALAKIREV, ROSS MCDONALD, Los Alamos National Laboratory, JIE WU, ANTHONY BOLLINGER, XI HE, IVAN BOZOVIC, Brookhaven National Laboratory — We report magnetoresistance in thin films of the cuprate superconductor $La_{2-x}Sr_xCuO_4$ in pulsed magnetic fields up to 65 tesla. The films are synthesized using combinatorial molecular beam epitaxy, which allows for continuous tuning of doping. They are patterned into an array of pixels with steps of $\Delta x \approx 0.0002$, which is 25 times smaller than experiments using conventional sample growth methods. These films allow a detailed analysis of the doping evolution of non-Fermi liquid magnetoresistance in the vicinity of optimal doping.

4:54PM D11.00013 Magnetic field induced ordering and phase diagram in underdoped LSCO, JESSE HALL, McMaster University, TOOMAS RÖÖM, URMAS NAGEL, DAN HUVONEN, National Institute for Chemical Physics and Biophysics, D. HAWTHORNE, S. WAKIMOTO, H. ZHANG, University of Toronto, JUNGSEEK HWANG, Sungkyunkwan University, SEIKI KOMIYA, Central Research Institute of Electric Power Industry, THOMAS TIMUSK, McMaster University — The existence of ordered phases in superconducting cuprates has come under intense scrutiny with the revelation of charge-ordering near the superconducting transition in YBCO. Previous results demonstrating the existence of exotic ordered phases, including the existence of stripe order, and the richness of the magnetic-field/doping/temperature phase diagram, suggest that the underdoped region of the phase diagram may contain a wealth of information that has yet to be revealed. We turn our attention to $La_{2-x}Sr_xCuO_4$ on the boundary of superconductivity by studying the far-infrared optical properties of three single crystals with $x=0.05$, 0.06, and 0.07: the first is non-supercconducting, the others have transition temperatures of 6 K and 12 K respectively. By applying a magnetic field up to 17 T we are able to suppress superconductivity where it exists and compare the field-induced normal state to that induced by temperature or by doping. By studying the optical conductivity of these materials and the changes in the spectral weight with temperature and field, we can gain insight into the field induced ordered states of underdoped cuprate superconductors.

5:06PM D11.00014 Doping-dependent critical Cooper-pair momentum $p_c$ in thin underdoped cuprate films 1, THOMAS LEMBERGER, JOHN DRASKOVIC, STANLEY STEERS, THOMAS MCIJUNKIN, ADAM ANMED, Ohio State Univ - Columbus — We apply a low-field ($< 100$ G) technique to measure the critical Cooper pair momentum $p_c$ in thin, underdoped films of $Y_{0.9}Cu_{0.9}Ba_2Cu_3O_{7-δ}$ and $Bi_2Sr_2CaCu_2O_{8+δ}$, where doping is effected by adjusting the oxygen stoichiometry through post-deposition annealing. The technique is based on applying a perpendicular magnetic field to the center of a superconducting film and measuring the field at which the screening of the field catastrophically fails. Theory together with measurements on thin films of conventional superconductors Nb and MoGe argue for the validity of the technique. In underdoped cuprates, spectroscopy identifies multiple characteristic energy scales, e.g., the pseudogap and the “nodal” gap, neither of which is proportional to $T_c$. On general grounds, we expect to find that $p_c \propto T_c$ is proportional to the characteristic superconducting energy scale. We observe that $p_c \propto T_c^\alpha$, where $\alpha \approx 0.75$ decreases with underdoping, identifying $k_BT_c$ as the characteristic energy. While this result is trivial in conventional superconductors whose spectroscopic gaps are proportional to $T_c$, it is significant in cuprates.

1Research supported by DOE-Basic Energy Sciences through Grant No. FG02-08ER46533.

5:18PM D11.00015 A mean-field phase diagram with a pair density wave state in relation to cuprate phenomenology 1, AKASH MAHARAJ, LAIMEI NIE, Stanford University, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign, STEVENC KIVELSON, Stanford University — The possible role of the pair density wave (PDW) phase in the cuprate phase diagram is discussed. We examine the mean field Landau theory which intertwines PDW order with uniform superconduct- tivity as well as incommensurate spin- and charge-density wave order, and show how many unique experimental features of different cuprate families are qualitatively reproduced naturally from this perspective. In particular, we focus on the existence of the twodimensional charge order – both in the presence and absence of a magnetic field – and show that various observed trends can be understood from this perspective. This, in turn, is consistent with the supposition that the charge ordering phenomena observed in different cuprates have a common underlying origin.

1The National Science Foundation through the grant No. DMR 1265953, and DOE Office of Basic Energy Sciences under contract No. DEAC02- 76SF00515.
Molecular Dynamics Study of Heat Transport in Silicon–Germanium Nanoscale Metamaterials, Weinan Chen, Materials Science Department, Pennsylvania State University, Gerald Mahan, Vincent Crespi, Department of Physics, Pennsylvania State University, Ismaila Dabo, Materials Science Department, Pennsylvania State University — We have studied the thermal properties of Si–Ge metamaterials with lattice constants of up to tens of nanometers using molecular dynamics simulations and the Green–Kubo method. Validation of this approach is provided by comparing computed thermal conductivities to experimental data for bulk Si–Ge alloy systems. Close agreement with experiment in a large temperature range is found when isotopic effects are taken into account and interatomic potentials are directly parameterized against higher-level semilocal density-functional theory calculations. These simulations highlight the importance of surface morphology, isotopic substitution, alloy fraction, and superlattice periodicity in determining the thermal properties of these metamaterials, suggesting design strategies to control heat transport in nanostructures.

2:42PM D12.00002 First principles study of thermoelectric properties of IV-VI semiconductor superlattices, P.D. Borges, Universidade Federal de Víciosa, Brazil, J.E. Petersen, L. Scolfaro, Texas State University, USA, H.W. Leite Alves, Universidade Federal de São João del Rei, Brazil, T.H. Myers, Texas State University, USA — Thermoelectric materials (TE) have attracted great attention due to their ability to convert heat directly into electricity. However, to be commercially competitive with existing technology, TE devices must have a higher value of figure of merit ZT. It has been proposed to improve ZT by using multilayered systems or superlattices (SLs) resulting in 1D or 2D carrier confinement, reduction of the phonon thermal conductivity, and introduction of anisotropy effects. Here we study the TE properties of IV-VI derived semiconductor SLs. By using the Boltzmann transport theory, within the constant scattering time approximation, in conjunction with first principles calculations, we study the Seebeck coefficient (S) and ZT of PbTe/SnTe SLs. The calculated S shows good agreement with recent experimental data. An anisotropic behavior is observed for low carrier concentrations less than 10^18 cm^-3. For T = 900 K, a large value of ZT parallel to the SL axis equal to 2.6 is predicted for n = 1.2 x 10^18 cm^-3, whereas ZT perpendicular to the SL axis peaks at the value 1.4 for n = 5.5 x 10^17 cm^-3. Both electrical conductivity enhancement and reduction of thermal conductivity are analyzed, and a comparison with other multilayered systems such as planar-doped PbTe is done.

1Support from CNPq and Texas State University

2:54PM D12.00003 How bilayer excitons can greatly enhance thermoelectric efficiency, Kai Wu, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, LOUK Rademaker, Kavli Institute for Theoretical Physics, University of California Santa Barbara, Jan Zaanen, Institute-Lorentz for Theoretical Physics, Leiden University — Presently, a major nanotechnological challenge is to design thermoelectric devices that have a high figure of merit. To that end, we propose to use bilayer excitons in two-dimensional nanostructures. Bilayer exciton systems are shown to have an improved thermopower and an enhanced electric counterflow and thermal conductivity, with respect to regular semiconductor-based thermoelectrics. We suggest an experimental realization of a bilayer exciton thermocouple. Based on current experimental parameters, a bilayer exciton heterostructures of p- and n-doped Bi$_2$Te$_3$ can enhance the figure of merit an order of magnitude compared to bulk Bi$_2$Te$_3$. Another material suggestion is to make a bilayer out of electron-doped SrTiO$_3$ and hole-doped Ca$_3$Co$_4$O$_9$.

3:06PM D12.00004 Effect of phonon-blocking at sintered interfaces, Junichiro Shiomi, The University of Tokyo — With an aim to develop high-figure-of-merit silicon nanocrystalline thermoelectrics, controllability of thermal conductivity is demonstrated by combining computation, measurement, and material synthesis. Direct measurements of interfacial thermal conductance at sintered interfaces using a 2D model interface reveal that the interfacial thermal conductance can be greatly reduced by precipitating silicon oxide crystalline nano-dots at the interface. Furthermore the impact of the reduction in interfacial thermal conductance on the overall thermal conductivity of the bulk nanocrystalline material is identified by multiscale phonon transport calculation using intrinsic phonon properties obtained from first principles. These analyses help us identify the required interfacial structure and grain size (mean value and distribution) for targets thermal conductivity. Attempts to implement this in the actual material development will be also introduced.

1The work is supported in parts by JST PRESTO and JSPS KAKENHI 26709009

3:42PM D12.00005 Thermal boundary resistance in Si/Ge interfaces determined by approach-to-equilibrium simulations, Marcello Puligheddu, Konstanz Hahn, Claudio Melis, Luciano Colombo, Department of Physics, University of Cagliari, Italy — Nanostructured materials hold great promises as efficient thermoelectrics. In such materials, the propagation of phonons is hindered by the internal interfaces (grain boundaries), leading to a reduced overall thermal conductivity and, therefore, to a larger figure of merit. Any further improvement in this field does, however, require a better fundamental understanding of the specific interface effects on thermal transport. In the present work we use approach-to-equilibrium molecular dynamics simulations (AEMD) [1] to investigate the interfacial thermal resistance (ITR) of Si/Ge interfaces, occurring in very promising nanostructured SiGe alloys [2]. We discuss how ITR depends on the thickness of the interface layer, as well as on its composition. Furthermore, the effect of the heat flux direction has been investigated at ambient temperature showing lower ITR for thermal transport from Si to Ge than vice versa. This feature is discussed in connection to possible rectification effects.


1Present address: The Institute for Molecular Engineering, University of Chicago

Enhancing the thermoelectric performance and bridging the $p$- and $n$-type carrier asymmetry of Bi$_2$Te$_3$ thin films via topological surface states

We acknowledge financial support from the National Natural Science Foundation (Grant Nos. 51172167 and 1134006) and MOST of China (Grant Nos. 2013CB632502 and 2014CB921103).

Specific Heat and Thermoelectric Power of Germananene

This work is supported by the NSF EFRI-2DARE project EFRI-1433467.

Length scale dependent of thermal conductivity of Si-Ge alloys

Calculations of the thermopower in materials with nano-inclusions using quantum mechanical simulations

Calculations of the thermopower in materials with nano-inclusions using quantum mechanical simulations

Electronic structure and thermoelectric properties of (PbSe)$_m$/((SnSe)$_n$ superlattice: A first principles study

Tuning thermal transport ultra-thin silicon membranes: Influence of surface nanostructures

Acknowledgment: This project is funded by the program FP7-ENERGY-2012-1-2STAGE under contract number 309150.
5:06PM D12.00012 Thermal Conductivity of Nanocrystalline Silicon Prepared by Chemical-Vapor Deposition

Lifetime decreasing with increasing QD size. Data from TA experiments using a white light probe is also used to study the picosecond carrier dynamics. These PL decays for CdSe QDs with MPA, DDT and Cys ligands compared to OA and TOPO. The PL decay shows multi-exponential behavior with the average intensity accompanied by a larger surface trap state to excitonic PL intensity ratio. This is consistent with the TRPL measurements, which show faster exciton excitonic PL and a broad surface trap state PL. The ligand exchange of OA CdSe QDs with MPA, DDT and Cys leads to quenching of excitonic PL.

Combined with ab-initio calculations, we demonstrate that the rock-salt structure of this system has an intrinsic lattice instability similar to the resonant bond oxide (TOPO), oleic acid (OA), dodecanethiol (DDT), mercaptopropionic acid (MPA), and L-cysteine (Cys). These ligands have different chemical structures and which effects the optical properties of the QDs. Measurements were conducted on QD sizes ranging from Ø 2.5nm to 4.6nm with smaller QDs showing a higher quantum yield of the CdSe/CdS NCs.

Reasons for the higher quantum yield of the CdSe/CdS NCs.

The core of the NCs, and the e-h Coulomb interaction energies. We argue that although both types of core-shell NCs have similar confinement of the WFs, models, compared to the properties of CdSe/CdS NCs. We further looked into the spatial confinement of the HOMO and LUMO wavefunctions (WFs) within different diameters, 2.4 nm and 3.0 nm. We show that the electronic and optical properties of the CdS/ZnS NCs are influenced more by the different structural models, compared to the properties of CdSe/CdS NCs. We further looked into the spatial confinement of the HOMO and LUMO wavefunctions (WFs) within the core of the NCs, and the e-h Coulomb interaction energies. We argue that although both types of core-shell NCs have similar confinement of the WFs, the lowering of the e-h Coulomb interaction energies, hence increasing the AR lifetimes, in the CdSe/CdS NCs, compared to the CdSe/ZnS NCs, is one of the main reasons for the higher quantum yield of the CdSe/CdS NCs.

Monday, March 2, 2015 2:30PM - 5:30PM – Session D13 DCMP DMP: Focus Session: Optical Properties of Semiconductor Nanostructures

2:30PM D13.00001 Comparative study of the electronic and optical properties of core-shell nanocrystals. VANCHO KOCEVSKI, JAN RUSZ, OLLE ERIKSSON, Department of Physics and Astronomy, Uppsala University, Uppsala, D.D. SARMA, Department of Physics and Astronomy, Uppsala University, Uppsala; Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore — The photoluminescence (PL) properties of semiconducting nanocrystals (NCs) can be notably improved by capping the NCs with a shell of another semiconductor, making core-shell structures. Furthermore, their PL properties can be manipulated by changing the core type or the interface between the core and the shell. Here we present a comparative first-principles study of the electronic and optical properties of two different types of core-shell NCs, CdSe/CdS and CdS/ZnS, with four different structural models: pure core, graded core, alloyed interface and graded interface. For the purpose of the study we made NCs with two different diameters, 2.4 nm and 3.0 nm. We show that the electronic and optical properties of the CdS/ZnS NCs are influenced more by the different structural models, compared to the properties of CdSe/CdS NCs. We further looked into the spatial confinement of the HOMO and LUMO wavefunctions (WFs) within the core of the NCs, and the e-h Coulomb interaction energies. We argue that although both types of core-shell NCs have similar confinement of the WFs, the lowering of the e-h Coulomb interaction energies, hence increasing the AR lifetimes, in the CdSe/CdS NCs, compared to the CdSe/ZnS NCs, is one of the main reasons for the higher quantum yield of the CdSe/CdS NCs.

2:42PM D13.00002 Effect of Different Ligands on Carrier Dynamics of CdSe Quantum Dots for Solar Cells Applications

BAICHHABI R. YAKAMI, URICE TOGHA, University of Wyoming, MEG MAHAT, University of North Texas, SHASHANK N. NANDYALA, MILAN BALAZ, JON M. PIKAL, University of Wyoming, DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING TEAM, DEPARTMENT OF CHEMISTRY TEAM, DEPARTMENT OF PHYSICS TEAM — We have carried out steady state absorption and photoluminescence (PL), as well as time resolved PL and ultrafast transient absorption (TA) studies of CdSe quantum dots (QD) with five different capping ligands: trioclyphosphine oxide (TOPO), oleic acid (OA), dodecanethiol (DDT), mercaptopropionic acid (MPA), and L-cysteine (Cys). These ligands have different chemical structures and which effects the optical properties of the QDs. Measurements were conducted on QD sizes ranging from Ø = 2.5nm to 4.6nm with smaller QDs showing an excitonic PL and a broad surface trap state PL. The ligand and exchange of OA CdSe QDs with MPA, DDT and Cys leads to quenching of excitonic PL intensity accompanied by a larger surface trap state to excitonic PL intensity ratio. This is consistent with the TRPL measurements, which show faster exciton PL decays for CdSe QDs with MPA, DDT and Cys ligands compared to OA and TOPO. The PL decay shows multi-exponential behavior with the average lifetime decreasing with increasing QD size. Data from TA experiments using a white light probe is also used to study the picosecond carrier dynamics. These measurements shed light on the role of capping ligands on the carrier dynamics of the QD used as sensitizers in solar cells.
2:54PM D13.00003 Ultrafast Electron Trapping in Ligand-Exchanged Quantum Dot Assemblies

J. M. KIKKAWA, M. E. TURK, P. M. VORA, A. T. FAFARMAN, B. T. DIROLL, C. B. MURRAY, C. R. KAGAN, University of Pennsylvania — We use time-integrated and time-resolved photoluminescence and absorption to characterize the low-temperature (10 K) optical properties of CdSe quantum dot (QD) solids with different ligand and annealing preparation. Close-packed CdSe quantum dot solids are prepared with native aliphatic ligands and with thiocyanate with and without thermal annealing. Using sub-picosecond, broadband time-resolved photoluminescence and absorption, we find that ligand exchange increases the rate of carrier surface trapping. We further determine that holes within the QD core, rather than electrons, can bleach the band-edge transition in these samples at low temperature, a finding that comes as a surprise given what is known about the surface treatment in these QDs. We find that our ligand treatments lead to faster electron trapping to the quantum dot surface, a greater proportion of surface photoluminescence, and an increased rate of nonradiative decay due to enhanced interparticle coupling upon exchange and annealing.

3:06PM D13.00004 Van der Waals materials for the passivation of monolayer closed-packed films of CdSe quantum dots.

DENNIS ZI-REN WANG, DATONG ZHANG, RICHARD CRESWELL, Columbia University, CHENGUANG LU, National Center for Nanoscience and Technology, JIAYANG HU, IRVING P. HERMAN, Columbia University — Van der Waals (vdW) materials are shown to protect CdSe quantum dots (QDs) from oxidation. Few-layer vdW materials, e.g. graphene and MoS2, were transferred onto a monolayer closed-packed CdSe quantum dots and were examined by photoluminescence (PL) after different time periods. By comparing the PL of CdSe QDs in uncovered areas and those covered by different numbers of layers of graphene and MoS2, we saw that vdW encapsulation slows down the aging of CdSe QDs dramatically. PL mapping results clearly showed better protection of the CdSe QDs under the central part of the vdW material compared to that at the edge; this can be explained by the diffusion of oxygen and water vapor from the edge of the vdW materials.


YOUNG-SHIN PARK, CHTM, University of New Mexico, Albuquerque, NM, and Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM, WAN-KI BAE, Photoelectronic Hybrid Research Center, Korea Institute of Science and Technology, Seoul, Korea, ANDREW FIDLER, TOMAS BAKER, JAEOHUN LIM, JEFFREY PIETRYGA, VICTOR KLIMOV, Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM — We report amplified spontaneous emission (ASE) and lasing with very low thresholds obtained using thin films made of engineered thick-shell CdSe/CdS QDs that have a CdSeS alloyed layer between the CdSe core and the CdS shell. These “alloyed” QDs exhibit considerable reduction of Auger decay rates, which results in high bieicton emission quantum yields (Q_{bix}) of ~12%) and extended bieicton lifetimes (τ_{bix} of ~4ns). By using a fs laser (400 nm at 1 kHz repetition rate) as a pump source, we measured the threshold intensity of bieicton ASE as low as 5 µJ/cm^2, which is about 5 times lower than the lowest ASE thresholds reported for thick-shell QDs without interfacial alloying. Interestingly, we also observed bieicton random lasing from the same QD film. Lasing spectrum comprises several sharp peaks (linewidth ~0.2 nm), and the heights and the spectral positions of these peaks show strong dependence on the exact position of the excitation spot on the QD film. Our study suggests that further suppression of nonradiative Auger decay rates via even finer grading of the core/shell characteristics of the transparency. The study tests the molecular polaron formation as a function of the longitudinal acoustic phonon density of states in the optical phonons and we investigate an analogous transparency induced by acoustic phonons. Photoluminescence excitation spectroscopy is used to probe the quantum interference between discrete interdot excitons and continuum single dot-like polaron states [1] revealed the molecular polaron. It has been shown that the phonon-induced transparency is highly controllable by electric field, excitation energy and power. Here we review the molecular polaron formation via optical phonons and we investigate an analogous transparency induced by acoustic phonons. Photoluminescence excitation spectroscopy is used to probe the characteristics of the transparency. The study tests the molecular polaron formation as a function of the longitudinal acoustic phonon density of states in the range from 10 meV to 20 meV above the bare single dot-like neutral exciton ground state transition. [1] M. L. Kerfoot et al., Nat. Commun. 5, 3299 (2014).
4:06PM D13.00009 Quantum-confined Stark shifts of quantum-dot like states in GaAs/AlGaAs core multi-shell nanowires, TENG SHI, BEKELE BADADA, HOWARD JACKSON, LEIGH SMITH, Dept. of Physics, Univ of Cincinnati, CHANGXIN ZHENG, JOANNE ETHERIDGE, Monash Centre for Electron Microscopy, Monash University, NIAN JIANG, QIANG GAO, HOE TAN, CHENNUPATI JAGADISH, Dept. of Electronic and Materials Engineering, Australian National University — A 4nm GaAs quantum well tube sandwiched by AlGaAs barriers is formed surrounding a central 50nm GaAs core. The GaAs/AlGaAs core multi-shell nanowires were grown by MOCVD. Single nanowire devices were fabricated through photolithography followed by deposition of Ti/AI metal contacts. We observed photoluminescence (PL) emission with multiple sharp peaks on a single nanowire device at 10K. We attribute this quantum-dot (QD) like states to well width and alloy fluctuations. We apply a bias across the device to investigate the quenching of PL due to external field ionization of excitons and the Stark shifts in these QD like states. Integrated PL emission show quenching on the high energy side at a lower bias voltage compared to the low energy side. Quantum confined Stark shifts on individual QDs are observed in the range of couple hundreds of micro-eV, suggesting QD sizes varying from 7 to 15nm. We acknowledge the NSF through DMR-1105362, 1105121 and ECCS-1100489, and the Australian Research Council.

4:18PM D13.00010 Probing the band-structures and carrier dynamics of single GaAsSb nanowire heterostructures, YUDA WANG, BEKELE BADADA, HOWARD JACKSON, LEIGH SMITH, Dept. of Physics, Univ of Cincinnati, XIAOMING YUAN, PHILIPPE CAROFF, LAN FU, HOE TAN, CHENNUPATI JAGADISH, Dept. Electronic and Materials Engineering, Australian National University — We present the band structure and carrier relaxation of MOVCD grown single GaAs1-xSbx using photocurrent (PC) spectroscopy and transient Rayleigh Scattering (TRS) spectroscopy techniques. The PC spectroscopy was performed on nanowire devices fabricated using e-beam lithography and deposition of Ti/Au as contacts. The devices show nearly Ohmic behavior and are photosensitive. PC spectra shows an onset of absorption at room temperature in agreement with reported values of bulk GaAs0.6Sb0.4. We also used low temperature (10K) transient Rayleigh scattering (TRS) spectroscopy to measure the band structure as well as carrier relaxation dynamics of individual GaAsSb (x=30% and 40%) nanowires with and without InP passivation layers. The band gaps extracted from the TRS experiments are consistent with both photoluminescence (PL) measurements and theoretical predictions. The InP passivated GaAsSb shows smaller Eg due to the tensile strain from InP on GaAsSb as well as longer lifetimes due to the surface passivation. The carrier density and temperature are extracted by a phenomenological fitting model based on band to band transition theory. We acknowledge the NSF through DMR-1105362, 1105121 and ECCS-1100489, and the Australian Research Council.

4:30PM D13.00011 Superfluorescence from semiconductor quantum wells: magnetic field, temperature, and density dependence, KANKAN CONG, Rice University, JI-HEE KIM, Sungkyunkwan University, G. TIMOTHY NOE II, Rice University, STEPHEN A. MCGILL, National High Magnetic Field Laboratory, Florida State University, YONGRUI WANG, ALEXEY A. BELYANIN, Texas A&M University, JUNICHIRO KONO, Rice University, STEPHEN A. MCGILL COLLABORATION, ALEXEY A. BELYANIN COLLABORATION — In the phenomenon of superfluorescence (SF), a macroscopic polarization spontaneously builds up from an initially incoherent ensemble of excited dipoles and then cooperatively decays, producing giant pulses of coherent radiation. SF arising from electron-hole recombination has recently been observed in semiconductor quantum wells, but its observability conditions have not been fully understood. Here, by fully mapping out the magnetic field (B), temperature (T), and pump power (P) dependence of SF intensity and linewidth, we have constructed a “phase” diagram, showing the B-T-P region in which SF is observable. In general, SF can be observed only at low enough temperatures, high enough magnetic fields, and high enough laser powers with characteristic threshold behaviors. For example, for the (11) inter-Landau-level transition, when B = 17.5T and P = 4mW, SF can be observed only when T < 105K; at B = 17.5T and T = 4K, SF can only be induced by excitation power P > 0.05mW. These results lay the foundation of our understanding of electron-hole SF and provide guidelines for our search for a Bardeen-Cooper-Schrieffer state of excitons.

4:42PM D13.00012 Artificial graphene in nanopatterned GaAs Quantum Wells1, SHENG WANG, DIEGO SCARABELLI, Department of Applied Physics, Columbia University, ANTONIO LEVY, Department of Physics, Columbia University, LOREN PFEIFFER, KEN WEST, Department of Electrical Engineering, Princeton University, VITTORIO PELLEGRINI, Italian Institute of Technology, Genoa, Italy, MICHAEL J. MANFRA, Department of Physics and Astronomy, and School of Materials Engineering, and School of Electrical and Computer Engineering, Purdue University, SHALOM WIND, Department of Applied Physics, Columbia University, ARON PINCZUK, Department of Physics and Department of Applied Physics, Columbia University — Electrons in graphene have linear energy-momentum dispersion, making them massless Dirac fermions. An alternative way to achieve massless Dirac-fermions in a controllable and tunable manner is to construct a honeycomb lattice potential for a 2D electron gas in a semiconductor quantum well. We report realization of very short period (as small as 40 nm) honeycomb lattice pattern using e-beam lithography and drying etching on a GaAs quantum well and scanning electron microscopy (SEM) images of the honeycomb pattern. We acknowledge the NSF through DMR-1105362, 1105121 and ECCS-1100489, and the Australian Research Council.

4:54PM D13.00013 Nanoscale light emission: direct bandgap versus indirect bandgap1, JUN-WEI LUO, SHU-SHEN LI, Institute of Semiconductors, Chinese Academy of Sci (CAS) — The electron-hole Coulomb interaction bounds an electron and a hole together forming an exciton and the e-h exchange interaction lifts the spin-allowed bright exciton state up with respect to the spin-forbidden dark state by an energy of ~1 meV to tens meV depending on the NCs size. The recombination dynamics of the NC exciton remains open to debate, especially at high temperatures (T > 20 K). One perception is a weak exchange interaction of dark excitons with the ensemble of dangling bonds on the NC surface, resulting in spin flip assisted recombination directly from the dark state. Another perception is thermal redistribution of excitons between the dark and bright states. By performing atomistic pseudopotential calculations of indirect bandgap Si NCs and direct bandgap InAs NCs in a large range of NC sizes, we found that the predicted recombination rates of NC excitons are in excellent agreement with experimental data provided by various groups. This agreement confirms the explanation of thermal activation of bright state of excition recombination dynamics in NCs. We also found that the exciton recombination rates, as function of confinement energy, of indirect bandgap NCs is distinct from direct bandgap NCs. More detail theoretical analyses will be presented.

1Supported by DOE-BES Award DE-SC0010695

3JL is supported by the National Young 1000 Talents Plan and the National Science Foundation of China
5:06PM D13.00014 White and Red Light Photoluminescence of ZnS:Eu$^{3+}$ - CMC Nanophosphors, AHEMEN IKORKYA, Department of Physics, University of Agriculture Makurdi, Nigeria, DILIP DE, Department of Physics, Covenant University, Ota, Ogun State, Nigeria, OSITA MELEDU, Department of Physics, Modibo Adamawa University of Technology, Yola, Adamawa, Nigeria, V. BRUNO, Laboratoire de Chimie de la Matière Condensée de Paris — White and red photoluminescence based on europium-doped zinc sulfide nanocrystals capped with sodium carboxymethyl cellulose (ZnS: Eu$^{3+}$ - CMC) was synthesized using precipitation technique with Eu$^{3+}$ ions doping concentrations of 1 mol% and 5 mol%. Some portions of the doped samples were annealed at 300 °C in a sulfur-rich atmosphere. All samples show cubic (zinc blende) structure with crystal sizes; 2.56 nm and 2.91 nm, for the as-synthesized samples, 4.35 nm and 3.65 nm for thermally treated samples, respectively. The as-synthesized samples have equal energy band gap of 4.2 eV, but decreased to 3.76 eV and 3.81 eV after heat treatment. Photoluminescence studies indicate defect emission bands and Eu$^{3+}$ ion lines for the as-synthesized samples. The as-synthesized samples gave pure orange-red emission when excited at wavelength of 394 nm and 465 nm. After thermal annealing of the samples, a broad emission band in the blue-green region assigned to defect related states emerged or were enhanced. Also enhanced were the emission lines of Eu$^{3+}$ ions in the orange-red region. A combination of these two transitions gave white light of different shades depending on Eu concentration or excitation wavelength. Different shades of white light from cool white through Day-light to warm white light were recorded on the CIE 1931 chromaticity diagram. The source excitation wavelengths range from UV-330 nm through near UV ~ 396 nm to blue - 465 nm wavelengths which are in the range of InGaN - based LEDs emissions.

5:18PM D13.00015 The Influence of Impurity Doping On the Phase Transition and Morphology Tuning of Sr/CaFCl: Yb$^{3+}$, Er$^{3+}$ Nanoparticles, YUE CUI, Wake Forest Univ, SULING ZHAO, Beijing Jiaotong University, WENXIAO HUANG, Wake Forest Univ, ZHENGYU XU, Beijing Jiaotong University, YUAN LI, DAVID CARROLL, Wake Forest Univ, SULING ZHAO TEAM — Upconversion nanoparticles (UCNPs) are well-known for their unique luminescent properties that enable the conversion of low-energy photons into high-energy photons by multiphoton processes. In this work, Sr/CaFCl: Yb$^{3+}$,Er$^{3+}$ NCs with a wide range of ions dopant concentrations were synthesized, and strong green and red upconversion fluorescence were observed under laser excitation at a wavelength of 980 nm. The influence and mechanism of ions dopant are demonstrated and discussed. The ions doped concentration has a significant influence on the phase-transfer of the host material and on the corresponding upconversion emissions, and the mechanism of which was studied. In addition, the optimized concentration represents a good balance between the occurrence of the phase transition and concentration quenching. These high-efficiency nanoparticles have potential applications in the fields of optical nanodevices and biomedicine.

Monday, March 2, 2015 2:30PM - 5:30PM
Session D14 DCMP: Invited Session: Bulk and Surface Spectroscopy of Mixed Valence Topological Insulator Samarium Hexaboride 008A - James W. Allen, University of Michigan

2:30PM D14.00001 Quantum Oscillations in Kondo Insulator SmB$_6$, LU LI, University of Michigan — In Kondo insulator samarium hexaboride SmB$_6$, strong correlation and band hybridization lead to a diverging resistance at low temperature. The resistance divergence ends at about 3 Kelvin, a behavior recently demonstrated to arise from the surface conductance. However, questions remain whether and where a topological surface state exists. Quantum oscillations have not been observed to map the Fermi surface. We solve the problem by resolving the Landau Level quantization and Fermi surface topology using torque magnetometry. The observed angular dependence of the Fermi surface cross section suggests two-dimensional surface states on the (101) and (100) plane. Furthermore, similar to the quantum Hall states for graphene, the tracking of the Landau Levels in the infinite magnetic field limit points to -1/2, the Berry phase contribution from the 2D Dirac electronic state.

3:06PM D14.00002 Spin- and angle-resolved photoemission on the first topological Kondo Insulator: SmB$_6$, MING SHI, Paul Scherrer Institute — The concept of a topological Kondo insulator (TKI) has been brought forward as a new class of topological insulators in which non-trivial surface states appear in the bulk Kondo band gap at low temperatures due to the strong spin-orbit coupling. Theoretical considerations have shown that SmB$_6$ is a promising candidate for the first realization of TKIs. In this contribution we will present comprehensive studies of the bulk and surface electronic structures of SmB$_6$. Using high-resolution angle-resolved photoemission spectroscopy (ARPES) we revealed that the two-dimensional surface states reside within a bulk Kondo gap and form three Fermi surfaces in the surface Brillouin zone [1]. The odd number of surface bands crossing the Fermi level fulfills the necessary condition of topologically nontrivial surface states and is in good agreement with the theoretical prediction. Applying spin-resolved ARPES to SmB$_6$, we show that the energy bands of the surface states around the X bar points are spin-polarized. The spins of the surface states are locked to crystal momentum and the spin-helical structure fulfills the requirement of time-reversal symmetry [2]. Our results prove that SmB$_6$ is the first realization of strongly correlated topological Kondo insulator. We will also show the evolution of the bulk electronic structure from a metallic state at high temperatures to a Kondo insulating phase, and how the non-trivial states appear in the system [3].


This work was supported by the Sino-Swiss Science and Technology Cooperation and the Swiss National Science Foundation.

3:42PM D14.00003 Interaction-driven sub-gap resonance in the topological Kondo insulator SmB$_6$, WESLEY FUHRMAN, Johns Hopkins University — Samarium hexaboride (SmB$_6$) is a strongly correlated Kondo Insulator with a non-trivial band-structure topology. I will discuss recent neutron scattering experiments and analysis that expose a 14 meV resonant mode in SmB$_6$ and relate it to the low energy insulating band structure. Repeating outside the first Brillouin zone, the mode is coherent with a 5d-like magnetic form factor. I will discuss how band inversion can be inferred from neutron scattering and show that a perturbative slave boson treatment of a hybridized 2 species (d/f) band structure within an Anderson model can produce a spin exciton with the observed characteristics. This analysis provides a detailed physical picture of how the SmB$_6$ band topology arises from strong electron interactions, and accounts for the 14 meV resonant mode as a magnetically active exciton.

This work was supported by the US Department of Energy, office of Basic Energy Sciences, Division of Material Sciences and Engineering under grant DE-FG02-08ER46544.
4:18PM D14.00004 Surface structure of SmB$_6$ investigated by STM and HAXPES. STEFFEN WIRTH, MPI for Chemical Physics of Solids Dresden, Germany — The intermediate-valence compound SmB$_6$ is typically considered a “Kondo insulator” albeit the concept of the Kondo effect does, in principle, not hold for an intermediate-valence material. Nonetheless, the hybridization between conduction electrons and the strongly interacting Sm $f$-electrons results in a gap at the Fermi energy and hence, an insulating ground state arises at temperatures below about 40 K. Recently, SmB$_6$ has become of enormous topical interest because it is a candidate material for hosting topologically protected surface states. The intermediate valence of Sm in SmB$_6$ was confirmed by HAXPES measurements down to 5 K. Such measurements conducted at high photon energies for improved probing depth are of importance in view of valency limits given for strong topological insulators [1]. Scanning tunneling microscopy (STM) has the unique capability of providing combined topographic and spectroscopic information. We conducted STM on numerous samples cleaved in situ at around 20 K [2]. Cleavage along the (001) plane of the cubic structure through breaking inter-octahedral B-B bonds gives rise to polar surfaces. In result, we found disordered chain-like as well as ordered (2 x 1) surface reconstructions. Occasionally, we also observed patches of non-reconstructed surface areas of both, Sm and B termination. On such areas, we found indications for the Kondo effect being at play. Also, for non-reconstructed surface areas of some ten nanometers in size the $dI/dV$-curves can be well described by a Fano resonance. Thus, the hybridization picture typically considered for this material could be fully confirmed. All types of surfaces, reconstructed and non-reconstructed, displayed a finite zero-bias conductance of considerable magnitude. This finding, in spite of different surface topologies, confirms the robustness of the metallic states and is in line with the proposal of SmB$_6$ being a topological insulator.


1Partly supported by NSF DMR-0801253

4:54PM D14.00005 Temperature dependence, termination dependence, and the spin chirality of the electronic structure of a mixed-valent topological insulator: SmB$_6$. BYUNG IL MIN, POSTECH — A great deal of recent effort has been paid to demonstrate the topological origin of a strongly correlated mixed-valent insulator SmB$_6$. Despite extensive research, however, there is no consensus yet on the topological nature of the Kondo insulator SmB$_6$. In this respect, the works reported so far need be reexamined carefully to see whether the reported results are relevant to the intrinsic property or not. For example, the termination-dependent physical properties of the surface in-gap states in SmB$_6$ have hardly been examined seriously. Also it is important to investigate the spin chirality of the surface states in SmB$_6$. Furthermore, if bulk SmB$_6$ is really a Kondo insulator, its energy gap should have a many-body origin. Then the temperature-dependent evolution of electronic structure is expected in both the bulk and surface bands, which can be measured by ARPES. We have investigated the topological properties of SmB$_6$, based on the dynamical mean-field theory (DMFT) calculations [1] and the density-functional theory (DFT) slab calculations [2], and compared them with those of a similar mixed-valent system of golden phase SmS and other hexaboride systems.


Monday, March 2, 2015 2:30PM - 5:30PM —
Session D15 DCMP: Invited Session: Quantum Criticality at the Superconductor-Insulator Transition and the Higgs Mode 008B — Subir Sachdev, Harvard University


1Support of US-Israel Binational Science Foundation is gratefully acknowledged

3:06PM D15.00002 Quantum critical dynamics without quasiparticles. WILLIAM WITCZAK-KREMPA, Perimeter Institute for Theoretical Physics — Understanding the real-time behavior of quantum systems without long-lived excitations (quasiparticles) constitutes a challenging problem. I’ll discuss recent progress concerning the dynamics of quantum critical systems, in which quantum fluctuations destroy quasiparticles. I’ll show concrete results stemming from an interdisciplinary approach combining field theory, quantum Monte Carlo simulations, and the holographic gauge/gravity duality (AdS/CFT). In particular, experimental predictions will be made regarding the charge response near the superfluid-insulator quantum critical transition of bosons on a 2d lattice. Extensions to other observables and universality classes will be discussed.

3:42PM D15.00003 Evolution of the electronic spectral function and dynamical conductivity across the disorder-tuned superconductor-insulator transition¹. NANDINI TRIVEDI, The Ohio State University, Columbus, OH 43220 — I will discuss the behavior of the single particle electronic spectral function, the bosonic (pair) spectral function \( P(\omega) \), and the dynamical conductivity \( \sigma(\omega) \) across the superconductor-insulator transition (SIT) calculated using quantum Monte Carlo simulations [1]. The transition is driven by tuning the charging energy relative to the Josephson coupling or by varying the degree of disorder. We identify a prominent Higgs mode in the superconductor, and characteristic energy scales in the insulator, that vanish at the transition due to enhanced quantum phase fluctuations, despite the persistence of a robust fermionic gap across the SIT [2]. Disorder leads to increased absorption at low frequencies compared to the SIT in a clean system. Disorder also expands the quantum critical region, due to a change in the universality class, with an underlying \( T=0 \) critical point. Obtaining the conductivity at the transition has been problematical because of analytic continuation of numerical data. We propose a well-defined integrated low-frequency conductivity that can be reliably estimated and discuss its universality.


¹I acknowledge support from DOE DE-FG02-07ER46423

4:18PM D15.00004 Emergence of nanoscale inhomogeneity and finite frequency superfluid response in disordered superconductors, PRATAP RAYCHAUDHURI, Tata Institute of Fundamental Research, Mumbai — The notion of spontaneous formation of an inhomogeneous superconducting state is at the heart of most theories attempting to understand the superconducting state in the presence of strong disorder. Using a combination of low-temperature scanning tunneling spectroscopy and high resolution scanning transmission electron microscopy, we experimentally demonstrate that under the competing effects of strong homogeneous disorder and superconducting correlations, the superconducting state of a conventional superconductor, NbN, spontaneously segregates into domains. Tracking the superconducting state as a function of temperature we show that these superconducting domains persist across the bulk superconducting transition, \( T_c \), and disappear close to the pseudogap temperature, \( T^* \), where signatures of superconducting correlations disappear from the tunneling spectrum and the superfluid response of the system. These results along with complementary measurements of the superfluid stiffness at microwave frequencies underpins the importance of phase fluctuations in strongly disordered s-wave superconductors.

4:54PM D15.00005 The Higgs Mode in Disordered Superconductors Close to a Quantum Phase Transition¹. AVIAD FRYDMAN, Bar Ilan University — The Higgs theory, which generates mass for elementary particles, was inspired by screening of magnetic fields in superconductors. The same theory also predicts an amplitude mode whose high-energy-physics analogue is the famous Higgs particle. It is somewhat disappointing that in superconductors, the Higgs-amplitude mode has not yet been observed, partially because it can rapidly decay into unpaired electrons. Nevertheless, recent theories show that if the Higgs mass could be softened below the pairing gap it should be visible in two dimensions. Such conditions can be met by tuning a superconducting film towards a quantum critical point (QCP). I will report on spectroscopic studies in the terahertz frequency regime of thin superconducting films for which the superconductor to insulator transition (SIT) is tuned by disorder. Tunneling spectroscopy determines the pairing gap \( 2\Delta \) which remains finite on both sides of the SIT. In contrast, the threshold frequency for dynamical conductivity, which in BCS theory is associated with the gap, vanishes critically toward the SIT. The excess optical spectral weight below \( 2\Delta \) is identified as an unambiguous observation of the Higgs mode in a superconductor.

¹Supported by GIF grant # I-1250-303.10/2014.

Monday, March 2, 2015 2:30PM - 5:18PM — Session D16 DMP: Focus Session: Machine Learning For Materials Discovery 101AB - Marco Nardelli, University of North Texas

2:30PM D16.00001 Machine Learning methods in fitting first-principles total energies for substitutionally disordered solid¹. QIN GAO, SANXI YAO, MICHAEL WIDOM, Carnegie Mellon University — Density functional theory (DFT) provides an accurate and first-principles description of solid structures and total energies. However, it is highly time-consuming to calculate structures with hundreds of atoms in the unit cell and almost not possible to calculate thousands of atoms. We apply and adapt machine learning algorithms, including compressive sensing, support vector regression and artificial neural networks to fit the DFT total energies of substitutionally disordered boron carbide. The nonparametric kernel method is also included in our models. Our fitted total energy model reproduces the DFT energies with prediction error of around 1 meV/atom. The assumptions of these machine learning models and applications of the fitted total energies will also be discussed.

¹Financial support from McWilliams Fellowship and the ONR-MURI under the grant NO. N00014-11-1-0678 is gratefully acknowledged.

2:42PM D16.00002 Phase Transitions of Boron Carbide: Pair Interaction Model of High Carbon Limit. SANXI YAO, MICHAEL WIDOM, Carnegie Mellon University, WILLIAM HUHN, Duke University, QIN GAO, Carnegie Mellon University — Boron carbide is a structure that exhibits a broad composition range, implying a degree of intrinsic substitutional disorder. While the observed symmetry is rhombohedral, the enthalpy minimizing structure has lower, monoclinic, symmetry. With high melting temperature, it is difficult to experimentally study its phase transition at low temperature and there is discrepancy among different research groups. Moreover, the widely-accepted phase diagram suggests substitutional disorder at low temperature, implying a non vanishing entropy. Here we use computational method to study its phase transition. We implement a pair interaction model and fit to a database of structural energies. Utilizing histogram methods to analyze Monte Carlo simulations of this model, we investigate the symmetry-restoring phase transition that explains the observed rhombohedral symmetry at high temperatures.
2:54PM D16.00003 Unsupervised machine learning on atomistic configurations: examples on amorphous defects and energy landscapes, EKIN CUBUK, Harvard University, SAMUEL SCHOENHOLZ, ANDREA LIU, University of Pennsylvania, EFTIMIOS KAXIRAS, Harvard University — Due to the recent availability of very large datasets, machine learning (ML) methods are gaining popularity as approximation and optimization tools in solid state physics. We have recently shown that supervised ML can also be used to identify and analyze soft particles, particles susceptible to rearrangement, in amorphous solids [1]. Our method can be used to understand what makes certain configurations of particles more prone to rearrangement, and design stronger materials. We use unsupervised ML and nonlinear dimensionality reduction methods, where we do not need a “training set” to train the algorithm, to explore better representations of atomic configurations. These representations are shown to provide important physical insights into the structure of soft spots and stable regions in several computational and experimental glassy systems, as well as the energy landscapes of quantum mechanical systems based on Density Functional Theory calculations. By discovering an improved representation and visualization of relevant energy landscapes, discovery and optimization efforts can be simplified.


3:06PM D16.00004 Machine Learning Methods for the Sampling of Chemical Space From First Principles, RAGHU RAMAKRISHNAN, University of Basel — Computational brute force high-throughput screening of compounds is beyond any capacity for all but the most restricted systems due to the combinatorial nature of chemical space, i.e. all the compositional, constitutional, and conformational isomers. Efficient computational materials design algorithms must therefore make good trade-offs between the accuracy of the applied model and computational speed. Overall, rapid convergence in terms of number of compounds visited is highly desirable. In this talk, I will describe recent contributions in this field based on statistical approaches that can serve as inexpensive surrogate models to reduce the computational load of quantum mechanical calculations. Such surrogate machine learning (ML) models infer quantum mechanical observables of novel materials, rather than solving approximate variants of Schrodinger’s equation. We developed accurate ML models for the rapid prediction of atomization energies and enthalpies, cohesive energies, and electronic properties that conventionally can only be predicted using quantum mechanics. All our ML models have been trained using large data bases containing properties of thousands of chemical compounds and materials. I will exemplify our approach for the prediction of properties from scratch for out-of-sample compounds. These predictions reach quantum chemical accuracy and are basically instantaneous, i.e. at a computational cost reduced by several orders of magnitude.

3:42PM D16.00005 Informatics guided Search for Magnetic Apatites, PRASANNA V. BALACHANDRAN, TURAB LOOKMAN, Los Alamos National Laboratory — Materials with apatite crystal structure have applications ranging from biomaterials to electrolytes for solid oxide fuel cells. Their chemical flexibility and structural diversity provide a fertile ground to tune functionalities as potential candidates for many applications. However, magnetic apatites are rare. In this work, we use machine learning methods to rapidly screen a vast chemical space and identify novel apatite compositions with magnetic ions. We first construct a database of known materials from searching the experimental literature. We then augment the database with features that capture the trends in geometry and bonding characteristics of apatites. Supervised classification learning forms the basis of our machine learning approach through which we uncover design rules that enable prediction of potentially stable magnetic apatite compositions, prior to experimental synthesis. Finally, we validate our predictions using density functional theory calculations.

3:54PM D16.00006 Using Data Mining Algorithms in Solid State Physics, TROY LYONS, Central Michigan University, NICHOLAS MECHOLSKY, The Catholic University of America, STEFANO CURTAROLO, Duke University, MARCO BUONGIORNO NARDELLI, University of North Texas, MARCO FORNARI, Central Michigan University — We processed large materials databases with data mining methods such as clustering and classification in order to assign specific questions in the field of thermoelectric materials and transparent conductors. Our goal is to extract meaningful information from band structures repositories such as AFLLOWLIB. Our implementation is validated using a toy database that mimics the complexity of AFLLOWLIB, which has also been solved analytically. We found that even when the analytical solution is known, proper data analysis can help to understand physical phenomena.

4:06PM D16.00007 Interplay of Atomic and Electronic Structure in Second Harmonic Generating Nonlinear Optical Materials, ANTONIO CAMMARATA, Czech Technical University in Prague, JAMES RONDINELLI, Northwestern University — Group theoretical methods and ab initio electronic structure calculations are combined to formulate a general Symmetry-Assisted Functional Optical Response (SAFOR) protocol to understand and predict the second harmonic generation (SHG) response in nonlinear optical crystals. We show that the SHG coefficients may be decomposed into atomic contributions from various inversion symmetry lifting distortions, which we parametrize as symmetry-adapted displacement patterns that transform as irreducible representations of a relevant centrosymmetric parent structure. The SAFOR protocol is then combined with an electronic descriptor for bond covalency to explain the origin of SHG in noncentrosymmetric-nonpolar JTeMoO$_6$ telluromolybdate compounds. We show that the SHG response has a complex dependence on the asymmetric geometry of the polyhedral units and the orbital character at the valence band edge. The atomic scale and electronic structure understanding of the macroscopic SHG behavior obtained with these descriptions is then used to identify hypothetical HgTeMoO$_6$ as a candidate telluromolybdate, which we predict should exhibit the largest SHG response in the JTeMoO$_6$ family.

4:18PM D16.00008 Materials Cartography: Representing and Mining Material Space Using Structural and Electronic Fingerprints, COREY OSES, Duke Univ, OLEXANDR ISAYEV, DENIS FOURCHES, EUGENE MURATOVI, UNC Chapel Hill, KEVIN RASCH, Duke Univ, ALEXANDER TROPISHA, UNC Chapel Hill, STEFANO CURTAROLO, Duke Univ, CENTER FOR MATERIALS GENOMICS, DUKE UNIVERSITY COLLABORATION, LABORATORY FOR MOLECULAR MODELING, UNC CHAPEL HILL COLLABORATION — As the proliferation of high-throughput approaches in materials science is increasing the wealth of data in the field, the gap between accumulated-information and derived-knowledge widens. We address the issue of scientific discovery in materials databases by introducing novel analytical approaches based on structural and electronic materials fingerprints. The framework is employed to (i) query large databases of materials using similarity concepts, (ii) map the connectivity of the materials space (i.e., as a materials cartogram) for rapidly identifying regions with unique organizations/properties, and (iii) develop predictive Quantitative Materials Structure-Property Relationships (QMSPR) models for guiding materials design. In this study, we test these fingerprints by seeking target material properties. As a quantitative example, we model the critical temperatures of known superconductors. Our novel materials fingerprinting and materials cartography approaches contribute to the emerging field of materials informatics by enabling effective computational tools to analyze, visualize, model, and design new materials.
several decades ago, enabled an average success in classification of (non-rocksalt structures and thus performed a binary classification task. We found that using the standard indices various forms of cross-validation, for the task of classifying the crystal structures of the octet AB solids. We partitioned a set of 75 solids into rocksalt and PILANIA, T. LOOKMAN, Los Alamos National Laboratory — We explored the use of machine learning methods, specifically support vector machines and in GNEMR and may help further study of the intrinsic electrical properties of the materials under strain. model-based fittings determine the intrinsic stain and mass of graphene samples accurately. Our devices allow thorough exploration of the nonlinear dynamics the model and matches with experimental data. Results from numerical simulation demonstrate also the transition in the nonlinear behavior. Additionally, the nanoelectromechanical resonators (GNEMR) on flexible substrates. The intrinsic stain in graphene is tuned by bending the substrate, during which a transition from hardening to softening resonance behavior and a minimum resonance frequency are observed. To explain these observations, a resonator model taking from hardening to softening resonance behavior and a minimum resonance frequency are observed. To explain these observations, a resonator model taking 1Supported by the Department of Energy.

4:42PM D16.00010 Structure classification of AB solids via machine learning1, J.E. GUBERNITIS, G. PILANIA, T. LOOKMAN, Los Alamos National Laboratory — We explored the use of machine learning methods, specifically support vector machines and various forms of cross-validation, for the task of classifying the crystal structures of the octet AB solids. We partitioned a set of 75 solids into rocksalt and non-rocksalt structures and thus performed a binary classification task. We found that using the standard indices (rσ, rπ), suggested by St. John and Bloch several decades ago, enabled an average success in classification of 92%. Our main new result is our finding that using just rσ and the excess Born effective charge ∆Z_A of the A atom, computed by DFT, enabled an average success of 98%, prompting us to propose (rσ, ∆Z_A) as a replacement for the St. John-Bloch pair. In general, we found that adding one or two other features to the St. John-Bloch pair, unless they include the excess Born effective charge, generally decreases the average success rate.

5:06PM D16.00012 Force field development from first principles for materials design, MARIA CHAN, ALPER KINACI, BADRI NARAYANAN, FAITH SEN, STEPHEN GRAY, MICHAEL DAVIS, SUBRAMANIAN SANKARANARYANAN, Argonne National Laboratory — The ability to perform accurate calculations efficiently is crucial for computational materials design. In this talk, we will discuss a stream-lined approach to force field development using first principles density functional theory training data and machine learning algorithms. We will also discuss the validation of this approach on precious metal nanoparticles.


2:30PM D17.00001 Graphene Electrostatic Microphone, QIN ZHOU1, SEITA ONISHI2, A. ZETTL3, Department of Physics, University of California - Berkeley — We demonstrate a wideband electrostatic graphene microphone displaying flat frequency response over the entire human audible region as well as into the ultrasonic regime. Using the microphone, low-level ultrasonic bat calls are successfully recorded. The microphone can be paired with a similarly constructed electrostatic graphene loudspeaker to create a wideband ultrasonic radio.

3Materials Sciences Division, Lawrence Berkeley National Laboratory Kavli Energy NanoSciences Institute at the University of California - Berkeley

4Materials Sciences Division, Lawrence Berkeley National Laboratory Kavli Energy NanoSciences Institute at the University of California - Berkeley

4:24PM D17.00002 Nonlinear dynamics in tunable graphene nanoelectromechanical systems, FEN GUAN, PIRANAVAN KUMARAVADIVEL, DIMITRI AVERIN, XU DU, Stony Brook University — We report the fabrication and characterization of graphene nanoelectromechanical resonators (GNEMR) on flexible substrates. The intrinsic stain in graphene is tuned by bending the substrate, during which a transition from hardening to softening resonance behavior and a minimum resonance frequency are observed. To explain these observations, a resonator model taking into account the intrinsic strain and electrostatic force is developed. Including higher-order nonlinear terms, a minimum frequency is obtained analytically from the model and matches with experimental data. Results from numerical simulation demonstrate also the transition in the nonlinear behavior. Additionally, the model-based fittings determine the intrinsic strain and mass of graphene samples accurately. Our devices allow thorough exploration of the nonlinear dynamics in GNEMR and may help further study of the intrinsic electrical properties of the materials under strain.
2:54PM D17.00003 High frequency nanomechanical resonators in ultraclean suspended graphene pn junctions, MINKYUNG JUNG, PETER RICKHAUS, SIMON ZIHMANN, PETER MAKK, Department of Physics, University of Basel. ALEXANDER EICHLER, Department of Physics, ETH Zurich, MARKUS WEISS, CHRISTIAN SCHÖNENBERGER, Department of Physics, University of Basel. DEPARTMENT OF PHYSICS, UNIVERSITY OF BASEL TEAM, DEPARTMENT OF PHYSICS, ETH ZURICH TEAM — Here, we demonstrate high frequency nanomechanical resonators in ultraclean suspended graphene pn junctions. The suspended graphene resonators are fabricated on two bottom gates (left and right) covered with lift-off resist (LOR) by using a mechanical transfer technique. After current annealing, the device exhibits a clear charge neutrality point around zero gate voltage. Depending on the left and right bottom gate voltages, the device shows four different conductance regimes: pp, np, pn and pp regimes. The clear Fabry-Perot interference pattern is observed, indicating ballistic transport behavior over 1 μm-long channel. Then, the mechanical resonance is measured in the same device with a frequency modulation (FM) mixing technique at 4.2 K in the vacuum chamber. The resonance frequency is about 405 MHz. By fitting resonance frequency, we deduce both the mass density and the built-in tension in the graphene sheet. In a similar device structure with different strain environment, we observe a resonance frequency as high as 1.17 GHz for the fundamental mode.

3:06PM D17.00004 Angle dependent phonon spectra and thermal properties of misoriented bilayer graphene, MAHESH NEUPANE, Department of Electrical and Computer Engineering, Univ of California - Riverside, PANKAJ RAMNANI, Department of Chemical and Environmental Engineering, Univ of California, Riverside, SUPENG GE, Department of Physics and Astronomy, University of California, Riverside, ASHOK MULCHANDANI, Department of Chemical and Environmental Engineering, Univ of California, Riverside, ROGER LAKE, Department of Electrical and Computer Engineering, Univ of California - Riverside — The Raman spectra of misoriented bilayer graphene (MBG) show angle dependent signatures of the misorientation angle (θ) in the low frequency breathing modes. We investigate these low frequency modes using molecular dynamics including temperature dependent phonon anharmonicity. The calculated vibrational and thermal properties are compared against our experimental data. Our theoretical investigations reveal that the layer breathing mode (LBM) frequencies at 100 ± 10 cm⁻¹ for angles 6° ≤ θ ≤ 30° are consistent with the observed frequencies of ZO modes in the Raman spectrum. For the smaller θ (or larger L), the reduced BZ leads to the zone-folding of the phonon dispersion and doping depends on the orientation of the lattice specific heat capacity.

3:18PM D17.00005 Strain in Transferred Graphene at Low Temperatures, JUAN AGUILERA-SERVIN, ADRIAN NOSEK, CHENG PAN, MARC BOCKRATH, Univ of California - Riverside — Strain in graphene layers produces synthetic gauge fields that may be used to modify the properties of its electron system [1,2]. We study single layers of graphene transferred over Ti/Au electrical contacts on oxidized Si wafers with etched triangular holes in the oxide. The layers are strainied by applying pressure electrostatically using a gate voltage and hydrostatically using an external inert gas. We investigate electronic transport in this suspended variable-strain graphen system at low temperatures. We will discuss our latest results.

3:30PM D17.00006 Control Over the Adhesion and Strain on Graphene Using Arrays of Mesoscale Pyramids, STEPHEN GILL, University of Illinois at Urbana-Champaign, SHUZE ZHU, University of Maryland, J. HENRY HINNEFELD, WILLIAM SWANSON, University of Illinois at Urbana-Champaign, TENG LI, University of Maryland, NADYA MASON, University of Illinois at Urbana-Champaign — Applying non-uniform shear stress to graphene can lead to new electronic states. For example, strain having triangular symmetry has been shown theoretically and experimentally to generate a nearly uniform pseudo-magnetic field [1,2]. However, the lack of methods to control non-uniform strain in graphene devices has limited the ability to explore transport phenomena tuned by strain. In this talk, we demonstrate that the adhesion and strain of graphene can be controlled by using arrays of mesoscale pyramids. By manipulating the arrangement of pyramids and the aspect ratio of the array, graphene’s adhesion to the array range from conformal to suspended between pyramids. Strain in graphene adhered to pyramids is revealed by Raman spectroscopy, and the amount of strain experienced is shown to depend on the adhesion to the pyramids. Support calculations demonstrate the pseudo-magnetic field profile for graphene adhered to pyramids for different strains. These results indicate a potential route for exploring strain-controlled transport phenomena in graphene.

3:42PM D17.00007 Electron-phonon interactions in bilayer graphene, HELI VORA, NIST-Boulder, XU DU, Department of Physics and Astronomy, Stony Brook University — We report measurements on electron thermal conductance in bilayer graphene due to cooling via phonons. The measurements were carried out using bilayer graphene-superconductor tunnel junctions, where the superconducting contacts effectively confine the hot electron inside the graphene channel, allowing access to the electron cooling at low temperatures. We show results on the temperature and doping dependence of the cooling power in bilayer graphene. Contrary to what was observed in monolayer graphene, the phonon cooling power decreases with increasing carrier density in bilayer graphene. The temperature dependence of the phonon cooling power can be described by a power law with a power factor ~ 5, again, qualitatively different from the T^3 temperature dependence observed in the disordered monolayer graphene. These new results may shed light on the dominating mechanisms for hot electron cooling bilayer graphene.

3:54PM D17.00008 Dissipation and feedback cooling of graphene and MoS2 nanomechanical resonators, RONALD VAN LEEUWEN, GARY STEELE, WARNER VENSTRA, HERRE VAN DER ZANT, Delft Univ of Tech, KAVLI INSTITUTE OF NANOSCIENCE TEAM — The interesting mechanical and electronic properties of 2-dimensional materials make them candidates for nano-electromechanical systems. Remarkably, the mechanical resonance linewidth of such suspended structures is found to be invariably low at room temperature. Time-domain measurements were used as a tool to differentiate between dissipation and non-dissipative frequency fluctuations, thus providing more insight in the origin of the low linewidth. We perform time-domain measurements on MoS2 resonators with thickness down to a single layer, and compare the relaxation times obtained from ringdown measurements to the resonance linewidth obtained from Brownian motion and driven frequency responses. We conclude that dephasing plays a negligible role in the thermal relaxation process as the finite damping linewidth is limited by the signal to noise ratio. To improve the damping we introduce an optical feedback technique. We demonstrate continuous tuning of the oscillator linewidth, by modifying the linewidth over 2 orders of magnitude. Feedback also enables cooling of the fundamental mode of graphene and MoS2 drum resonators down to an effective temperature of 100 K.

4:06PM D17.00009 Electron transport in graphene with uniaxial local strain, HIKARI TOMORI, Japan Science and Technology Agency and Univ. Tsukuba, RINEKE HIRAIIDE, HIROKAZU TANAKA, YU ITOU, KENTA KATAKURA, YOUSHI OOTUKA, AKINOBU KANDA, Univ of Tsukuba — Transport engineering is a promising method for controlling electron transport in graphene; Spatial variation of pseudo-vector potential and pseudo-scalar potential induced by lattice strain modulate transport property of graphene. We have succeed in fabricating a graphene FET with uniaxial local strain, and observed clear deformation in gate voltage dependence of conductivity (σ – Vg curve). From a comparison with numerical calculation, we conclude that strain-induced scalar potential is responsible for the deformation of the σ – Vg curve.
4:30PM D17.00011 Thermal Conductance of Epitaxial and Transferred CVD-Grown Graphene, JOYCE COPPOCK, PAVEL NAGORNYKH, IAN MCADAMS, BRUCE KANE, University of Maryland, College Park — Two-dimensional materials such as graphene tend to ripple in the out of plane direction. These ripples arise both due to thermal fluctuations and uneven stress forces at the boundary. In this work, we study the effect of the rippling on the effective mechanical properties of graphene: Young’s modulus and bending rigidity. To accomplish this, we developed a non-contact technique that allows probing mechanical properties of graphene at temperatures between 4K and 400K. We use a high voltage electrostatic force to pull on graphene and high-resolution optical interferometric profilometry to measure its mechanical response. We find that the effective Young’s modulus of graphene is significantly softened and the bending rigidity is increased due to rippling.

4:42PM D17.00012 Graphene Mechanical Resonators under Large Strain, SEITA ONISHI1, QIN ZHOU2, ALEX ZETTL3, Department of Physics, University of California, Berkeley, CA 94720, USA — Graphene has shown promise as a high frequency mechanical resonator due to its high Young’s modulus and light mass [1]. With large strains, theoretical predictions anticipate even changes to graphene’s band structure [2]. We developed an integrated platform to apply large strains on suspended graphene with a MEMS based actuator. We will show preliminary results on the optical detection of the change in resonance frequency as the graphene mechanical resonator is strained.


1Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA
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4:54PM D17.00013 Thermal and Thermoelectric Transport across Graphene/BN and Graphene/BN/Graphene Heterostructures, NIRAkar Poudel, University of Southern California — We report thermal and thermoelectric transport measurements across graphene/hexagonal boron nitride (h-BN)1 and graphene/hexagonal boron nitride (h-BN)/graphene2 heterostructure devices. Using an AC lock-in technique, we are able to separate the thermoelectric contribution to the I - V characteristics of these important device structures. The temperature gradient is measured using optical Raman spectroscopy, which enables us to explore thermoelectric transport produced at material interfaces, across length scales of just 1-2 nm. A temperature drop of 60 K can be achieved across this junction at high electrical powers (14 mW). Based on the temperature difference and the applied power data, we determine the thermal interface conductance of this junction to be 7.4 x108 W/m2·K, which is below the 10^-10 W/m2·K values previously reported for graphene/SiO2 interface. Based on the observed thermoelectric voltage (∆V) and temperature gradient (∆T), a Seebeck coefficient of 99.3 µV/K is ascertained for the heterostructure device.

5:06PM D17.00014 Development of a quadrupole trap apparatus for UHV measurements of levitated graphene, JOYCE COPPOCK, PAVEL NAGORNYKH, IAN MCADAMS, BRUCE KANE, University of Maryland, College Park — Completely decoupling graphene from any substrate opens up new possibilities for measurement of its electrical and mechanical properties as well as the exploration of novel methods of crystal growth and fabrication of 2D materials. We levitate a charged micron-scale few-layer graphene-like flake on copper foil and after it is transferred to a deposited copper substrate. It is found out that the thermal conductance of un-annealed transferred SLG on copper foil is around 20 MW/m·K, much lower than that of SLG grown on copper foil which is approximately 30 MW/m·K. Annealing in forming gas/vacuum causes the thermal conductance of transferred SLG to increase to 31 MW/m·K. X-ray spectroscopy (XPS) and Atomic force microscopy (AFM) are employed to investigate the various factors, (i.e., copper oxide, polycarbonate (PC) residue, roughness and conformity) that may cause a decrease in thermal conductance after the transfer. XPS measurement results show an absence of PC residue, even before annealing. The results also reveal that annealing in forming gas reduces the copper oxide thickness by about 2.5nm, and such a small reduction in oxide thickness is not sufficient to cause a drastic increase of approximately 10MW/m·K in thermal conductance. AFM results show that before annealing, the SLG has elongated ridges-like morphology. This morphology is different from that of copper which has circular-like features. After annealing, the SLG morphology becomes very similar to that of copper — both exhibiting circular-like features. This shows that the SLG can conform better to the copper surface after annealing.

5:18PM D17.00015 Effect of stray electric fields on cooling of center of mass motion of levitated graphite flakes, PAVEL NAGORNYKH, JOYCE COPPOCK, BRUCE KANE, University of Maryland, College Park — Levitation of charged multilayer graphite flakes in a quadrupole ion trap provides a unique way to study graphene in isolated conditions. Cooling of a flake in such a setup is necessary for high vacuum measurements of the flake and is achieved by using a parametric feedback scheme [1]. We present data showing the strong dependence of the cooling of the flake’s center of mass motion on the stray electric fields. We achieve this by using auxiliary electrodes to shift the position of the trap center in space. Once the point of minimum interaction between the trap fields and the particle is found (leading to cooling of the flake motion to temperatures below 20K at pressure of 10^-7 Torr), we can estimate charge and mass of the flake by observing quantized discharge of the particle and measure transient dynamics of the center of mass motion by tuning the cooling off and on. As an additional benefit, the behavior of the flake away from the optimum trap position can be used to quantify stray fields’ effect on the particle motion by measuring its spinning orientation and frequency dependence on offset from the optimum position.

2:30PM D18.00001 Constructing and Deconstructing Non-Abelian Anyons, BELÉN PAREDES, Instituto de Física Teórica UAM/CSIC — Non-Abelian anyons are profoundly unintuitive quasiparticles. When braiding them, the order of the braids matters, dramatically changing the properties of the underlying piece of quantum matter. They are predicted to occur as excitations of certain quantum Hall liquids and as Majorana fermions attached to vortices in special superconductors. But their experimental realization remains a major challenge, possibly because our theoretical understanding of non-Abelian matter is also far from complete. In this talk I will deconstruct non-Abelian anyons, revealing that they are made of clusters of Abelian quasiparticles, Abelian anyons, which become indistinguishable. I will show that deconstruction into identical indistinguishable components is a useful framework for the theoretical understanding of non-Abelian anyons, providing an intuitive picture for the physical mechanism leading to their emergence. Moreover, deconstruction opens a route for the construction and characterization of non-Abelian physical models and for their experimental realization in nature. To illustrate the approach, I will construct and characterize a non-Abelian spin-1 lattice model, discussing directions to detect the emergent non-Abelian anyons in experiments with ultracold atoms.

3:06PM D18.00002 Novel ways of creating and detecting topological order with cold atoms and ions1, MACIEJ LEWENSTEIN, ICF0 - Institut de Ciències Fotòniques and ICREA - Institució Catalana de Recerca i Estudis Avançats — In my talk I will focus on novel physics and novel quantum phases that are expected of lattice systems of ultra-cold atoms or ions in synthetic gauge fields, generated via lattice modulations and shaking. I will discuss fractal energy spectra and topological phases in long-range spin chains realized with trapped ions or atoms in nanofibers, and synthetic gauge fields in synthetic dimensions. I will spend large part of the talk discussing the ways to detect topological effects and order, via tomography of band insulators from quench dynamics, or via direct imaging of topological edge states.

3:42PM D18.00003 Effects of Berry Curvature in Ultracold Atomic Gases1, NIGEL COOPER, T.C.M. Group, Cavendish Laboratory, University of Cambridge — Topological energy bands exhibit many fascinating physical phenomena. For instance, topological invariants underlie both the quantum Hall effect and more general topological insulators. There is currently great interest in exploring such physics in ultracold gases. Recent experiments have explored optical lattices with novel geometrical and topological features, and there is much ongoing activity to extend to other situations. Less widely appreciated is the fact that the energy bands of these new forms of optical lattice also have important geometrical properties. In particular, the Berry curvature is a geometrical property of the energy eigenstates, defined locally in the Brillouin zone. When integrated over the Brillouin zone of a two-dimensional band, it gives the Chern number, the topological invariant of the quantum Hall effect. The Berry curvature has many physical consequences in 2D and 3D systems, such as in the anomalous quantum Hall effect. I shall summarize how the Berry curvature can manifest itself in experimental measurements of transport and of collective modes in ultracold atomic gases.

This work was supported by ERC AdG OSYRIS, EU IP SIQS, EU STREP EQUAM and Spanish Ministry Grant FOQUS.

4:18PM D18.00004 Realization of the topological Haldane model, RÉMI DESBUQUOIS, ETH - Zurich — A topologically non-trivial band structure appears in a hexagonal lattice if time-reversal symmetry is broken, as suggested by F. D. M. Haldane. He further pointed out that, in combination with broken inversion symmetry, this gives rise to a phase diagram containing topologically distinct phases, yet without the necessity of a magnetic field. Studying the band structure of a hexagonal lattice with broken time reversal symmetry induced by complex valued next-nearest neighbor couplings, he showed that the boundaries of the topologically different phases are gap opening-and-closing transitions at the Dirac points. Whilst a realization of this model in a material was hardly conceivable, it provided the conceptual basis for other topological insulators and the quantum spin Hall effect. Prospects to realize the model with cold atoms emerged by advances in generating effective magnetic fields for neutral atoms and the idea to employ time-dependent fields to break time-reversal symmetry in a hexagonal lattice. Here we report on the implementation of the Haldane model in a periodically driven honeycomb optical lattice and the characterization of the topological Bloch bands using non-interacting fermionic atoms. Modulating the position of the lattice sites along a circular trajectory generates complex next-nearest-neighbor tunneling and a gap opens at the Dirac points, which we measure using momentum-resolved inter-band transitions. In analogy to a Hall conductance we observe a characteristic displacements of the atomic cloud under a constant force. By additionally breaking the inversion-symmetry, we identify the closing of the gap at an individual Dirac point, associated with the transition between the topologically distinct phases, obtaining good agreement with the calculated phase diagram. Whilst the physics of the non-interacting system is determined by the single-particle band structure, as studied in this work, the cold atom systems is also suited to explore the interplay between topology and interactions.

4:54PM D18.00005 An Aharonov-Bohm interferometer for determining Bloch band topology, ULRICH SCHNEIDER, LMU & MPQ Munich — The geometric structure of an energy band in a solid is fundamental for a wide range of many-body phenomena in condensed matter and is uniquely characterized by the distribution of Berry curvature over the Brillouin zone. In analogy to an Aharonov-Bohm interferometer that measures the magnetic flux penetrating a given area in real space, we realize an atomic interferometer to measure Berry flux in momentum space. We demonstrate the interferometer for a graphene-type hexagonal lattice, where it has allowed us to directly detect the singular x-Berry flux localized at each Dirac point. This interferometer enabled us to determine the distribution of Berry curvature with high momentum resolution. In addition, I will present results on extending these ideas to two-band models, where Berry phases generalize to Wilson loops and give rise to even richer geometric structures. This work can form the basis for a general framework to fully characterize topological band structures and can also facilitate holonomic quantum computing through controlled exploitation of the geometry of Hilbert space.

Monday, March 2, 2015 2:30PM - 5:30PM – Session D19 DCOMP DPOLY GSOFT/DBIO: Invited Session: Fifty Years of Molecular Dynamics Simulations II: Past, Present and Future Mission Room 103B - Rajiv Kalia, University of Southern California

2:30PM D19.00001 A Variational Approach to Enhanced Sampling and Free Energy Calculations, MICHELE PARRINELLO, ETH Zurich and Università della Svizzera italiana, Lugano, Switzerland — The presence of kinetic bottlenecks severely hampers the ability of widely used sampling methods like molecular dynamics or Monte Carlo to explore complex free energy landscapes. One of the most popular methods for addressing this problem is umbrella sampling which is based on the addition of an external bias which helps overcoming the kinetic barriers. The bias potential is usually taken to be a function of a restricted number of collective variables. However constructing the bias is not simple, especially when the number of collective variables increases. Here we introduce a functional of the bias which, when minimized, allows us to recover the free energy. We demonstrate the usefulness and the flexibility of this approach on a number of examples which include the determination of a six dimensional free energy surface. Besides the practical advantages, the existence of such a variational principle allows us to look at the enhanced sampling problem from a rather convenient vantage point.
1:30PM D19.00002 Bridging scales: from atoms to coarse-grained models for soft matter systems, CHRISTINE PETER, University of Konstanz, Konstanz, Germany — Molecular simulation has extended to increasingly complex soft matter systems, and time-scale and system-size requirements have instigated the use of simulation models on multiple levels of resolution. On the classical particle-based level, a large variety of methods to develop coarse grained (CG) simulation models has emerged, an important subgroup being those scale-bridging methods where the CG model is derived from and systematically linked to an underlying atomistic description. In my talk, I will introduce a few of these methods, address the underlying concepts as well as some of the ongoing challenges that are inherent to coarse graining. A natural consequence of reducing the level of resolution in a simulation model is a loss of transferability, i.e. a decreasing ability to correctly describe a system at several thermodynamic state points. Intimately linked to this is a loss of the ability to correctly represent all structural, thermodynamic and dynamic properties of the system. Examples for these limitations are easily found in all CG simulations of multicomponent or multiphase soft matter systems – ranging from liquid crystals, biomolecular aggregates, biomaterials to hard/soft nanocomposites. A correct representation of phase transitions, phase coexistence, environment-induced conformational transitions, or effects due to surfaces and interfaces is a severe challenge for bottom-up CG models. Addressing this challenge requires both a method of generating CG potentials as well as finding and rationalizing an appropriate reference state point to start out from. I will illustrate several of these aspects using examples from the biomolecular and (biomimetic-) materials world.

3:42PM D19.00003 Polymers at Surfaces and Interfaces1. MESFIN TSIGE, The University of Akron — Interfaces between solids, liquids, and gases play an important role in a wide range of practical applications and have been a subject of scientific interest since Poisson showed in 1831 that the order parameter of liquids near interfaces must deviate considerably from its bulk value. In particular, polymers at surfaces and interfaces have been the subject of extensive theoretical, experimental and computational studies for a long time due to their use in many diverse applications ranging from antifouling coatings to flexible electronic devices. Understanding the structure and thermodynamic properties of polymers at surfaces and interfaces is thus an area of fundamental and current technological interest. Although encouraging experimental progress has been made over the years in understanding the molecular structure of polymers in contact with various environments, selectively probing their structure and dynamics at surfaces and interfaces has been extremely difficult. Computer simulations, especially molecular dynamics (MD) simulations, have proven over the years to be an invaluable tool in providing molecular details at interfaces that are usually lacking in the experimental data. In this talk, I’ll give an overview of some previous simulation efforts to understand the structure and dynamics of polymers at surfaces and buried interfaces. I will conclude by presenting our current and ongoing work on combining ab initio calculations and MD simulations with Sum Frequency Generation (SFG) Spectroscopy to study polymer surfaces. This approach demonstrates the future role of MD in surface science.

1 Work supported by NSF (DMR0847580 and DMR1410290) and Petroleum Research Fund of the American Chemical Society.

4:18PM D19.00004 Systematic Coarse-graining of Molecular Dynamics Simulations, GREGORY VOTH, University of Chicago — Coarse-grained (CG) models can provide a computationally efficient means to study biomolecular and other soft matter processes involving large numbers of atoms that are correlated over distance scales of many covalent bond lengths and at long time scales. Systematic variational coarse-graining methods based on information from molecular dynamics simulations of finer-grained (e.g., all-atom) models provide attractive tools for the systematic development of CG models. Examples include the multiscale coarse-graining (MS-CG) and relative entropy minimization methods, and results from the former theory will be presented in this talk. In addition, a new approach will be presented that is appropriate for the “ultra coarse-grained” (UCG) regime, e.g., at a coarse-grained resolution that is much coarser than one amino acid residue per CG particle in a protein. At this level of coarse-graining, one is faced with the possible existence of multiple metastable states “within” the CG sites for a given UCG model configuration. I will therefore describe newer systematic variational UCG methods specifically designed to CG entire protein domains and subdomains into single effective CG particles. This is accomplished by augmenting existing effective particle CG schemes to allow for discrete state transitions and configuration-dependent resolution. Additionally, certain aspects of this work connect back to single-state force matching and open up new avenues for method development. This general body of theory and algorithm provides a formal statistical mechanical basis for the coarse-graining of fine-grained molecular dynamics simulation data at various levels of CG resolution. Representative applications will be described as time allows.

4:54PM D19.00005 Multiscale Simulations of Membranes, MICHAEL KLEIN, Temple University — No abstract available.

Monday, March 2, 2015 2:30PM - 5:30PM
Session D20 DPOLY: Invited Session: Physics of Glass-Forming Liquids: Challenges and Surprises II Ballroom B - Sindee Simon, Texas Tech University

2:30PM D20.00001 The structure of glass as revealed by dynamical large deviation methods, JUAN P. GARRAHAN, School of Physics & Astronomy, University of Nottingham — The dynamics of many-body systems is often richer than what one can directly infer from their static properties. This dynamical richness is revealed by considering strictly dynamical observables. The full statistical characteristics of such quantities encode the dynamical properties of the system at hand. By considering their large deviations it is possible to derive a statistical mechanics of trajectories, which is to trajectories of the dynamics what equilibrium statistical mechanics is to configurations of the statics. In this talk I will describe this approach and how it can be applied to the glass transition problem. I will show how the underlying kinetic phenomenon of glass formation is a novel class of order disorder transitions in trajectory, rather than configuration, space. I will consider the connection between the inactive dynamical phases this approach reveals and glasses prepared by more standard means. A significant prediction from this approach is the emergence of non-trivial correlations that distinguish glass from its reversible melt. Time permitting I will discuss how these ideas extend to the area of quantum glasses.

3:06PM D20.00002 Approaching the Glass Transition from Various Directions3, JANE LIPSON, Dartmouth College — In recent years a significant amount of experimental work has appeared on glassy systems, both polymeric and small molecule. However, this rich explosion in data has not been met with a concomitant leap in fundamental understanding. We have developed a number of approaches to elucidate some of the underlying mechanisms of behaviour in bulk and confined glassy systems. Using our Limited Mobility (LM) coarse-grained simulation model we have characterized the dynamic heterogeneity associated with approaching the glass transition, explored interfacial behaviour when layering materials of differing mobility, and analyzed the effect of a free surface on a supported thin film. Approaching related problems from a different direction we have modified a simulation technique designed primarily for bulk-bulk and for molecules deposited on a film surface, and substrate interactions in the case of supported films. Characterizing the systems via bulk data alone, we find our film-averaged predictions for the effects of confinement agree well with experimental data on several freestanding and supported polymer films. That work deals with confined systems; a fundamental understanding of bulk glass transitions also remains incomplete. Most recently we have been applying our Locally Correlated Lattice (LCL) equation of state model, which has met with success in modeling polymer melt and mixture behaviour, to reveal hints of the underlying glassy nature of a bulk polymer sample, even while above its transition temperature (Tg). Correlations between Tg and a variety of equilibrium bulk quantities have lead us to make connections not only with a substantive amount of experimental data on a wide range of polymers, but also with other models of glassy polymeric systems. This talk will comprise an efficient summary of past progress from these different directions, and will then focus on our most recent results and current understanding.

3 This work has been supported by NSF-DMR and GAANN.
the mechanisms leading to these striking observations in depth in this presentation. The band gap can be modulated by nearly 3 eV. We will consider distortions are understood in terms of a balance between the electrostatic and mechanical boundary conditions governing the two systems. Below 5 unit cells terminated with negatively charged NiO2-planes are insulating with strongly distorted Ni-O bonds. The differences in the observed structural found. We find that films terminated with positively charged LaO planes preserve bulk-like Ni-O bonding and are metallic. In contrast, films with thicknesses have arisen due to their inherently high carrier densities, as well as the strong coupling of their electronic and magnetic order parameters to structural degrees of freedom. Understanding the structural-property relations in these systems is crucial for designing heterostructure devices for a wide range of applications including KUMAH, ANDREI MALASHEVICH, ANKIT DISA, Yale University, DARIO ARENA, Brookhaven National Laboratory, FRED WALKER, SOHRAB ISMAIL-

1Partial support from The Welch Foundation and the Gulf of Mexico Research Initiative.

Monday, March 2, 2015 2:30PM - 5:30PM –
Session D21 DCMP: Nickelates and Other Transition Metal Oxides 201 - Jack Chakhalian, University of Arkansas

2:30PM D21.00001 Pseudo-gaps at the Mott quantum critical point in the perovskite rare earth nickelates1, S. JAMES ALLEN, Univ of California - Santa Barbara, ADAM HAUSER, EVGENY MIKHEEV, UC Santa Barbara, ANKIT DISA, FRED WALKER, Yale University, NELSON MORENO, UC Santa Barbara, CHARLES AHN, Yale University, LEON BALENTS, SUSANNE STEMMER, SUSANNE STEMMER, UC Santa Barbara — We explore the behavior of the pseudo-gap in the vicinity of the quantum critical point of charge transfer Mott insulators. We focus on NdNiO3 and LaNiO3, which as bulk material bracket the quantum critical point, but tune the nature of the transition in epitaxial ultra-thin films by substrate strain, film thickness and Nd/LaNiO3 composition. We expand our earlier work [1] that documented the energy gaps and pseudo gaps in thick films using tunneling spectroscopy between Al and nickelate films with 1nm Al2O3 barriers. We focus on the relative importance of disorder scattering and electron correlation in the pseudogaps.

1Supported by the MURI program of the ARO “Emergent Phenomena at Complex Oxide Interfaces” - Grant # W911-NF-09-1-0398.

2:42PM D21.00002 Carrier localization in correlated nickelates by electron doping1, YOU ZHOU, JIAN SHI2, SHRIRAM RAMANATHAN, Harvard University — The electronic properties of transition metal oxides are often sensitive to the orbital occupancy of the 3d electrons due to non-degenerate energy levels and strong electron correlations. A prototypical rare earth nickelate, SmNiO3 exhibits thermally driven insulator-metal transition at 400 K with one to two orders of magnitude change in its resistivity, characterized by charge ordering of the Ni sites. In this work, by modifying the φ0 orbital filling of Ni through electron doping with reversible hydrogenation and lithium/magnesium intercalation, we realize a deep insulating phase with greater than eight orders of magnitude change in resistivity at room temperature. The band gap can be modulated by nearly 3 eV. We will consider the mechanisms leading to these striking observations in depth in this presentation.

2We acknowledge National Science Foundation grants CCF- 0926148, National Academy of Sciences and NSF DMR-0952794 for financial support.

2:54PM D21.00005 Fluids with short-range attractions and longer-range repulsions1, THOMAS TRUSKETT, The University of Texas at Austin — Many complex fluids comprise particles with effective interactions that include short-range attractions and longer-range repulsions. In this talk, I explore—using a simple theoretical model—what behaviors one should expect to find in such systems, including the possibility of equilibrium “cluster” formation and its associated implications for dynamics near structural arrest. I also discuss how one might predict the onset of cluster formation from the static structure factor. Finally, some implications for concentrated liquid formulations of therapeutic proteins are addressed.

1Supported by the MURI program of the ARO “Emergent Phenomena at Complex Oxide Interfaces” - Grant # W911-NF-09-1-0398.

2:30PM D21.00002 Carrier localization in correlated nickelates by electron doping1, YOU ZHOU, JIAN SHI2, SHRIRAM RAMANATHAN, Harvard University — The electronic properties of transition metal oxides are often sensitive to the orbital occupancy of the 3d electrons due to non-degenerate energy levels and strong electron correlations. A prototypical rare earth nickelate, SmNiO3 exhibits thermally driven insulator-metal transition at 400 K with one to two orders of magnitude change in its resistivity, characterized by charge ordering of the Ni sites. In this work, by modifying the φ0 orbital filling of Ni through electron doping with reversible hydrogenation and lithium/magnesium intercalation, we realize a deep insulating phase with greater than eight orders of magnitude change in resistivity at room temperature. The band gap can be modulated by nearly 3 eV. We will consider the mechanisms leading to these striking observations in depth in this presentation.

2We acknowledge National Science Foundation grants CCF- 0926148, National Academy of Sciences and NSF DMR-0952794 for financial support.

2Now with Department of Materials Science and Engineering, Rensselaer Polytechnic Institute
3:06PM D21.00004 Electrically induced metal-insulator transition in epitaxial SmNiO$_3$ thin films$^1$, TOYANATH JOSHI, West Virginia University, NIKHIL SHUKLA, SANDEEPAH DASGUPTA, Pennsylvania State University, PAVEL BORISOV, West Virginia University, SUMAN DATTA, Pennsylvania State University, DAVID LEDERMAN, West Virginia University — Materials with metal-insulator transitions (MITs) above room temperature are potentially interesting for electronic applications, inter alia, to design a new class of the so-called Mott field transistors. We studied a member of the rare-earth nickelates family, SmNiO$_3$, with the bulk MIT transition temperature close to 400K. Thin films of SmNiO$_3$ were grown using pulsed laser deposition. Epitaxial structural quality was verified by reflection high-energy electron diffraction, x-ray diffraction, x-ray reflectometry, x-ray photoelectron spectroscopy and atomic force microscopy. Temperature-dependent resistivity measurements showed MIT temperatures close to the bulk values. Electrically driven MIT in two terminal SmNiO$_3$ thin film devices was demonstrated using DC and pulsed mode I-V measurements in the temperature range 273-348 K. The differential conductance $dI/dV$ peaked in the DC mode at switching field of 80 kV/cm at 273 K. The switching behavior became less pronounced with increasing measurement temperature and decreasing time period of the voltage pulses. By analysis of the experimental data we conclude the electrically-driven MIT in SmNiO$_3$ is due to the current-induced Joule self-heating. These findings should contribute to utilization of novel electronic applications.

\textsuperscript{1}This work was supported at WVU and PSU by STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA, Office of Naval Research through award.

3:18PM D21.00005 Anti-ferromagnetically driven Mott transition in ultrathin NdNiO$_3$ epitaxial films , MIKHAIL KAREEV, D. MEYERS, Univ of Arkansas-Fayetteville, JIAN LIU, University of California-Berkeley, S. MIDDEY, Univ of Arkansas-Fayetteville, J.W. FREELAND, P. RYAN, Advanced Photon Source, J. CHAKHALIAN, Univ of Arkansas-Fayetteville — The independent roles of anti-ferromagnetism and charge ordering in the realization of the temperature induced Mott metal-to-insulator transition within heteroepitaxial nickelate films remain to be disentangled hindering true understanding of the nature of the hotly debated ground state. To this end, we have investigated ultra thin, fully epitaxial films of the strongly correlated electron system NdNiO$_3$ with hard and soft resonant x-ray scattering. We find a robust E0-type antiferromagnetic transition, identical to the bulk ordering, occurs despite the ultra thin nature of the films. However, many discrepancies with the bulk like charge ordering are found.

3:30PM D21.00006 ABSTRACT WITHDRAWN —

3:42PM D21.00007 Evolution of antiferromagnetic order in rare-earth nickelates probed by muon spin relaxation , BENJAMIN FRANDESEN, LIAN LIU, SKY CHEUNG, YASUTOMO J. UEMURA, Columbia University, TIMOTHY MUNSIE, MURRAY WILSON, ALANNAH HALLAS, GREAME M. LUKE, McMaster University, BJULIAN CHEN, CHANGQING JIN, Institute of Physics, Beijing, CUI DING, FANLONG NING, Zhejiang University, JOSE ALONSO, Instituto de Ciencia de Materiales de Madrid (ICMM) — The rare-earth nickelates with structural formula RNiO$_3$ comprise a well-known family of Mott insulators that exhibits a gradual suppression of the metal-insulator transition and antiferromagnetic (AF) order with increasing rare-earth ionic size, resulting in a zero-temperature quantum phase transition at a rare-earth ionic radius of $\sim$1.17 Å. We present detailed muon spin relaxation ($\mu$SR) measurements of RNiO$_3$ ($R=$Sm,Nd,Pr,La) to investigate the evolution of the antiferromagnetic order across the phase diagram. In the compounds with lower ordering temperatures near the quantum phase transition, we observe a “stretched” Mott transition with phase separation between magnetic and paramagnetic regions over a wide temperature interval. We also find that the suppression of the magnetic order at the quantum phase transition occurs in a first-order manner, with the ordered volume fraction decreasing to zero while the moment size remains large and constant. We compare these observations to other Mott insulator systems and discuss generic behavior.

3:54PM D21.00008 Non-Gaussian resistance noise across the metal-insulator transition in epitaxial NdNiO$_3$ films , ALI ALSAQQA, SUJAY SINGH, State Univ of NY - Buffalo, SRIMANTA MIDDEY, MICHAEL KAREEV, JAN CHAKHALIAN, University of Arkansas - Fayetteville, G. SAMBANDAMURTHY, State Univ of NY - Buffalo — The rich phase diagrams exhibited by strongly correlated rare earth nickelates provide a great playground to investigate the electronic, magnetic and structural properties using a variety of experimental tools. NdNiO$_3$ thin films exhibit a temperature-driven metal-insulator transition (MIT) and the transition temperature is controlled by the interface strain. We present results from transport measurements and noise spectroscopy studies in strained, ultrathin (15 unit cells) NdNiO$_3$ across the MIT. Resistance noise spectroscopy (in the frequency range below 10 Hz) is a powerful tool to statistically investigate the fluctuations of the microscopic scatterers that can dramatically affect macroscopic properties. In our samples, we find that the noise spectrum follows a $1/f$ behavior, however the noise magnitude dramatically peaked in the DC mode at switching field of 80 kV/cm at 273 K. The switching behavior became less pronounced with increasing measurement temperature and decreasing time period of the voltage pulses. By analysis of the experimental data we conclude the electrically-induced MIT in SmNiO$_3$ is due to the current-induced Joule self-heating. These findings should contribute to utilization of novel electronic applications.

4:06PM D21.00009 Nanostructure Investigations of Nonlinear Differential Conductance in NdNiO$_3$ Thin Films , WILL HARDY, HENG JI, Department of Physics and Astronomy, Rice University, EVGENY MIKHEEV, SUSANNE STEMMER, Materials Department, University of California, Santa Barbara, DOUGLAS NATELSON, Department of Physics and Astronomy, Rice University — Transport measurements on thin films of NdNiO$_3$ reveal a crossover to a regime of pronounced nonlinear conduction below the well-known metal-insulator transition temperature. The evolution of the transport properties at temperatures well below this transition appears consistent with a gradual formation of a gap in the hole-like Fermi surface of this strongly correlated system. As $T$ is decreased below the nominal transition temperature, transport becomes increasingly non-Ohmic, with a model of Landau-Zener breakdown becoming most suited for describing $I(V)$ characteristics as the temperature approaches 2 K.

4:18PM D21.00010 ABSTRACT MOVED TO J15.00013 —

4:21PM D21.00011 ABSTRACT MOVED TO J15.00012 —

4:21PM D21.00012 Comparative study of Raman excitations in YVO$_3$ and HoVO$_3$, BENOIT ROBERGE, SERGE JANDL, Université de Sherbrooke, AGUSTINUS AGUNG NUGROHO, Institut Teknologi Bandung, THOMAS PALSTRA, University of Groningen — First-order Raman scattering and multiphonons are studied in RVO$_3$(R=Ho and Y) as a function of temperature in the orthorhombic and monoclinic phases. Below $T_{O-O} = 200$ K in YVO$_3$ and $T_{O-O} = 188$ K in HoVO$_3$, a G-type orbital ordering (G-OO) with a concomitant monoclinic transition occurs. The orbital ordering enhances the phonon polarizabilities, it also allows the resolution of room-temperature phonons, and activates new excitations around 700 cm$^{-1}$. Below $T_{N} = 114$ K (in both compounds), a C-type magnetic ordering (C-SO) occurs and some phonon frequency softening or frequency hardening are observed. Following the structural and magnetic transitions, below 40 K in YVO$_3$ and $T_{N}$ = 40 K in HoVO$_3$, important changes are observed in Raman excitations of both compounds. Even if R ionic radii of HoVO$_3$ and YVO$_3$ are nearly equal ($\bar{R}_{Ho} = 192$ pm and $\bar{R}_{V} = 190$ pm), we observe some differences that we report.
5:06PM D21.00014 Self-interaction corrected electronic structure of Ti4O7, TiO2 and Ti2O3
, XIAOLIANG ZHONG, Argonne National Laboratory, IVAN RUNGGER, Trinity College, PETER ZAPOL, OLLE HEINONEN, Argonne National Laboratory — Titanium oxides have a range of applications in, e.g., catalysis and resistive switching. There are many oxide structures with different ground states and electronic properties that have to be understood for potential applications to be possible. We have studied rutile TiO2, Ti2O3, and Magnéli phase Ti3O6 using density functional theory with self-interaction corrections to account for electronic correlations, which are important in these structures. The ground state of the low temperature (LT) phase of Ti3O6 is found to be a new semiconducting state with antiferromagnetic coupling between two sublattices. Depending on the charge screening strength, different Ti-O phases are best described by applying different values of an empirical parameter \( \alpha \), which represents the magnitude of the applied self-interaction correction. We will show that Pauli paramagnetism of the metallic high-temperature Ti3O6 phase is predicted using \( \alpha \approx 0 \), that the band gaps of small-gap LT-Ti3O6 and Ti2O3 are captured by \( \alpha \approx 0 \), while the large band gap of TiO2 is reproduced using \( \alpha \approx 0 \). Nevertheless, restricting \( \alpha \) to a standard value of 0.5 for transition metal oxides is found to be a good compromise describing reasonably well the electronic structures of all these oxides. We gratefully acknowledge the computing resources provided on Blues, a high-performance computing cluster operated by the Laboratory Computing Resource Center at Argonne National Laboratory. Argonne National Laboratory’s work was supported under U.S. Department of Energy contract DE-AC02-06CH11357.

5:18PM D21.00015 ABSTRACT WITHDRAWN —

Session D22 DCMP: Theory of Exotic States of Matter 202A - Eun-Ah Kim, Cornell University

Monday, March 2, 2015 2:30PM - 5:18PM —

2:30PM D22.00001 Algebraic spin liquids with emergent generalized gauge boson excitations, ALEX RASMUSSEN, CENKE XU, ZHEN BI, YI-ZHUANG YOU, Univ of California - Santa Barbara — According to an early proposal by Hermele, et.al., (cond-mat/0404751), an algebraic spin liquid state with gapless emergent photon excitations can exist in quantum spin ice systems. This algebraic spin liquid is stable against any weak perturbation. Further work by Xu and Ho?ava (arxiv:1003.0009) concluded that certain lattice models give rise to more exotic stable spin liquid states with graviton-like excitations. In this talk we will show how these algebraic spin liquid states can be generalized to even more exotic types of gapless excitations and then demonstrate that these new phases are stable against weak perturbations.

2:42PM D22.00002 (Almost) naked quantum criticality with non-Fermi liquid behavior at the onset of inhomogeneous Larkin-Ovchinikov superfluidity in two dimensions, PHILIPP STRACK, Harvard University, FRANCESCO PIÀZZA, TU Muenchen — We present a renormalization group analysis for the non-Fermi liquid behavior and quantum criticality arising in coupled quantum wires of attractively interacting fermions with spin imbalance in two spatial dimensions.

2:54PM D22.00003 Topological Phases of Interacting Bosons on the Kagome Lattice, KRISHANU ROYCHOWDHURY, SUBHRO BHATTACHARJEE, FRANK POLLMANN, MPIPKS, Dresden — We consider an extended Hubbard model of hard core bosons including nearest-neighbour hopping and long range repulsive interactions on a kagome lattice. The system is an insulator at commensurate fillings of 1/6, 1/3 and 1/2 and can be mapped to different dimer triangular lattice (depending on the filling). We focus on the filling of 1/3, which transforms to a fully packed loop (FPL) model, and derive the full phase diagram in the low-energy subspace. Similar to the quantum dimer model and easy-axis kagome antiferromagnetic model studied before, we find an extended region of a gapped \( Z_3 \) liquid with vison excitations. The gauge fluctuations, responsible for the vison modes, are dictated by the action of an even Ising gauge theory. In the ordered phase, where the vison gap closes, we observe a 3-fold rotationally symmetric loop order and present the critical theory for the amplitude fluctuations of the condensed modes. We also speculate the phase diagram for the fermionic counterpart of the model at all the above mentioned fractional fillings.

3:06PM D22.00004 Spontaneous Anomalous Hall states in metals, WATHID ASSAWASUNTHONNET, VICTOR CHUA, EDUARDO FRADKIN, Univ of Illinois - Urbana — We explore two phases in 2-D electron fluids with two Fermi surfaces in which the time-reversal symmetry is broken spontaneously by using the method of higher dimensional bosonization. Earlier mean-field calculations [1] showed that the order parameter for both phases can be expressed as two two-component real vectors. There are two phases: the beta phase in which the two order parameters are perpendicular to each other and the alpha phase in which they are parallel. The beta phase exhibits nonvanishing un-quantized spontaneous anomalous Hall effect at zero external magnetic fields, which is determined by a Berry curvature associated with Fermi surfaces. The alpha phase does not have that property. To go beyond mean-field, we use higher-dimensional bosonization. We have identified the two phases as topological phases. In the ordered phase, where the vison gap closes, we observe a 3-fold rotationally symmetric loop order and then present the critical theory for the amplitude fluctuations of the condensed modes. We also speculate the phase diagram for the fermionic counterpart of the model at all the above mentioned fractional fillings.

3:18PM D22.00005 Transition of a \( Z_3 \) topologically ordered phase to a trivial phase\(^1\), CHING-YU HUANG, Tzu-Chieh Wei, C. N. Yang Institute for Theoretical Physics and Department of Physics and Astronomy, State University of New York at Stony Brook — Topologically ordered quantum systems have robust physical properties, such as quasiparticle statistics and ground-state degeneracy, which do not depend on the microscopic details of the Hamiltonian. We consider a topological phase transition under a string tension \( g \) on a \( Z_3 \) topological state. This is first studied numerically in terms of the gauge-symmetry preserved quantum state renormalization group proposed by He, Moradi and Wen (arXiv:1401.5557). Modular matrices \( S \) and \( T \) can be obtained and used as parameters to determine the critical string tension \( g_c \). Then from a mapping to a classical 2D three-state Potts model on square lattice we obtain analytically the transition \( g_c \) via the transition temperature of the three-state Potts model. We find the numerically determined \( g_c \) agrees well with the analytic result via the mapping.

\(^1\)This work was supported in part by the National Science Foundation.

3:30PM D22.00006 Pairing instabilities of a Non-Fermi liquid in the presence of nematic and gauge fluctuations\(^2\), ANDREJ MESAROS, MICHAEL J. LAWLER, EUN-AH KIM, Cornell University — In the absence of Fermi-liquid starting point, instabilities of non-Fermi liquids are theoretically challenging problems. Here we note that a non-Fermi liquid state occurring at \( v = 1/2 \) may be a promising concrete case for theoretical investigation of the issue for two reasons. Firstly, exotic ordered states observed in half-filled Landau levels, namely the FQH state at \( v = 5/2 \) which is most likely best described as a paired state, and the quantum Hall nematic state at \( v = 9/2 \), present a compelling possibility that the non-Fermi liquid state with gauge fluctuations at \( v = 1/2 \) is close to instabilities towards these ordered states. Secondly, a recent theoretical progress [Metlitski et al., arXiv:1403.3694] offers a scheme for a controlled renormalization group study of the problem. We will discuss competition between the two fluctuations in promoting or suppressing a superconducting instability, based on the phase diagram we obtain from a renormalization group calculation.

\(^2\)This research was supported by NSF through CAREER grant DMR-0955822.
The dimerized spin-1/2 Heisenberg ladder is topologically characterized from the viewpoints of symmetry protection and bulk-edge correspondence. Our focus is on the plateau phase at the half of the saturation induced by dimerization and magnetic field. The Berry phase associated with the twisted boundary condition is employed as a topological order parameter. The magnetic field reduces the symmetry of the system, but there is a topological phase protected by a spatial inversion symmetry that is characterized by a Berry phase quantized to $0/\pi$. For a Berry phase quantization, usage of a symmetry-preserving boundary, which leaves at least one inversion center after the system is cut at the boundary, is essential. As a comparison, a symmetry-breaking boundary is also analyzed. Naively, such a boundary is inadequate to make the Berry phase quantized and topological. However, for a specific type of boundary, we found a unique quantization of the Berry phase into $\pm \pi/2$, instead of $0/\pi$ [T. Kariyado and Y. Hatsugai, Phys. Rev. B 90, 085132 (2014)]. Further, for the case of $\pm \pi/2$-quantization, there appears an edge state distinct from the one for the $0/\pi$-quantization, which reveals new aspects of the bulk-edge correspondence for symmetry-breaking boundary.

3:54PM D22.00008 Josephson-coupled Moore-Read states , LAYLA HORMOZI, Massachusetts Institute of Technology, GUNNAR MOLLER, University of Cambridge, JOOST SLINGERLAND, National University of Ireland, STEVEN SIMON, University of Oxford — We study a quantum Hall bilayer system of bosons at total filling fraction $\nu = 1$, and analyze the the coupled Moore-Read state [PRL 108, 256809 (2012)] that results from the interplay between short-ranged interactions and interlayer pair-tunneling terms. Supported by the exact solution of the full zero-energy quasihole spectrum and a conformal field theory analysis, we develop an intuitive picture of this system as two coupled composite fermion superconductors. In this language, pair tunneling plays the role of Josephson coupling between the superconducting phases of the two layers, which gaps out the Goldstone mode associated with interlayer particle distribution. This coupling further implies that non-Abelian quasiparticles are confined between the layers. In the bulk, the resulting phase has the topological order of the Halperin 220 state i.e. $U(1)_2 \times U(1)_2$, but the edge spectrum at a fixed particle number reveals an unexpected $U(1)_3 \times U(1)$ structure. We attribute this behavior to the fact that this state is realized in a rotated basis of layer index, where the charged and neutral sectors are separated. With the charge quantum number being conserved but without any such restriction on the neutral sector we show that the edge spectrum must take the observed form.

4:06PM D22.00009 ABSTRACT WITHDRAWN —

4:18PM D22.00010 Ground State Degeneracy of Topological Phases on Open Surfaces , YIDUN WAN, Perimeter Institute for Theoretical Physics, JANET HUNG, Department of Physics and Center for Field Theory and Particle Physics, Fudan University — we relate the ground state degeneracy (GSD) of a non-Abelian topological phase on a surface with boundaries to the anyon condensates that break the topological phase to a trivial phase. Specifically, we propose that gapped boundary conditions of the surface are in one-to-one correspondence to the sets of condensates, each being able to completely break the phase, and we substantiate this by examples. The GSD resulting from a particular boundary condition coincides with the number of confined topological sectors due to the corresponding condensation. These lead to a generalization of the Laughlin-Wu-Tao charge-pumping argument for Abelian fractional quantum Hall states to encompass non-Abelian topological phases, in the sense that an anyon loop of a confined anyon winding a non-trivial cycle can pump a condensate from one boundary to another. Such generalized pumping may find applications in quantum control of anyons, eventually realizing topological quantum computation.

4:30PM D22.00011 Parent Hamiltonians for Bosonic Symmetry-Protected States , LUZ SANTOS, Perimeter Institute — A platform for constructing parent Hamiltonians describing bosonic symmetry-protected (SPT) states will be presented. The Hamiltonians we consider are examples of frustration-free Kitaev-Kivelson models, which are known to be in one-to-one correspondence with classical stochastic systems in the same spatial dimensionality. By exploring this classical-quantum mapping we are able to propose Hamiltonians which, in a closed manifold, yield a unique gapped symmetric ground state describing the universal properties of SPT states. Specific examples which illustrate our approach shall be discussed.

4:42PM D22.00012 Quasi-one-dimensional superfluid criticality , PIERRE-FRANCOIS DUC, MICHEL SAVARD, MATEI PETRESCU, McGill University, ADRIAN DEL MAESTRO, University of Vermont, GUILLAUME GERVAIS, McGill University — In one of the most celebrated examples of the theory of universal critical phenomena, superfluid $^4$He state belongs to the same three dimensional O(2) universality class as the onset of ferromagnetism in a lattice of XY spins. Its ability to flow without viscosity below the $\lambda$-transition temperature is a paradigmatic manifestation of emergent phenomena and macroscopic quantum coherence, driven by both strong interactions and bosonic quantum statistics. As the number of spatial dimensions decreases, it is expected that enhanced thermal and quantum fluctuations should push $T_{\lambda} \rightarrow 0$. However, in the one dimensional limit, the universal quantum hydrodynamics of Luttinger liquid theory should apply, providing a host of theoretical predictions including the simultaneous algebraic spatial decay of both density-density and superfluid correlation functions. At McGill University, we have designed an experiment and measured the DC mass flow of superfluid helium in single nanopores with radii down to 3 nm. For the smaller aperture, in which helium is expected to be in a ‘quasi-one-dimensional’ regime, the universal critical exponent for the superfluid velocity is found to deviate significantly from its bulk value, $\nu = \frac{3}{2}$.

1NSERC(Canada), FQRNT(Quebec),CIFAR

4:54PM D22.00013 Electronic properties in a superlattice of strongly correlated electron systems , SUGURU UEDA, NORIO KAWAKAMI, Department of Physics, Kyoto University, Kyoto 606-8502, Japan — We theoretically investigate the superlattice consisting of a Mott insulator and a metal by using the dynamical mean-field theory. At low temperature, the quasi-particle state appears in the density of states of the Mott insulator layers. We address how the structure of the superlattice affects the stability of this Fermi liquid state. It is elucidated that the quasi-particle weight shows the characteristic even-odd oscillation depending on the thickness of the metal domain. We confirm this even-odd dependence in the electrical resistivity, and find that the Fermi liquid state is further stabilized by the superlattice with a certain periodicity. We also discuss the importance of our findings comparing with the recent experiments.

5:06PM D22.00014 The theory of cluster Mott insulator: charge fluctuation and spin liquids , GANG CHEN, HAE-YOUNG KEE, YONG BAEK KIM, University of Toronto — I will present recent theoretical work on cluster Mott insulators (CMI) in which interesting physics such as emergent charge lattices, charge fractionalization and quantum spin liquids are proposed. For the anisotropic Kagome system like LiZn2Mo3O8, we find two distinct CMIs, type-I and type-II, can arise from the repulsive interactions. In type-I CMI, the electrons are localized in one half of the triangle clusters of the Kagome system while the electrons in the type-II CMI are localized in every triangle cluster. Both CMIs are $U(1)$ quantum spin liquids (QSL) with a unique $\pi$-band regime with a spin Fermi surface and gapped charge excitations. In type-II CMI, however, the charge fluctuations lead to a long-range plaquette charge order that breaks the lattice symmetry, gives rise to an emergent charge lattice and reconstructs the mean-field spinon band structure of the underlying $U(1)$ QSL. Such a reconstruction gives a consistent prediction of the “fractional spin susceptibility” that is observed in LiZn2Mo3O8. For the pyrochlore system, the CMI can further support a charge fractionalization with an emergent gauge photon in the charge sector in addition to the spin fractionalization in the spin sector. Experimental connection with the several cluster magnets such as LiZn2Mo3O8.
2:30PM D23.00001 Modeling of Singlet Fission Kinetics for a Wide Range of Molecules. SHANE YOST, Lawrence Berkeley National Laboratory — Singlet exciton fission is a process that occurs in organic molecules where one high energy singlet exciton decays into two low energy triplet excitons. Over the years since its first discovery in the 1960s a number of different singlet fission materials have been discovered with a wide range of rates and yields. The mechanism for singlet fission in these materials is still not fully understood, and no method is able to accurately reproduce fission rates over a wide range of timescales. In order to gain a better understanding of the singlet fission mechanism a group of fission materials with vastly different crystal structures and fission rates were modeled. Using a first principles expression the rates were computed with constrained density functional theory with configuration interactions. The computed rates successfully predict the fission rates in the different materials studied. For the slow, weak intermolecular coupling materials singlet fission obeys Marcus theory, but for faster, larger intermolecular coupling materials the rate becomes diabatic in nature. This work alters the guidelines for tailoring molecular properties from a focus on crystal packing and intermolecular coupling to properties like solubility and energy level alignment while maintaining the high fission yield required for photovoltaic applications.

3:06PM D23.00002 GW-BSE, self-consistency, and vertex corrections applied to group IB/IIB atoms and oxide molecules1. LINDA HUNG, SERDAR OGUT, University of Illinois at Chicago — Time-dependent density functional theory (TDDFT), the GW approximation, and the Bethe-Salpeter equation (BSE) are often used for the first-principles calculation of excited-state properties of materials that contain transition metals. Accuracy is improved compared to mean-field theories such as Kohn-Sham DFT or Hartree-Fock; however, predicted quasiparticle levels and optical spectra can still differ from experiment. We model Cu, Zn, Ag, and Cd atoms and their oxide molecules to assess various approximations in many-body perturbation theory methods that contribute to these differences. In particular, we examine how self-consistent iterations and/or a two-point vertex function affect the predicted excitation energies, compared to “one-shot” GCW0 calculations. Experimental measurements of optical spectra and ionization energies for charged and neutral atoms are widely available, and allow us to evaluate excitations from both s and d states. Differences between TDDFT and BSE spectra are also discussed. Calculations are performed with RGWBS, a software suite which uses a basis of transition space and quasiparticle wavefunctions.

3:18PM D23.00003 Quasiparticle Band Gap Renormalization in Doped Two-Dimensional Materials1. YUFENG LIANG, Lawrence Berkeley National Lab, LI YANG, Department of Physics, Washington University in St. Louis — Recently, atomically thin two-dimensional (2D) materials have emerged as new prototypes for a variety of electronic and optoelectronic devices, for which charge carrier doping is an effective approach for modifying their intrinsic properties. In the process of producing monolayer metal dichalcogenides, doping can occur naturally and may lead to exotic many-body phenomena as evidenced in recent optical experiments. Despite the common occurrence of doping in 2D structures, little knowledge has been obtained for the evolution of the band gap with the carrier concentration, which is key to harnessing the electronic properties and understanding more complicated many-body effects. Here, we investigate how the band gap changes with doping density in various 2D structures. Based on the conventional GW method for semiconductors, we devised and implemented an efficient calculation scheme to capture the unique dielectric screening arising from intraband transitions in low-dimensional structures, specifically MoS2 and MoSe2. We reveal that an enhanced band gap renormalization of a few hundred meV can be achieved and the band gap evolution displays an unusual nonlinear behavior with doping density. Our calculated band gap is in excellent agreement with the recent ARPES experiments on MoSe2.

3:30PM D23.00004 Band Structures of Plasmonic Polarons. FABIO CARUSO, HENRY LAMBERT, FELICIANO GIUSTINO, University of Oxford — In angle-resolved photoemission spectroscopy (ARPES), the acceleration of a photo-electron upon photon absorption may trigger shake-up excitations in the sample, leading to the emission of phonons, electron-hole pairs, and plasmons, the latter being collective charge-density fluctuations. Using state-of-the-art many-body calculations based on the ‘GW plus cumulant’ approach, we show that electron-plasmon interactions induce plasmonic polaron bands in group IV transition metal dichalcogenide monolayers (MoS2, MoSe2, WS2, WSe2). We find that the energy vs. momentum dispersion relations of these plasmonic structures closely follow the standard valence bands, although they appear broadened and blueshifted by the plasmon energy. Based on our results we identify general criteria for observing plasmonic polaron bands in the angle-resolved photoelectron spectra of solids.

3:42PM D23.00005 Recent Progress in GW-based Methods for Excited-State Calculations of Reduced Dimensional Systems. FELIPE H. DA JORNADA, University of California at Berkeley and Lawrence Berkeley National Laboratory — Ab initio calculations of excited-state phenomena within the GW and GW-Bethe-Salpeter equation (GW-BSE) approaches allow one to accurately study the electronic and optical properties of various materials, including systems with reduced dimensionality. However, several challenges arise when dealing with complicated nanostructures where the electronic screening is strongly spatially and directionally dependent. In this talk, we discuss some recent developments to address these issues. First, we turn to the slow convergence of quasiparticle energies and exciton binding energies with respect to k-point sampling. This is very effectively dealt with using a new hybrid sampling scheme, which results in savings of several orders of magnitude in computation time. A new ab initio method is also developed to incorporate substrate screening into GW and GW-BSE calculations. These two methods have been applied to mono- and few-layer MoS2, and yielded strong environmental dependent behaviors in good agreement with experiment. Other issues that arise in confined systems and materials with reduced dimensionality, such as the effect of the Tamm-Dancoff approximation to GW-BSE, and the calculation of non-radiative exciton lifetime, are also addressed. These developments have been efficiently implemented and successfully applied to real systems in an ab initio framework using the BerkeleyGW package. I would like to acknowledge collaborations with Diana Y. Qiu, Steven G. Louie, Meiyue Shao, Chao Yang, and the experimental groups of M. Crommie and F. Wang.

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2 This work is supported by NSF DMR-1207141 and was done at Washington University.

3 This work was supported by Department of Energy under Contract No. DE-AC02-05CH11231 and by National Science Foundation under Grant No. DMR10-1006184.
4:18PM D23.00006 Ultrafast Hot Carrier Scattering and Generation from Surface Plasmons in Noble Metals, MARCO BERNARDI, JAMAL MUSTAFA, Department of Physics, University of California, Berkeley, and Materials Science Division, Lawrence Berkeley National Lab, Berkeley, CA 94720, USA, JEFFREY B. NEATON, Molecular Foundry, Lawrence Berkeley National Lab, Berkeley, CA 94720, USA, STEVEN G. LOUIE, Department of Physics, University of California, Berkeley, and Materials Science Division, Lawrence Berkeley National Lab, Berkeley, CA 94720, USA — Non-equilibrium “hot” carriers in materials are challenging to study experimentally as they thermalize at subpicosecond time and nanometer length scale. Recent experiments employed hot carriers generated by light absorption or surface plasmon annihilation in noble metals (e.g., Au and Ag) for catalysis and solar cells. The energy distribution and transport of the generated hot carriers play a key role in these experiments. We present ab initio calculations of the energy distribution of hot carriers generated by surface plasmons in noble metals, and the relaxation time and mean free path of the hot carriers along different crystal directions within 5 eV of the Fermi energy. Our calculations show the interplay of the noble metal s and d bands in determining the damping rate of the plasmon and the mean free path of the hot carriers. The trends we find as a function of surface plasmon momentum and frequency allow us to define optimal experimental conditions for hot carrier generation and extraction. Our approach combines density functional theory, GW, and electron-phonon calculations. Our work provides microscopic insight into hot carriers in noble metals, and their ultrafast dynamics in the presence of surface plasmons.

4:30PM D23.00007 First-Principles Simulation of Hot Electron Dynamics at Silicon-Molecule Interfaces, LESHENG LI, YOSUKE KANAI, Univ of NC - Chapel Hill, KANAI GROUP TEAM — Hot carrier relaxation process at an interface between semiconductor and molecular ligands is of great importance for a number of technological applications ranging from photo-electrochemical cells to quantum-dot light emitting diodes. Although a number of spectroscopic experiments suggest important role of molecular ligands at surface in the hot carrier relaxation, a quantitative understanding has not been developed. We investigate the hot electron relaxation process through synergistic use of first-principles molecular dynamics (FPMD), fastest switch surface hopping (FSSH) algorithm, and GW calculations. Using FSSH stochastic dynamics simulation based on non-adiabatic couplings from FPMD and quasi-particle energy level alignment at the interface, we investigate the role of molecular passivation at silicon (111) surface as a representative example. We will discuss how different types of molecules influence the relaxation process and elucidate important factors controlling the relaxation time scale.

4:42PM D23.00008 Improved Description of Electron-Plasmon Coupling In Green’s Function Calculations, JIANQIANG ZHOU, LUCIA REINING, Laboratoire des Solides Irradies, Ecole Polytechnique, CNRS-CEA/DSM, F-91128 Palaiseau, France. European Theoretical Spectroscopy Facility (ETSF) — Green’s function (GF) methods have been very successful for describing one- or two-particle excitations in solids. The GW approximation [1] is a well established approach for describing quasi-particle peaks in the spectral function. Beyond GW, the cumulant expansion, which is based on a hole-boson coupling model, gives a better description of plasmon satellites [2,3]. However, this traditional time-ordered cumulant (TOC) is only valid far from the Fermi level. Recent development [4] of a generalized cumulant (GC) improves the spectral function close to the Fermi level, but a framework for systematically improving is still missing. Here we show how GW, TOC and GC can be derived as a successive series of approximations in a unified way, and how one can go beyond today’s state-of-the-art methods. Results for spectral functions and total energies of an exactly solvable model show that systematic improvement is obtained.

1Work supported by FP7/ERC Grant Agreement n. 320971

4:54PM D23.00009 Plasmon Pole Approximation within the GW Lanczos approach, VINCENT GOSSELIN, BRUNO ROUSSEAU, MICHEL COTE, Univ of Montreal — The well-known DFT gap problem is adressed by computational methods that are more resource intensive both in terms of memory and time requirements. Amongst other methods, the GW approach has known great success in the field of electronic structure calculations. Addressing the main bottlenecks impeding one shot GW calculations, a sum over all conduction states and an integral over all frequencies must be carried. Within an implementation of the GW method based on the Lanczos algorithm, the sum over conduction states is treated with a Sternheimer method whereas the frequency integral is carried out numerically. In this talk, I will present an implementation of a plasmon-pole model combined with the Lanczos method that allows a treatment of this integral that is computationally favorable.

5:06PM D23.00010 Applications of the Retarded Cumulant Expansion to Realistic Systems, J.J. KAS, J.J. REHR, U. Washington — The cumulant expansion of the one-electron Green’s function has proved extremely useful in describing electron correlation in materials beyond the one-electron approximation. For example, the approach improves on the GW approximation, accounting for multiple satellites in the spectral function and x-ray photoemission spectra. Previous implementations based on the time ordered representation ignore diagrams which lead to partial occupations and satellite features in the spectral function above and below the Fermi surface. Recently we have shown that these difficulties can be overcome with a cumulant expansion of the retarded Green’s function. This model was tested on the homogeneous electron gas, giving good results for the spectral function, correlation energies, and occupation numbers. In this follow-up, we discuss the extension of the approach to realistic condensed matter systems, using GW calculations of the self-energy to approximate the cumulant. Results are presented for the spectral function and occupation numbers, and compared to experimental XPS data.

5:18PM D23.00011 Photoelectron spectra of copper oxide (Cu_{x}O_{y} , x = 1 – 2 , y = 1 – 4) clusters from first principles, BIN SHI, University of Illinois at Chicago, SHIRA WEISSMAN, Weizmann Institute of Science, LINDA HUNG, University of Illinois at Chicago, LEEÖR KRONIK, Weizmann Institute of Science, SERDAR OGUT, University of Illinois at Chicago — Copper oxide clusters are systems of current technological and fundamental interest. They have unique electronic and optical properties due to the exchange and correlation effects of their f electrons, which also make their modeling from first principles computationally demanding. We optimize the ground-state structures of copper oxide Cu_{x}O_{y} (x = 1 – 2 and y = 1 – 4) cluster anions using density functional theory (DFT). We compare photoelectron spectra determined at two levels of theory: DFT and the GW approximation. DFT calculations use Perdew-Burke-Ernzerhof (PBE), hybrid, and range-separated exchange-correlation functionals. The calculated photoelectron spectra are compared with available experimental measurements to identify the nature of the observed electronic excitations.

1Supported by DOE DE-FG02-97ER45623
4Supported by DOE Grant No. DE-SC0001853 and the European Research Council.
2:30PM D24.00001 Quantum-classical Adaptive Coupling in Grand-Canonical like Adaptive Resolution Simulations, ANIMESH AGARWAL, LUIGI DELLE SITE, Institute for Mathematics, Warmlmalle 6, D-14195, Freie Universität, Berlin, Germany — We have extended the recently developed Grand Canonical AdResS (GC-AdResS) [1,2] to quantum-classical adaptive coupling where the quantum delocalisation of an atom is described by the path integral formalism. Compared to standard adaptive coupling approaches [3], the advantage of GC-AdResS is that there is no need to obtain a coarse-grained model that correctly reproduces the structural and thermodynamic properties of a full PI (path integral) system, thereby eliminating the need to run a full PI simulation before starting the adaptive simulation. In this context, we have shown that spherical molecules described by a simple generic WCA potential in the coarse-grained region, act as a particle reservoir for the PI region. The resulting Grand Canonical set up is such that the structural and dynamical properties of quantum flexible water models in the PI subregion in AdResS are consistent with the properties obtained in the same subregion in full PI simulations.


1This work was supported by the Deutsche Forschungsgemeinschaft (DFG)

2:42PM D24.00002 Efficient cluster Monte Carlo algorithm for Ising spin glasses in more than two space dimensions, ANDREW J. OCHOA, ZHENG ZHU, HELMUT G. KATZGRABER, Texas A&M University — A cluster algorithm that speeds up slow dynamics in simulations of nonplanar Ising spin glasses away from criticality is urgently needed. In theory, the cluster algorithm proposed by Houdayer poses no advantage over local moves in systems with a percolation threshold below 50%, such as cubic lattices. However, we show that the frustration present in Ising spin glasses prevents the growth of system-spanning clusters at temperatures roughly below the characteristic energy scale $J$ of the problem. Adding Houdayer cluster moves to simulations of Ising spin glasses for $T \sim J$ produces a speedup that grows with the system size over conventional local moves. We show results for the nonplanar quasi-two-dimensional Chimera graph of the D-Wave Two quantum annealer, as well as conventional three-dimensional Ising spin glasses, where in both cases the addition of cluster moves speeds up thermalization visibly in the physically-interesting low temperature regime.

2:54PM D24.00003 A new class of scalable parallel pseudorandom number generators based on Pohlig-Hellman exponentiation ciphers, PAUL BEALE, University of Colorado Boulder — We propose a new class of pseudorandom number generators based on Pohlig-Hellman exponentiation ciphers. The method generates uniform pseudorandom streams by encrypting simple sequences of short integer messages into ciphertexts by exponentiation modulo prime numbers. The advantages of the method are: the method is trivially parallelizable by parameterization with each pseudorandom number generator derived from an independent prime modulus, the method is fully scalable on massively parallel computing clusters due to the large number of primes available for each implementation, the seeding and initialization of the independent streams is simple, the method requires only a few integer multiplications per pseudorandom number drawn. The state of each instance is defined by only a few integer values, the period of each instance is different, and the method passes a battery of intrastream and interstream correlation tests using up to $10^{15}$ pseudorandom numbers per test. We propose an implementation using 32-bit prime moduli with small exponents that require only a few 64-bit multiply-mod operations that can be executed directly in hardware. The 32-bit implementation we propose has millions of possible instances, all with periods greater than $10^{18}$.

3:06PM D24.00004 Crossover behavior of the thermal conductance and Kramers’ transition rate theory, SUBIN SAHU, Department of Physics, Oregon State University, Corvallis OR, KIRILL VELIZHANIN, Theoretical Division, Las Alamos National Lab, Los Alamos NM, CHIH-CHUN CHIEN, School of Natural sciences, University of California, Merced CA, YONATAN DUBI, Department of Chemistry, Ben-Gurion University of Negev, Israel, MICHAEL ZWOLAK, National Institute of Standards and Technology, Gaithersburg MD — Heat transport plays opposing roles in nanotechnology, hindering the miniaturization of electronics on one hand and forming the core of novel heattronics devices on the other. Moreover, heat transport in one-dimensional nanostructures has become a central tool in studying the onset of Fourier’s law of heat conduction, a yet unresolved puzzle in theoretical physics. We study the paradigmatic setting of heat transport in one-dimensional systems, a lattice coupled to two heat baths held at different temperatures. Using both numerical and analytical tools, we demonstrate that the heat conductance displays a crossover behavior as the coupling to the thermal reservoirs is tuned. We provide evidence that this behavior is universal by examining harmonic, anharmonic, and disordered systems, and discuss the origin of this effect using an analogy with Kramers’ transition state theory for chemical reaction rates. This crossover behavior has important implications in the analysis of numerical results, and suggests a novel way to tune the conductance in nanoscale devices.

3:18PM D24.00005 Accelerated rare event sampling, DAVID YEVICK, University of Waterloo — We suggest a strategy for biased transition matrix Monte-Carlo calculations that both ensures the most rapid coverage of the entire computational window in the macroscopic variables of interest $E$ and yields estimates of transition probabilities between states that are equally accurate in low and high probability regions. Further, paths between different low probability regions are sampled at regular intervals. For the case of a single $E$ variable, a random system realization for which the value of $E$ falls in e.g. the $i$th histogram bin is generated. This state is perturbed and the resulting realization is rejected until a transition is observed to a neighboring bin, taken here as $i + 1$. All accepted and rejected transitions are simultaneously employed to generate the elements of a transition matrix. Subsequently, only a transition to bin $i + 2$ is accepted and this procedure is continued until the last of the $N$ bins comprising the computational window is sampled. The procedure is then repeated but in the direction of decreasing bin number. The probability distribution of $E$ can then be obtained by e.g. repeatedly multiplying a random vector by the transition matrix.

3:30PM D24.00006 The Transition Matrix in Flat-histogram Sampling, GREGORY BROWN, Florida State University, M. EISENBACh, Y. W. LI, G. M. STOCKS, Oak Ridge National Laboratory, D. M. NICHOLSON, University of North Carolina Asheville, KH. ODBADRRAK, University of Tennessee, P. A. RIKVOLD, Florida State University — Calculating the thermodynamic density of states (DOS) via flat-histogram sampling is a powerful numerical method for characterizing the temperature-dependent properties of materials. Since the calculated DOS is refined directly from the statistics of the sampling, methods of accelerating the sampling, e.g. through windowing and slow forcing, skew the resulting DOS. Calculating the infinite-temperature transition matrix during the flat-histogram sampling decouples the sampling from estimating the DOS, and allows the techniques of Transition Matrix Monte Carlo to be applied. This enables the calculation of the properties for very large system sizes and thus finite-size scaling analysis of the specific heat, magnetic susceptibility, and cumulant crossings at critical points. We discuss these benefits in the context of models for magnetocaloric and spin-crossover materials. This work was performed at the Oak Ridge National Laboratory, which is managed by UT-Battelle for the U.S. Department of Energy. It was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Office of Advanced Scientific Computing Research, and the Oak Ridge Leadership Computing Facility. PAR is supported by the National Science Foundation.

3:42PM D24.00007 ABSTRACT WITHDRAWN —
A More Direct Approach to Finding Phase Transitions in Realistic Alloy Models

1 DWO acknowledges support by NSF (DMR-0908753). GLWH and CWR was supported by ONR (MURI N00014-13-1-0635).

Nonstandard Finite-Size Scaling at First-Order Phase Transitions

Nontrivial nonequilibrium critical relaxation in cluster algorithms and universal nonequilibrium-to-equilibrium scaling procedure

A method for efficient structural simulation of carbon nanostructures and its application to irradiated graphene nanoribbons

ABSTRACT WITHDRAWN
5:18PM D24.00015 Molecular dynamics simulations of nanoscale Al structures for energetic formulations, N. SCOTT WEINGARTEN, U. S. Army Research Laboratory, MICHAEL ZACHARIAH, University of Maryland — The addition of metal microparticles, such as aluminum, to molecular explosives results in an increase in the heat of explosion, as well as higher temperatures. It is expected that the use of Al nanoparticles would further enhance these effects, but this has never been realized due to sintering of the nano-Al just prior to the energy release step. Recently, a capability emerged to produce macroscopic quantities of aluminum-based nanoclusters comprising near metallic state Al cores, passivated with an energetic gas generator. We are pursuing the possibility that these nanoclusters can be embedded in a mesoscopic spherical architecture which, upon heating, will lead to the decomposition of the gas generator. This would drive a volumetric expansion that liberates the aluminum nanoclusters which can subsequently undergo exothermic reaction. Atomistic simulations are used to explore the feasibility of this process, and determine the dynamics driving the ejection of the nano-Al particles.

Monday, March 2, 2015 2:30PM - 5:18PM –
Session D26 DCP: Focus Session: Water and Liquid Dynamics 204A - David Chandler, Sandia National Laboratories

2:30PM D26.00001 ABSTRACT WITHDRAWN

2:42PM D26.00002 New insights into the femtosecond-to-picosecond dynamics of liquid water from temperature dependence using terahertz spectroscopy studies and molecular dynamics simulations, CHOLA REGMI, DEEPU GEORGE, SHENGFENG CHENG, NGUYEN VINH, Virginia Polytechnic Institute and State University — Water plays an active and complex role in sustaining life. The hydrogen bonds between the water molecules exhibit the unique physical properties that distinguish water from other molecular liquids. Nevertheless, there is little agreement regarding the femtosecond to picosecond relaxation dynamics of water. In response, we have used the state-of-the-art terahertz spectroscopy (frequency-domain and time-domain) and molecular dynamics simulation techniques to study the molecular relaxation of water at different temperatures in the femtosecond to picosecond time scale. We show that the two-Debye model is insufficient to explain the observed relaxation dynamics of water and our results on the terahertz dielectric relaxation of water are best described as the sum of three-Debye processes. We compute the time autocorrelation function of the dipole moment of water molecules at different temperatures with molecular dynamics simulations and compare the calculations with the experimental data.

2:54PM D26.00003 Exploring the nonlocal dielectric susceptibility of liquid water in the terahertz regime - propagating modes, Debye relaxation and overscreening, DANIEL ELTON, MARIVI FERNANDEZ-SERRA, Stony Brook University — There is great interest in the dielectric and infrared spectra of water between 1-1000 cm⁻¹ (.03-30 THz). To gain insight into this region we study the nonlocal (wavelength dependent) dielectric susceptibility. A curious feature of water is the presence of a propagating mode in the librational band in the terahertz regime. For the first time we study the temperature dependence of this mode and its range of propagation. We show that the librational band has two components - non-dispersive and dispersive. Previously this mode was suggested to be analogous to an optical phonon propagating along the H-bond network. We suggest a possible alternative - that it is the dipolaron mode predicted for dipolar systems. Next we study the region of 1-10 THz which is relevant to understanding the coupling between proteins and water. We show that in addition to H-bond vibrations, intramolecular inertial relaxations also contribute. We find that the Debye peak is dispersive, confirming its long range cooperativity. We report the first temperature dependent study of the static nonlocal susceptibility, which exhibits a negative region, a phenomena called overscreening. We compare a rigid model (TIP4P/ε), a flexible model (TIP4P/2005f) and a polarizable model (TTM3-F).

3:06PM D26.00004 A Dataset of First-Principles Molecular Dynamics Simulations of Water, FRANCOIS GYGI, WILLIAM DAWSON, Univ of California - Davis — We present a dataset of first-principles molecular dynamics simulations [1] of water performed using Density Functional Theory. A set of 32 independent 64-molecule samples was used in separate, parallel simulations for a duration of 50 ps. An analysis of atomic trajectories is given focusing on correlations of the Kohn-Sham energy, ionic kinetic energy, pair correlation functions, diffusion coefficient, and vibrational spectrum. The availability of 32 independent simulations allows for an estimation of the variance of averaged quantities, both within MD runs and between samples. The variability of oxygen pair correlation functions across samples provides a measure of the uncertainty associated with that quantity. We observe several instances of large fluctuations in the oxygen pair correlation functions that can be associated with increases in the local structure index (LSI) proposed by Shiratani and Sasai [2] supporting the hypothesis that water undergoes frequent changes to locally highly structured configurations. Complete atomic trajectories and simulation output files are available online [3].

1 Supported by DOE/BES grant DE-SC0008938

3:18PM D26.00005 Mutual Exclusion of Urea and Trimethylamine N-oxide from Amino Acids in Mixed Solvent Environment, PRITAM GANGULY, Univ of California - Santa Barbara, TIMIR HAJIARI, TU Darmstadt, Germany, JOAN-EMMA SHEA, Univ of California - Santa Barbara, NICO F. A. VAN DER VEGT, TU Darmstadt, Germany — We study the solvation thermodynamics of individual amino acids in mixed urea and trimethylamine N-oxide (TMAO) solutions using molecular dynamics simulations and the Kirkwood-Buff theory. Our results on the preferential interactions between the amino acids and the cosolvents (urea and TMAO) show a mutual exclusion of both the cosolvents from the amino acid surface in the mixed cosolvent condition which is followed by an increase in the cosolvent-cosolvent aggregation away from the amino acid surface. The effects of the mixed cosolvents on the association of the amino acids and the preferential solvation of the amino acids by water are found to be highly non-linear in terms of the effects of the individual cosolvents. A similar result has been found for the association of the protein backbone, mimicked by triglycerine. Our results have been confirmed by different TMAO force-fields and the mutual exclusions of the cosolvents from the amino acids are found to be independent of the choice of the strength of the TMAO-water interactions. Based on our data, a general mechanism can potentially be proposed for the effects of the mixed cosolvents on the preferential solvations of the solutes including the case of cosolvency.

3:30PM D26.00006 ABSTRACT WITHDRAWN —
3:42PM D26.00007 Experiments on Tracer Diffusion in Water and Aqueous Mixtures

3:54PM D26.00008 Spectroscopic studies on di-porphyrin rotor as micro-viscosity sensor

4:06PM D26.00009 High pressure Raman spectroscopy of H_{2}O-CH_{3}OH mixtures

4:18PM D26.00010 Discovery of Water Structural Transitions near Interfaces of Polarizable Solutes

4:30PM D26.00011 Ionic liquid and water molecules diluted in hydrophobic solvent matrix investigated by infrared absorption spectroscopy

4:42PM D26.00012 Electrical Conduction in Pure Water – Trapping and Scattering of Positive Protons and Negative Proton Holes

4:54PM D26.00013 Surface-enhanced Raman mapping of chemical hot spots

1 NSF Research at Undergraduate Institutions
Clusters to Micron-scale Aerosol Particles

Session D27 DCP: Focus Session: Chemical Physics of Clusters: Bridging from Angstrom-scale Clusters to Micron-scale Aerosol Particles 1

204B - Bruce Garrett, Pacific Northwest National Laboratory

and a neutral Ar cluster is dominant in the formation of the cluster complex, \( \text{Co}^{+} \) low-energy collision between clusters. Here we present recent experimental results for the coupling of solution-phase compounds with an optical cavity. Solutions of \( \text{V}(\text{CO})_{6}, \text{Mo}(\text{CO})_{6} \), and NCS \(^{-}\) contained in cavities show strong coupling between the solute chromophores in the mid-infrared and cavity modes. We show that the methodology established with polymer-filled cavities is generally applicable to liquids but that the fluidity of the sample complicates the cavity construction. Varied cavity thicknesses can give rise to spatial gradients in coupling strength and difficulty in targeting a specific cavity-mode order. We also compare the transmission of the mixed vibrational-cavity modes in cavities constructed from either metallic or dielectric reflectors which impacts the cavity resonance line width.

Monday, March 2, 2015 2:30PM - 5:30PM –

Session D27 DCP: Focus Session: Chemical Physics of Clusters: Bridging from Angstrom-scale Clusters to Micron-scale Aerosol Particles I

2:30PM D27.00001 From Clusters to Atmospheric Aerosol Particles: Nucleation in the CLOUD Experiment at CERN

1 NRC Postdoctoral Fellow
2 NRC Postdoctoral Fellow
3 NRC Postdoctoral Fellow

The CLOUD (Cosmics Leaving OUtdoor Droplets) collaboration consists of 20 institutions from Europe and the United States and is funded by national funding institutions as well as the EU training network CLOUD-TRAIN (http://www.cloud-train.eu/)

3:06PM D27.00002 Aerosol Particle Interfacial Thermodynamics and Phase Partitioning Measurements Using Biphasic Microfluidics

1 NRC Postdoctoral Fellow
2 NRC Postdoctoral Fellow
3 NRC Postdoctoral Fellow

3:18PM D27.00003 Formation of Cluster Complexes by Cluster-Cluster-Collisions

1 NRC Postdoctoral Fellow
2 NRC Postdoctoral Fellow
3 NRC Postdoctoral Fellow

The CLOUD (Cosmics Leaving OUtdoor Droplets) collaboration consists of 20 institutions from Europe and the United States and is funded by national funding institutions as well as the EU training network CLOUD-TRAIN (http://www.cloud-train.eu/)

References

The CLOUD (Cosmics Leaving OUtdoor Droplets) collaboration consists of 20 institutions from Europe and the United States and is funded by national funding institutions as well as the EU training network CLOUD-TRAIN (http://www.cloud-train.eu/)
3:30PM D27.00004 Investigations of ice nanoparticles and aerosols in molecular beams\(^1\), MICHAL FARNIK, J. Heyrovsky Institute of Physical Chemistry, ASCR, Dalejovka 3, 18223 Prague 8, Czech Republic — We have recently set up a versatile experiment which allows for different experiments with molecular clusters and nanoparticles in molecular beams. Here we concentrate on the experiments with ice nanoparticles (large water clusters (H\(_2\)O)\(_x\), N \(\sim\)10\(^{-2}-10^3\)) doped with atmospherically relevant molecules, e.g., hydrogen halides, CFCs, nitric acid, N\(_2\)O\(_y\), etc. Such species are relevant to ozone depletion and other atmospheric processes. We investigate (1) the UV-photochemistry using velocity map imaging techniques, and (2) the uptake cross section for the molecules on the ice nanoparticles from velocity measurements. In addition, we record (3) mass spectra of the particles implementing different ionization methods: electron ionization (EI) at variable electron energies, photoionization, and special method of electron photodetachment after Na-doping (NaPI). The unique combination of all these different methods performed with the same nanoparticles provides detailed molecular level information about the studied species and their (photo)physics and chemistry. In particular, an investigation of mixed water-nitric acid particles by means of EI and NaPI revealed the prominent role of the HNO\(_3\) molecule as the condensation nuclei. The uptake of atmospheric molecules by ice nanoparticles has been studied, and the pickup cross sections for some molecules exceed significantly the geometrical sizes of the ice nanoparticles. It has been argued that the large particles composed of several hundred water molecules which grow in the supersonic expansions tend to have highly irregular shapes — nanosnowflakes. Photodissociation of hydrogen halides on ice nanoparticles has been investigated, and shown to proceed via excitation of aciddially dissociated ion pair and subsequent biradical generation and H\(_2\)O dissociation. The photodissociation of CF\(_4\)Cl\(_2\) molecules in clusters leads to efficient CI-fragment caging caused by formation of halogen bond\(^2\).

\(^1\)Grant agency of the Czech Republic, Grant No.: 14-08937S

4:06PM D27.00005 What is the structure of aqueous-alkane nanodroplets?\(^1\), BARBARA WYSLOUZIL, HARSHAD PATHAK, Ohio State Univ - Columbus, ABDALLA OBEIDAT, Jordan University of Science and Technology, GERALD WILEMSKI, Missouri University of Science and Technology — In situ small angle X-ray scattering (SAXS) experiments were conducted on D\(_2\)O-nonane nanodroplets produced in a supersonic nozzle. Fits to the scattering spectra, using standard models for multicomponent droplets such as well-mixed spheres and core-shell structures, were often poor and furthermore the amount of one of the condensed species often violated mass balance. Better fits were obtained using ‘lens-on-sphere’ models suggested by molecular dynamics simulations. Here the amount of nonane condensed, based on the SAXS fitting parameters, was quite close to that measured by infrared absorption spectroscopy although the amount D\(_2\)O condensed was only half of that measured spectroscopically.

\(^1\)Supported by NSF grants CBET 1033439 and CBET 1033387, and Jordan University of Science and Technology

4:18PM D27.00006 Nanodroplets of immiscible fluid pairs adopt nonspherical shapes\(^1\), GERALD WILEMSKI, Missouri University of Science and Technology, FAWAZ HRAHSHEH, King Fahd University of Petroleum and Minerals and Missouri University of Science and Technology — To help understand recent experimental results for nonane/water condensation [Pathak, et al. J. Chem. Phys. 140, 224318 (2014)], the structure of water/nonane nanodroplets was investigated using classical molecular dynamics (MD) simulations of SPC/E water and a unified atom model of nonane. Because nonane and water are essentially immiscible fluids that only partially wet each other, one might expect unusual nanodroplet structures to arise. Indeed, nonspherical, phase-separated Russian Doll (RD) structures were found to occur for these nanodroplets over the entire temperature range studied in the MD simulations, 220K – 300K. An idealized, but realistic lens-on-sphere model for the observed RD structures consists of a spherical nonane lens that partially wets a spherical water droplet. This model was used to analyze the experimental small angle X-ray scattering measurements. The simulated contact angle close to the experimental value of 33.6\(^o\) was confirmed.

\(^1\)Supported by NSF Grant No. CBET-1033387

4:30PM D27.00007 Vapor and Condensed Phase Clusters\(^1\), SHAWN KATHMANN, Pacific Northwest National Laboratory — Given the difficulty of directly observing clustering mechanisms underlying nucleation, classical and ab initio statistical mechanics provide crucial insight into the thermodynamics and kinetics of these processes. Recent experiments have shown nucleation can emit (e.g., crystalloluminescence) and be induced (e.g., IR lasers) by electromagnetic radiation. This opens up the possibility of using luminescence as an exquisite probe of the nucleation mechanism in addition to doing the reverse process by imposing external electromagnetic fields to activate specific modes of nucleation. The inclusion of electronic degrees of freedom as well as excited electronic states lies beyond classical theory. In addition, the osmotic coefficients of sub- and supersaturated aqueous electrolytes may provide quantitative insights into salt cluster distribution functions and free energies of crystal formation. Here we outline the chemical physics relevant to these findings and their consequences on how we understand and model nucleation to control and exploit the synthesis of matter.

\(^1\)This work is sponsored by the U.S. DOE, Office of Basic Energy Sciences, Division of Chemical Science, Geosciences, and Biosciences. Pacific Northwest National Laboratory is a multiprogram national laboratory operated for DOE by Battelle

5:06PM D27.00008 ABSTRACT WITHDRAWN —
consists of quasi-static (swept current) and pulsed-current regimes. Our aim is to investigate the dynamics and efficiency of spin-transfer switching. The layer stacks — We study current-induced switching of thin magnetic layers with perpendicular magnetic anisotropy using in-plane currents and the spin-Hall effect in the YU-MING HUNG, LAURA REHM, GEORG WOLF, ANDREW D. KENT, Department of Physics, New York University. Magnetic Anisotropy is a thousand times too small to account for the changes in switching fields that we observe. through magneto-Seebeck voltage measurements that the charge-currents that would be generated due to the temperature gradient would give rise to STT that significant TSTs in MTJs by generating large temperature gradients across ultrathin MgO tunnel barriers that considerably affect the switching fields of the thermal-spin-torques (TSTs) have been proposed, but so far these TSTs have not been large enough to influence MTJ switching. Here we demonstrate the spin-dependent thermoelectric properties of magnetic materials, novel means of generating spin-currents from temperature gradients, and their associated AAHAKSH PUSHP, TIMOTHY PHUNG, CHARLES RETTNER, BRIAN HUGHES, SEE-HUN YANG, STUART PARKIN, IBM Almaden Research Center —... devices using PMA magnets. using the Spin-Circuit Approach regarding the total energy, the switching speed and energy-delay products for different assisted writing approaches in STT-MTJ such as spin orbit torque, spin Hall effect, voltage controlled magnetic anisotropy and thermal excitation. In this work, we report on our comparative study of their switching properties as well as topography and current mapping by using nanoscale Conductive Atomic Force Microscopy. Our patterning method is based on using hydrogen silsesquioxane resist mask combined with ion beam etching. It allows to fabricate p-MTJ devices down to 40 nm in diameter while maintaining the magnetic quality of the multilayers. Repeatable, consistent switching behaviour has been observed in the obtained p-MTJ devices of 500 nm down to 40 nm with 10 – 800 mV voltage applied. Switching field increased as device diameter decreased, from 580 Oe at 500 nm (MR = 10%) to 410 Oe at 80 nm (MR = 9%). We discuss the effect of device sizes on the switching properties. 1 This work was supported by C-SPIN, one of the six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA. 1 This work was supported in part by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA and in part by the National Science Foundation through the NCN-NEEDS program, contract 1227020-EEC. 

3:30PM D28.00001 Minimization of the energy costs for operating magnetic tunnel junctions1, ILYAS A. H. FARHAT, E. GALE, Khalifa University - KUSTAR, A. F. ISAROVIC, Khalifa University - KUSTAR, KSRC — Increasing prospects of utilizing the STT-MRAM calls for the re-assessment of the overall energy (power) cost of operating magnetic tunnel junctions and related elements. This motivates our design, nanofabrication and characterization of simple tri-layer magnetic tunnel junctions which show measurable decrease in the operating energy cost. The MTJs we report about rely on nanoengineering interfaces between the insulating and magnetic layers in such a way that the area of the hysteresis loops can be controlled in one or both magnetic layers. Our TMR coefficient ranges from 45% to 130%, depending on the MTJ layer materials, and can be anticipated to be further increased. We also report the study of the TMR dependence on the RA product, as an important interface parameter. Lastly, we present an analysis of MTJ parameters affected by our approach and a perspective on further improvements, focusing on the device design parameters relevant for the integration of this type of MTJs. 1This work is supported by the SRC-ATIC grant 2012-VJ-2335. A part of this work is being performed at Cornell University CNF, a member of NNIN. We thank CNF staff for the support. 1 This work was supported by C-SPIN, one of the six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA. 1 This work was supported in part by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA and in part by the National Science Foundation through the NCN-NEEDS program, contract 1227020-EEC.

3:42PM D28.00002 Switching Properties of sub-100 nm Perpendicular Magnetic Tunnel Junctions1, LARYSA TRYPUTEN, Massachusetts Institute of Technology, STEPHEN PIOTROWSKI, MUKUND BAPNA, Carnegie Mellon University, CHIA-LING CHIEN, Johns Hopkins University, WEIGANG WANG, University of Arizona, SARA MAJETICH, Carnegie Mellon University, CAROLINE ROSS, Massachusetts Institute of Technology — Perpendicular magnetic tunnel junctions (p-MTJs) have great potential for realizing high-density non-volatile memory and logic devices. It is critical to solve scalability problem to implement such devices, to achieve low resistance area and to reduce switching current density while maintaining thermal stability. We present our recent results on fabrication of high resolution Ta/CoFeB/MgO/CoFeB/Ta p-MTJ devices and characterization of their switching properties as well as topography and current mapping by using nanoscale Conductive Atomic Force Microscopy. Our patterning method is based on using hydrogen silsesquioxane resin mask combined with ion beam etching. It allows to fabricate p-MTJ devices down to 40 nm in diameter while maintaining the magnetic quality of the multilayers. Repeatable, consistent switching behaviour has been observed in the obtained p-MTJ devices of 500 nm down to 40 nm with 10 – 800 mV voltage applied. Switching field increased as device diameter decreased, from 580 Oe at 500 nm (MR = 10%) to 410 Oe at 80 nm (MR = 9%). We discuss the effect of device sizes on the switching properties. 1 This work was supported by C-SPIN, one of the six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA.
3:42PM D28.00007 Low frequency noise peak near magnon emission energy in magnetic tunnel junctions, LIANG LIU, LI XUANG, HUIQIANG GUO, JIAN WEI, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China, DALAI LI, Z.H. YUAN, JIAFENG FENG, XIUFENG HAN, Beijing National Laboratory of Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, J.M.D. COEY, CRANN and School of Physics, Trinity College, Dublin 2, Ireland — We report on the low frequency noise in magnetic tunnel junctions (MTJs) below 4 K and at low bias, where thermal activation from the bath is suppressed and magnon emission from hot tunneling electrons dominates the transport. For one CoFeB/MgO/CoFeB MTJ, within a narrow range of bias voltage around magnon emission energy, a Lorentzian shape noise spectra is observed. For one CoFeB/AIOx/CoFeB MTJ, at similar bias voltage but within much wider bias range, a much larger Lorentzian shape noise spectra is observed and random telegraph noise is visible in the time traces. In both cases the Lorentzian spectra eventually disappears after repeated measurements, which in combination of the fitted parameters suggests magnon-assisted activation of defects as its origin.

3:54PM D28.00008 ABSTRACT WITHDRAWN —

4:06PM D28.00009 Iterative and self-consistent quantification of nonlocal spin valves with low-resistance oxide barriers, YUNJIAO CAI, Department of Physics and Astronomy, University of Delaware, YONGMING LUO, CHAO ZHOU, Department of Physics, Fudan University, CHUAN QIN, SHUHAN CHEN, Department of Physics and Astronomy, University of Delaware, YIZHENG WU, Department of Physics, Fudan University, YI JI, Department of Physics and Astronomy, University of Delaware — The standard method of quantifying nonlocal spin valves is to assume an exponential decay of the spin signal as a function of the channel length. Then the spin diffusion length and the spin polarization can be extracted via fitting. However, this method does not distinguish between the injection polarization and the detection polarization. In addition, the assumption that the channel length is the only varying parameter may not be always valid. In this work, a large number (>50) of Py-AIOx-Cu NLSV structures on a single substrate are investigated. The standard fitting of exponential decay is initially performed but appears unsatisfactory. We then assume an additional dependence of the spin polarization on the size of the Py/AIOx/Cu junctions, and normalize the spin signals by using the actual junction sizes in individual structures. By feeding the parameters iteratively, we are able to collapse all normalized spin signals on an exponential decay curve with good correlation. The injection/detection polarization strongly depends on the size of the Py/AIOx/Cu junctions. The coexistence of large Cu resistivity and long spin diffusion length points to interesting mechanism of spin relaxation.

4:18PM D28.00010 Inelastic electron tunnelling and noise spectroscopies in organic magnetic tunnel junctions with PTCDI barrier, FARKHAD ALIEV, ISIDORO MARTINEZ, Universidad Autonoma de Madrid, Spain, JHENDY- YONG HONG, National Taiwan University, Taiwan, JUAN PEDRO CASCALES, PABLO ANDRES, Universidad Autonoma de Madrid, Spain, MINN-TSONG LIN, National Taiwan University, Taiwan — The influence of internal barrier dynamics on spin, charge transport and their fluctuations in organic spintronics remains poorly understood. Here we present inelastic electron tunnelling spectroscopy (IETS) and low frequency noise (LFN) studies in magnetic tunnel junctions with thin (1.2-5nm) organic PTCDI barriers in the tunnelling regime at temperatures down to 0.3K. Shot noise is superpoisonian with a Fano factor exceeding 1.5-2 times the maximum values reported for magnetic tunnel barriers with inorganic barriers, indicating spin dependent bunching in tunneling [1]. IETS results show energy relaxation of tunneling electrons through the excitation of collective (librons) and internal (phonons) vibrational modes of the molecules. The bias dependence of the normalised 1/f noise studied up to 350mV reveals that the excitation of some phonon modes has a strong impact on LFN with over a 10-fold reproducible increase near some specific biases. The dependence of the IETS and LFN anomalies with the relative magnetic alignment of the electrodes will also be discussed. [1] J.P.Cascas et al., submitted to Applied Physics Letters

4:30PM D28.00011 Direct Observation of Magnetoresistance Variation in Molecular Junctions Induced by Electrode Geometry, XIANGMIN FEI, GUANGFEN WU, VANESSA LOPEZ, GANG LU, California State University, Northridge, HONG-JUN GAO, Institute of Physics, Chinese Academy of Sciences, LI GAO, California State University, Northridge — Spin-polarized electron transport in the Co/C60/Cu/Ni molecular junctions, in which the fullerene (C60) molecule is in electrical contact with electrodes, has been investigated using an ultra-high vacuum cryogenic scanning tunneling microscope (STM). By combining spin-polarized STM and current-displacement measurements, the spin-polarized contact conductance of molecular junctions has been measured at 5 K. Large tunnel magnetoresistance (TMR) values higher than ~60% have been observed. Depending on electrode geometry, the measured TMR values vary by a factor of ~1.5. The atomic-scale geometry of the electrode apex strongly impacts the spin-polarization of the electrodes and that of the interfacial hybrid molecular states. Our findings suggest that atomic-scale engineering of electrodes represents an additional dependence of the spin polarization on the size of the Py/AIOx/Cu junctions, and normalize the spin signals by using the actual junction sizes in individual structures. By feeding the parameters iteratively, we are able to collapse all normalized spin signals on an exponential decay curve with good correlation. The injection/detection polarization strongly depends on the size of the Py/AIOx/Cu junctions. The coexistence of large Cu resistivity and long spin diffusion length points to interesting mechanism of spin relaxation.

4:42PM D28.00012 Memristive behavior in tunnel junctions with graphene oxide barrier, MIRKO ROCCI, ANA PEREZ-MUÑOZ, JAVIER DEL VALLE, JOSE LUIS VICENT, CARLOS LEON, ZOHAIR SEFRIOU, JACOBO SANTAMARIA, Universidad Complutense de Madrid, FRANCESCO PERROZZI, LUCA OTTAVIANO, MICHELE NARDOINE, SANDRO SANTUCCI, Università degli Studi dell’Aquila, ITALY, EMANUELE TROESSI, CNR-ISOF and Laboratory MIST.E-R, Bologna, Italy, VINCENZO PALERMO, CNR-ISOF, Bologna, Italy — Resistive switching in Graphene Oxide (GO) structures has shown its potential for future nonvolatile memory applications. Here we report on GO (2-20 layers thick) as tunnel barriers in combination with half-metallic La0.75Sr0.25MnO3 (LSMO) manganites, Ag, and Ni as electrodes. Hybrid LSMO/GO/Ag junctions show a memristive-like behavior with more than 5 orders of magnitude resistance change (between high and low states) at low temperature. We explain the resistance switching in terms of (redox) generation of oxygen vacancies at the GO metal interfaces and their diffusion through the GO layer under the large applied electric fields (10^4 V/m). Magnetic tunnel junctions fabricated with Ni (instead of Ag) show a significant tunnelling magnetoresistance (TMR) combined with the nonvolatile memristor response. The sign of the TMR changes from positive to negative upon resistive switching of the GO. We interpret the sign inversion as due to changes in the Ni surface bonding state occurring as the result of the oxygen accumulation (depletion) at its surface.

4:54PM D28.00013 ABSTRACT MOVED TO G14.00004 —

5:06PM D28.00014 Fluorine Functionalized BNNT as a Spin Filter1, KAMAL DHUNGANA, RANJIT PATI, Michigan Technological University — Spin filtering is a phenomenon that allows one to generate spin-polarized carriers in a circuit comprised of a magnetic channel sandwiched between two non-magnetic electrodes. In recent years, the quest for a novel low-dimensional metal-free magnetic channel that would exhibit both magnetism at a higher temperature and excellent spin filtering property has been intensively pursued. Herein, using a first-principles approach, we study the magnetic property of fluorine functionalized boron nitride nanotube (F-BNNT). A long range ferromagnetic spin ordering is found to occur in the F-BNNT at temperature much above the room temperature. Our spin polarized transport study shows that the fluorine functionalization in BNNT not only enhances its conductance by more than two orders, which is in excellent agreement with the experimental report, but also makes it a perfect spin filter.

1This work is supported by the NSF through grant no. 1249504.
5:18PM D28.00015 Antiferromagnet controlled tunneling anisotropic magnetoresistance1. CHENG SONG, YUYAN WANG, FENG PAN, Tsinghua University, School of Materials Science and Engineering, Beijing, SPINTRONICS TEAM — We investigate tunneling anisotropic magnetoresistance (TAMR) in antiferromagnets (AFM)-based junctions, where Co/Pt magnetization drives partial rotation of AFM moments with the formation of exchange-spring [1]. The existence of exchange-spring is further confirmed by element specified x-ray magnetic dichroism [2]. Because of superior thermal tolerance of perpendicular exchange coupling and the stability of moments of ~ 6 nm-thick IrMn in [Pt/Co/IrMn/AOx/Pt] junctions, TAMR gets significantly enhanced up to room-temperature [1]. The TAMR behavior in [Pt/Co/IrMn/AOx/metal] junctions is insensitive to the top metal electrodes [3]. The situation turns out to be different when the top electrode is replaced by AFM. TAMR is observed in IrMn/AOx/IrMn junctions, where the resistance states are governed by the relative arrangement of the AFM moments adjacent to AOx [4]. Our findings would advance the process towards practical AFM spintronics.


1This work was supported by NSFC (Grant Nos. 51322101, and 51202125) and 863 project of China (Grant no. 2014AA032904).

Monday, March 2, 2015 2:30PM - 5:30PM –
Session D29 GMAG DMP FIAP: Focus Session: Ferromagnetic Metals 206A - Johan Akerman, University of Gothenburg

2:30PM D29.00001 ABSTRACT WITHDRAWN –

2:42PM D29.00002 High-frequency modes of a magnetic antivortex1. MARTIN ASMAT-UCEDA, GRANT RILEY, ARABINDA HALDAR, KRISTEN BUCHANAN, Colorado State University — Magnetic vortices have attracted considerable attention in recent years not only because of their interesting physical properties but also due to their potential for applications. The magnetic antivortex (AV), the topological counterpart of the magnetic vortex, possesses similarly rich dynamics and its spin configuration may prove advantageous for spin-wave-based devices, however, it has not been studied as intensely. Recent experiments show that AV’s will form naturally at the intersections of patterned pound-key-like nanostructures that are magnetically soft. Here we present micromagnetic simulations of the dynamics of AV’s in these structures. The simulations show that pound-key-like structures made of 30-nm thick Permalloy exhibit a complex dynamic profile that includes a number of discrete high-frequency modes (>1 GHz). Spatial maps of the dynamic modes that were constructed using Fourier analysis of the simulation results show modes that are in similar in character to the radial and azimuthal modes observed for magnetic vortices but the spin dynamics also differ from those of a vortex due to the presence of the elongated nanowires in the pound-key-like structure. The frequencies of the observed modes tend to decrease with increasing sample size, however, the general features of the modes remains relatively unaffected by the structure size. The simulations will be compared to Brillouin Light Scattering (BLS) experimental results.

1This work was supported by the US DOE-BES award #ER 46854.

2:54PM D29.00003 Control of magnetic damping and magnetic fluctuations by spin current . YONG PU, CHI ZHANG, SERGEI MANUILOV, EZEKIEL JOHNSTON-HALPERIN, FENGYUAN YANG, CHRIS HAMMEL, The Ohio State University — We use spin hall effect in a non-magnetic film (NM) to generate spin current, which can excite magnetic precesses and manipulate magnetic properties of an adjacent ferromagnetic thin film (FM). We show that both magnetic damping and magnetic fluctuations can be sufficiently suppressed or enhanced by the spin current. We find that the magnetic damping is linear with spin current that is consistent with previous reports; on the other hand, the quasi-uniform precession and magnetic fluctuations show strongly nonlinear behaviors at driving current approaching critical value. The observations suggest that spin current interacts with all allowed spin-wave modes and induces strong nonlinear influence. Our results give an insight of the complex spin-torque driven dynamics in FM/NM systems and suggest a route to control the magnetic damping and magnetic fluctuations in nanodevices.

3:06PM D29.00004 Co1.5Fe1.5Ge and Co2MnSi Half-Metal Magnetic behavior tested by spin-resolved photoemission and ferromagnetic resonance , STEPHANE ANDRIEU, Institut Jean Lamour - Universite de Lorraine — In a magnetic spin-valve or tunnel junction, a crucial parameter to get both large magnetoresistance (MR) and a good Spin Transfer Torque (STT) efficiency is the spin-polarization of the magnetic electrodes. So-called “Half-Metallic” Magnetic (HMM) materials are of interest for such devices due to the existence of a spin-gap at the Fermi level for minority spins [1]. Recently, MR enhancements have been observed by different groups on Co2-xFe1+xGe [1] and Co2MnSi [2] Heusler materials, suggesting HMM behavior. A second consequence of that minority spin gap is that very low magnetic damping is expected. Combining both properties in a device is a challenge for decreasing the critical current necessary to switch the magnetization using STT. Up to now, many Heusler alloys are claimed to get this HMM property [3], but direct demonstration using spin-resolved photoemission is often missing. Here we focus on 2 systems, (i) Co1.5Fe1.5Ge for which a significant increase of the GMR was observed in spin valves [1], and (ii) Co2MnSi for which very large TMR values were observed in MgO-based MTJs [2]. The Co1.5Fe1.5Ge and Co2MnSi(001) films (noted CFG and CMS) were prepared by Molecular Beam Epitaxy and PLD coupled to the Spin-Resolved PhotoEmission (SR-PES) set-up on CASSIOPEE beamline at SOLEIL synchrotron. The L21 chemical ordering was confirmed in CFG films by using anomalous diffraction on (001) Bragg peaks. The spin-polarization of the magnetic electrodes, measured by SR-PES experiments, do not show any HMM behavior on our CFG films [4]. Similar PES experiments performed on CMS showed that the minority spin density of states (DOS) drops down to zero at -0.4eV below EF, leading to a 100% spin polarization. However, we also observed an increase of the minority spin DOS at EF, not predicted by ab initio calculations on the bulk structure. The spin-gap is thus decreased due to the surface symmetry breaking. We will show however that this spin-gap can be enlarged when finishing the surface by 1 Mn atomic plane, or when covering with the MgO barrier. Extremely low damping (<10-3) are observed, making CMS a very good candidate for spintronics devices.


3:42PM D29.00005 ABSTRACT MOVED TO Q31.00006 –
Temperature dependent ferromagnetic relaxation and gyromagnetic ratio in Ni80Fe20/Gd thin films

We report on the temperature dependence of the magnetization dynamics of NiFe thin films (5nm & 10nm) capped with a 3nm Gd layer using broadband ferromagnetic resonance. We observe that the effective Gilbert damping parameter determined from the broadband measurements increases as the temperature approaches the Curie-temperature of the Gd layer. Part of the enhancement can be explained by an increase of the spin-pumping contribution to the relaxation [1,2] as the temperature approaches the Curie temperature of Gd. We also measure a strong increase of the gyromagnetic ratio with decreasing temperature which resembles the increase of the gyromagnetic ratio in rare earth containing transition metals near the compensation point [3,4]. This increase in the gyromagnetic ratio is expected to lead to an increased Gilbert type damping due to spin-orbit interaction [5,6], that likely also contributes to the increase in damping.


This work is supported primarily by C-SPIN (one of the six SRC STAR-net Centers) and partly by the MRSEC Program under Contract No. DMR-0819885.
4:54PM D29.00011 Symmetry-dependent electron-electron interaction in coherent tunnel junctions resolved by measurements of zero-bias anomaly  

JIAN WEI, LIANG LIU, JASEN NIU, LI XIANG, ICQM, Peking Univ, China, D.-L. LI, J.-F. FENG, X.-F. HAN, IOP, CAS, China, X.-G. ZHANG, Oak Ridge National Laboratory and Univ. of Florida, USA, J.M.D. COEY, Trinity College, Ireland — We provide conclusive experimental evidence that zero-bias anomaly in the differential resistance of magnetic tunnel junctions (MTJs) is due to electron-electron interaction (EEI), clarifying a long standing issue. The magnon effect that caused confusion is now excluded by measuring at low temperatures down to 0.2 K and with reduced ac measurement voltages down to 0.06 mV. The normalized change of conductance is proportional to $\ln(e^v/k_{B}T)$, consistent with the Alshuler-Aronov theory of tunneling that describes the reduction of density of states due to EEI, but inconsistent with magnetic impurity scattering. The slope of the $\ln(e^v/k_{B}T)$ dependence is symmetry dependent: the slopes for parallel and antiparallel states are different for coherent tunnel junctions with symmetry filtering, while nearly the same for those without symmetry filtering (amorphous barriers). This observation may be helpful for verifying symmetry preserved filtering in search of new coherent tunneling junctions, and for probing and separating electron Bloch states of different symmetries in other correlated systems.  

1Liu et al., arXiv:1410.3636, accepted by Phys. Rev. B

5:06PM D29.00012 Large resistivity modulation in mixed-phase metallic systems  

YEONBAE LEE, University of California, Berkeley, ZHIQI LIU, Oak Ridge National Laboratory, Center for Nanophase Materials Sciences, JOHN HERON, Cornell University, JAMES CLARKSON, JEONGMIN HONG, CHANGHYUN KO, University of California, Berkeley, MICHAEL BIEGALSKI, Oak Ridge National Laboratory, Center for Nanophase Materials Sciences, ULRICH ASCHAUER, ETH Zurich, SHANG-LIN HSU, MARK NOWAKOWSKI, JUNQIAO WU, University of California, Berkeley, HANS CHRISTEN, Oak Ridge National Laboratory, Center for Nanophase Materials Sciences, SAYEEF SALAHUDDIN, JEFFREY BOKOR, University of California, Berkeley, NICOLA SPALDIN, ETH Zurich, DARRELL SCHLOM, Cornell University, RAMAMOOARTHY RAMESH, University of California, Berkeley — We have investigated the effect of an electric field to FeRh/PMN-Pt heterostructures and report 8% change in the electrical resistivity of FeRh films. Such a “giant” electroresistance (GER) response is striking in metallic systems, in which external electric fields are screened and thus only weakly influence the carrier concentrations and mobilities. We show that our FeRh films comprise coexisting ferromagnetic and antiferromagnetic phases with different resistivities, and the origin of the GER effect is the strain-mediated change in their relative proportions. The observed behavior is reminiscent of colossal magnetoresistance in perovskite manganites, and illustrates the role of mixed-phase coexistence in achieving large changes in physical properties with low-energy external perturbation.

5:18PM D29.00013 Effect of annealing on the surface magnetic and magnetoimpedance properties of Co-based amorphous microwires  

V. KALAPPATTI, J. DEVKOTA, E. CLEMENTS, S. CHANDRA, Department of Physics, University of South Florida, J.S. LIU, H.X. SHEN, J.F. SUN, Institute of Materials Science and Engineering, Harbin Institute of Technology, H. SRIKANTH, M.H. PHAN, Department of Physics, University of South Florida — Magnetic domains of negative magnetostrictive amorphous microwires (AWs) form a core-shell type structure with the core and shell domains preferred along axis and circumference, respectively. In this work, we have studied the effect of a combined current modulation annealing on the bulk and surface magnetic properties of melt-extracted $\text{Co}_{0.55}\text{Fe}_{0.45}\text{B}_{1.5}\text{Si}_{1.5}$ and Co$_{3.3}$Fe$_{1.7}$B$_{1.0}$Si$_{1.5}$Nb$_{0.5}$ AWs and their correlations with the magnetoimpedance (MI) effect. The AWs were annealed by a combination of ac (90 mA, 50 Hz) and dc (60, 63, and 65 mA) currents for 480 seconds each, and magnetic hysteresis loops were measured by VSM and a magneto-optic Kerr effect (MOKE) magnetometer. Compared to VSM loops, MOKE loops for the annealed AWs showed higher coercive and anisotropy fields, indicating that the near-surface region was magnetically harder. The anisotropy fields of the AWs defined as the peaks of the MI spectra at 1 MHz and 500 MHz were found to have a correlation with those probed by VSM and MOKE, respectively. These findings are of practical importance in designing MI-based sensors.

Monday, March 2, 2015 2:30PM - 5:30PM —  
Session D30 GMAG DMP: Focus Session: Magnetic Domains and Domain Walls  
206B - Timothy Phung, IBM Almaden Research Center

2:30PM D30.00001 Highly efficient in-line magnetic domain wall injector  
TIMOTHY PHUNG, AAKASH PUSHP, LUC THOMAS, CHARLES RETTNER, SEE-HUN YANG, KWANG-SU RYU, JOHN BAGLIN, BRIAN HUGHES, STUART PARKIN, IBM Almaden Research Center — The creation and manipulation of domain walls (DWs) in magnetic nano-wires is of considerable interest, and forms the basis of several logic and memory devices. Traditionally, the DWs are created in the nano-wires using local magnetic fields from current injection lines fabricated orthogonal to the nano-wires, whereas the synchronous motion of a series of DWs along a nano-wire is achieved using spin transfer torque (STT) from charge currents that transport spin angular momentum. Here we demonstrate a highly efficient and simple DW injection scheme that uses a combination of STT from nanosecond long, uni-polar, current pulses that cross a $90^\circ$ magnetization boundary along with the fringing fields inherently prevalent at the boundary. The $90^\circ$ magnetization boundary is created by local ion-irradiation at the end of a nano-wire exhibiting perpendicular magnetic anisotropy. Remarkably, we find that the currents needed for this “in-line” DW injection scheme are at least one hundred times smaller than conventional methods. Additional advantages are its significantly smaller footprint than that of conventional methods, its compatibility to the smallest lithographic dimensions, and its ability to continuously inject DWs using uni-polar current. This simplified scheme bodes well for the fruition of spintronics based memory and logic devices.

2:42PM D30.00002 Domain wall motion in sub-100 nm magnetic wire  
SAIMA SIDDIQUI, SUMIT DUTTA, JEAN ANNE CURRIVAN, Electrical Engineering and Computer Science, Massachusetts Institute of Technology, CAROLINE ROSS, Department of Materials Science and Engineering, Massachusetts Institute of Technology, MARC BALDÒ, Electrical Engineering and Computer Science, Massachusetts Institute of Technology — Nonvolatile memory devices such as racetrack memory rely on the manipulation of domain wall (DW) in magnetic nanowires, and scaling of these devices requires an understanding of domain wall behavior as a function of the wire width. Due to the increased importance of edge roughness and magnetostatic interaction, DW pinning increases dramatically as the wire dimensions decrease and stochastic behavior is expected depending on the distribution of pinning sites. We report on the field driven DW statistics in sub-100 nm wide nanowires made from Co films with very small edge roughness. The nanowires were patterned in the form of a set of concentric rings of 10 $\mu$m diameter. Two different width nanowires with two different spacings have been studied. The rings were first saturated in plane to produce onion states and then the DWs were translated in the wires using an orthogonal in-plane field. The position of the DWs in the nanowires was determined with magnetic force microscopy. From the positions of the DWs in the nanowires, the strength of the extrinsic pinning sites was identified and they follow two different distributions in two different types of nanowire rings. For the closely spaced wires, magnetostatic interactions led to correlated movement of DWs in neighboring wires. The implications of DW pinning and interaction in nanoscale DW devices will be discussed.
2:54PM D30.00003 Reversible electrically-driven magnetic domain wall rotation in multiferroic heterostructures to manipulate suspended on-chip magnetic particles1. MARK NOWAKOWSKI, University of California, Berkeley, HYUNMIN SOHN, CHENG-YEN LIANG, JOSHUA HOCKEL, KYLE WETZLAR, SCOTT KELLER, University of California, Los Angeles, BRENDA MCELLENN, NYU Polytechnic School of Engineering, MATTHEW MARCUS, ANDREW DORAN, ANTHONY YOUNG, Advanced Light Source, Lawrence Berkeley National Lab, MATHIAS KLÄUI, University of Mainz, GREGORY CARMAN, JEFFREY BOKOR, University of California, Berkeley, ROBERT CANDLER, University of California, Los Angeles — We experimentally demonstrate reversible electrically-driven, strain-mediated domain wall (DW) rotation in Ni rings fabricated on piezolectric [Pb(Mg1/3Nb2/3)O3]0.66-PbTiO3]0.34 (PMN-PT) substrates. An electric field applied across the PMN-PT substrate induces a strain in the Ni rings producing DW rotation around the ring toward the dominant PMN-PT strain axis by inverse magnetostriiction. We observe DWs reversibly cycled between their initial and rotated state as a function of the applied electric field with x-ray magnetic circular dichroism photo-emission electron microscopy. The DW rotation is analytically predicted using a fully coupled micromagnetic/elastodynamic multi-physics simulation to verify that the experimental behavior is caused by the electrically-generated strain in this multiferroic system. Finally, this DW rotation is used to capture and manipulate magnetic particles in a fluidic environment to demonstrate a proof-of-concept energy-efficient pathway for multiferroic-based lab-on-a-chip applications.

1Supported by TANMS (NSF 11-537), E3S, US Dept of Energy (DE-AC02-06CH12311), EU, and DFG

3:06PM D30.00004 Nucleation of 360 deg DWs in a wire using a local circular field1, FIKRIYE IDIL KAYA, ANANDAKUMAR SARELLA, KATHERINE E. AIDALA, Mount Holyoke College — Understanding domain wall (DW) motion in ferromagnetic nanostructures is important to realize proposed magnetic data storage and logic devices. Interest in 360° DWs has increased recently with the recognition that their minimal stray field creates only short range interactions, leading to a potentially higher packing density compared to 180° DWs. Our simulations demonstrate the feasibility of nucleating a 360° DW at a specific location along a wire by applying a local circular field that is centered in close proximity to the wire. We simulate the field strength as if from a current carrying wire, which can be experimentally realized by passing current through the tip of an AFM [1, 2]. The successful nucleation of a 360° DW depends on the dimensions of the Py wire, on the strength of the circular field, and on the distance of the center of the field from the wire. Once a 360° DW is nucleated, its position shifts with time. We use a notch to stabilize the location of the 360° DW. We investigate the optimal size and spacing of the notches to allow the greatest packing density with control over the nucleation and annihilation of individual domain walls. [1] T Yang et al., Appl. Phys. Lett., 98, 242505 (2011). [2] http://math.nist.gov/omnef

1Supported by NSF DMR-1207924

3:18PM D30.00005 Reversal-mechanism of in-plane current-induced perpendicular switching: the role of controllable domain behaviors, J. BI, Institute of Microelectronics, Chinese Academy of Sciences, Beijing 100029, China, J.Q. XIAO, Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716, USA, M. LIU, Institute of Microelectronics, Chinese Academy of Sciences, Beijing 100029, China — We propose a magnetization reversal model to explain the perpendicular switching of a single ferromagnetic layer induced by an in-plane current [1]. Our model includes three ingredients: (1) a steady equilibrium magnetization state with equal up and down domains favored by an applied current; (2) domain Wall (DW) motion under the applied current; (3) the up-down (↑↓) DW and down-up (↓↑) DW motions are separately modulated by an applied field. We experimentally demonstrate ingredient (1) can be satisfied in symmetric Pt/Co/Ni/Co/Pt and asymmetric Pt/Co/AlOx structures arising from the magnon instability induced by conventional spin torques [2] and probable spin-Hall torques (SHT) in asymmetric structures. We show ingredient (2) and (3) can also be satisfied in these structures. This model indicates that SHTs mainly play the role of driving DW motion, and a required external field plays the role of modulating the relative velocity of ↑↓ and ↓↑ DWs and thus determines the switching directions. This model also predicts similar switching behaviors in skyrmin structures. [1]L. Liu et al. Science 336, 555 (2012); [2] J. Shibata et al. Phys. Rev. Lett. 94, 076601 (2005).

3:30PM D30.00006 Domain Wall structures in wide palmello strips, VIRGINIA ESTEVEZ, LASSE LAURSON, COMP Centre of Excellence and Helsinki Institute of Physics, Department of Applied Physics, Aalto University — We numerically analyze the equilibrium micromagnetic domain wall structures encountered in Palmello strips of a wide range of thicknesses and widths, with strip widths up to several micrometers. By performing a systematic set of micromagnetic simulations, we show that the equilibrium domain wall structure exhibits additional DWs with respect to the previously found structures (symmetric and asymmetric transverse wall and vortex wall) also a double-vortex domain wall for large enough strip widths and thicknesses. In general, shape anisotropy is less important for wider strips, and thus energy minima with more complex spin structures closing the flux more efficiently than those found for narrow strips may appear. Also several metastable domain wall structures are found, such as structures with three or four vortices or two vortices and an antivortex. We discuss the details of the relaxation process, including the effect of varying the magnitude of the Gilbert damping constant, and the role of using different initial conditions. Finally, we also consider the field-driven dynamics of the double-vortex domain wall.

3:42PM D30.00007 Lateral Domain Transfer In a Magnetic Nanowire With Perpendicular-to-Plane-Anisotropy For Three-Dimensional Memory Applications, AISHA GOKCE, OZHAN OZATAY, BUGRA BULUT, Bogazici University, COLEMAN RAINY, Colombia University, JORDAN A. KATINE, HGST, A Western Digital Company, THOMAS HAUET, Institut Jean Lamour, Nancy Université, ANNA GIORDANO, GIOVANNI FRINGCCHIO, University of Messina — Spin torque driven magnetic domain transport has been of great interest with potential applications in three dimensional magnetic race track memory and also for domain wall logic. Here we report on experimental and micromagnetic modelling results of spin torque driven magnetic domain transport in CoNi/Pd multilayers with perpendicular-to-plane anisotropy patterned to form magnetic nanowires with double constrictions where domains can be moved with spin polarized current pulses in between constricted sites. The domain nucleation was triggered by Joule heating in the presence of a magnetic tip a few nm above the surface which was otherwise in the remanent state. We show that with low or high amplitude nanosecond current pulses two different types of domain transfer behavior is possible: a replicated or partially displaced domain in the neighboring constriction, or an expansion of the domain into the spacer region and the neighboring pinning site. Micromagnetic modelling of the domain transport in such devices suggests that in addition to the experimentally observed behavior a third regime where the full transfer of a single domain is also attainable. Our study shows that CoNi/Pd nanowires can be of potential practical use in a three dimensional memory structure.

3:54PM D30.00008 ABSTRACT WITHDRAWN —

4:06PM D30.00009 Dzyaloshinskii-Moriya Domain Walls in Nanotubes, OLEG TRETIAKOV, IMR, Tohoku University, ARSENII GOUSSEV, Northumbria University, J.M. ROBBINS, VALERIY SLASTIKOV, University of Bristol — We study domain walls in thin ferromagnetic nanotubes with Dzyaloshinskii-Moriya interaction (DMI). Dramatic effects arise from the interplay of space curvature and spin-orbit induced DMI on the domain wall structure in these systems. The domain walls become narrower in systems with DMI and curvature. Moreover, the domain walls created in such nanotubes can propagate without Walker breakdown for arbitrary applied currents, thus allowing for a robust and controlled domain-wall motion. The domain-wall velocity is directly proportional to the non-adiabatic spin transfer torque current term and is insensitive to the adiabatic current term. Application of an external magnetic field along the nanotube axis triggers rich dynamical response of the curved domain wall. In particular, we show that the propagation velocity is a non-linear function of both the applied field and DMI, and strongly depends on the orientation and chirality of the wall.

1We acknowledge support by the Grants-in-Aid for Scientific Research (No. 25800184 and No. 25247056) from the MEXT, Japan and SpinNet.
4:18PM D30.00010 Thermodynamic theory for thermally driven domain wall motion in magnetic nanostructures\textsuperscript{1}, XIANG RONG WANG, Hong Kong Univ of Sci & Tech — It is well-established now that a thermal gradient can be used to manipulate spins in a magnetic texture like skyrmions and domain walls (DWs). A thermal gradient can interact with spins through different channels. For example, a thermal gradient can affect spins through the thermoelectric effects by which spin polarized electric current is generated in a ferromagnetic metal. In turn, the thermally generated electric current can interact with magnetic texture via spin-transfer torque (STT). A thermal gradient can also generate magnons or spin waves that interact with magnetic textures. This effect should be important in a ferromagnetic insulator. Spin waves (or magnons) interact with magnetic domain walls (DWs) in a complicated way that a DW can propagate either along or against magnon flow, similar to its electron counterpart. Probably different from its electron counterpart where one may attribute the “wrong” DW propagation direction to the Dzyaloshinskii-Moriya interaction and various types of torques due to spin-orbit interactions, it will be very difficult to understand why a DW can move along the magnon flow if the angular momentum transfer is the only mechanism behind the magnon driven DW motion. It will also be difficult to explain why “wrong” DW propagation direction has not been observed in thermally driven DW motion in both simulations and experiments. Thus, there must be other interaction(s) between spin waves and magnetic textures. In terms of thermal gradient driven DW propagation along a nanowire, a DW always propagates to the hot region of a magnetic insulator wire. We theoretically illustrate why it is surely so from thermodynamic viewpoint. It is shown that DW entropy is always larger than that of a domain. Equivalently, the free energy difference of a DW and a domain decreases as the temperature increases. The larger DW entropy is related to the increase of magnon density of states at low energy originated from the gapless bound spin waves in DWs. This theory should be applicable to other spin textures like skyrmions as well since bound spin waves generally exist in spin textures. The theory also naturally explains why the magnetic domain widths decrease with the increase of the temperature, a well-known experimental phenomenon. In collaboration with X.S. Wang, Hong Kong University of Science & Technology.


\textsuperscript{1}This work was supported by Hong Kong GRF Grant (605413) and the grant from NNSF of China (11374249).

4:54PM D30.00011 Asymmetric domain expansion and dendrite formation in thin films with strong Dzyaloshinskii-Moriya interaction, LUCAS CARETTA, MAXWELL MANN, AIK-JUN TAN, GEOFFREY BEACH, Massachusetts Inst of Tech-MIT — The Dzyaloshinskii-Moriya interaction (DMI) at heavy-metal/ferromagnet interfaces can stabilize chiral spin textures \textsuperscript{1}. It has been recently shown that field-driven bubble domain expansion in perpendicularly-magnetized thin films is asymmetric under the application of an in-plane field, which can be used to quantify the DMI effective field in the (DW). We have imaged domain expansion in Pt(3nm)/Co(0.9nm)/Pt(x)/GdOx(3nm) films using wide-field Kerr microscopy to characterize this behavior systematically as a function of DMI strength. In the case of null or weak DMI, realized when top and bottom Pt layers are of similar thickness, the in-plane field dependence of the DW velocity is well-described by the simple expansion model derived in Ref. \textsuperscript{2}. However, in the case of strong DMI, we find a strongly nonmonotonic behavior due to flattening of the DW, minimizing Zeeman energy and DMI energy. Moreover, we show that when the ratio of the DMI effective field to the perpendicular anisotropy field is large, expanding bubble domains leave behind fine-scale dendritic structures, consisting of coupled 360 degree DWs. We present modeling that qualitatively describes these behaviors. \textsuperscript{1} A. Fert et al., Nat. Nano., 8, 593 (2013). \textsuperscript{2} J. C. Slonczewski, J. Magn. Magn. Mater., 195, 222 (1999).

5:06PM D30.00012 Static and Dynamic Properties of Magnetic Antivortices in Asteroid-Shaped Permalloy Nanomagnets, ALI TAHA HABIBOGLU, VEDAT KARAKAS, MUSTAFA METE, AHMET COSKUNER, YEMLIHA BILAL KALYONCU, AISHA GOKCE, OZHAN OZATAY, Bogazici University, ANNA GIORDANO, MARIO CARPENTIERI, University of Calabria, GIOVANNI FINOCCHIO, University of Messina, FEDERICA CELEGATO, CNR Institute of Materials for Electronics and Magnetism, PAOLA TIBERTO, INRIM National Institute of Research Metrologia — Patterned nanomagnets display unconventional spin configurations like vortex, anti-vortex, bubble, which have unique static and dynamic properties. Such micro-magnetic structures are potentially applicable to ultrafast memory, rf oscillators and detectors. Studies on magnetic thin films containing vortex structures exhibit interesting behavior under external field and/or current bias like polarity switching, core displacement and core gyration with high fields [1]. In this study, we report on our investigation of stable anti-vortex formation conditions and the subsequent magnetic field/dc current driven excitations in 2x2um\textsuperscript{2} Permalloy based asteroid geometry devices which exhibit an anti-vortex pair nucleation at the center. The Magnetic Force Microscopy images show that the antivortex pair can be rotated around the center by an external magnetic field. We obtain a high frequency (GHz) signal measured via anisotropic magneto-resistance effect (AMR) under constant dc current-bias which triggers antivortex pair gyration around the center of the device through spin torque transfer. We study the dynamic response of the structure as a function of current and field to assess utilization of the device as a practical on-chip microwave oscillator.


5:18PM D30.00013 Micro-hysteresis in the Faraday Rotation of Bismuth Doped Iron Garnets\textsuperscript{1}, MANNIX SHINN, DONG HO WU, ANTHONY GARZARELLA, U. S. Naval Research Laboratory, RONGJIA TAO, Temple University — There is strong interest in using the Faraday effect (Magneto-optic effect) for non-invasive detection of weak magnetic fields, since in principle one can construct an ultra-sensitive MO-sensor that could be comparable to a SQUID. Bismuth doped rare earth iron garnets (Bi-RIGs) are a candidate material, however their polarization rotation is often measured at saturating fields. We have found that in some Bi-RIGs there is a coercive field that is less than the noise level of our probe beam, which can lead to mischaracterization of sensitivity. This coercivity appears related to magnetic domain wall motion. In this talk I will discuss our experiments and how domain walls can affect the sensitivity of our MO-sensor.

\textsuperscript{1}Supported by the U. S. Naval Research Laboratory.

Monday, March 2, 2015 2:30PM - 5:30PM – Session D31 GMAG DMP FIAP: Focus Session: Spin-Dependent Phenomena in Semiconductors: Magnetic Interactions in Semiconductors 207A - Olaf van ‘t Erve, Naval Research Laboratory
2:30PM D31.00001 GMAG Dissertation Award Talk: Zero-moment Half-Metallic Ferrimagnetic Semiconductors, MICHELLE E. JAMER, Physics, Northeastern University — Low- and zero-moment half-metallic ferrimagnetic semiconductors [1,2] have been proposed for advanced applications, such as nonvolatile RAM memory and quantum computing. These inverse-Heusler materials could be used to generate spin-polarized electron or hole currents without the associated harmful fringing magnetic fields. Such materials are expected to exhibit low to zero magnetic moment at room temperature, which makes them well-positioned for future spin-based devices. However, these compounds have been shown to suffer from disorder [3]. This work focuses on the synthesis of these compounds and the investigation of their structural, magnetic, and transport properties. CrMnCoGa and Mn2Al thin films were synthesized by molecular beam epitaxy, and VFeAl and Cr2CoAl were synthesized via arc-melting. Rietveld analysis was used to determine the degree of ordering in the sublattices as a function of annealing. The atomic moments were measured by X-ray magnetic circular and linear dichroism confirmed antiferromagnetic alignment of sublattices and the desired near-zero moment in several compounds.

In collaboration with George E. Sterbinsky, Photon Sciences Directorate, Brookhaven National Laboratory; Dario Arena Photon Sciences Directorate, Brookhaven National Laboratory; Laura H. Lewis, Chemical Engineering, Northeastern University; and Don Heiman, Physics, Northeastern University.


3:06PM D31.00002 A Designed Room Temperature Multilayered Magnetic Semiconductor, DINAH SIMONE BOUMA, MICHALIS CHARILAOÛ, CATHERINE BORDEL, UC Berkeley Physics Department, RYAN DUCHIN, UC Berkeley Materials Science and Engineering Department, ALEXANDER BARRIGA, ADAM FARMER, FRANCES HELLMAN, UC Berkeley Physics Department, MATERIALS SCIENCE DIVISION, LAWRENCE BERKELEY NATIONAL LAB TEAM — A room temperature magnetic semiconductor has been designed and fabricated by using a combination of antiferromagnet (NiO) grown in the (111) orientation, which gives surface uncompensated magnetism for an odd number of planes, layered with the lightly doped semiconductor Al-doped ZnO (AZO). Magnetization and Hall effect measurements of multilayers of NiO and AZO are presented for varying thickness of each. The magnetic properties vary as a function of the number of Ni planes in each NiO layer; an odd number of Ni planes yields on each NiO layer an uncompensated moment which is RKKY-coupled to the moments on adjacent NiO layers via the carriers in the AZO. This RKKY coupling oscillates with the AZO layer thickness, and it disappears entirely in samples where the AZO is replaced with undoped ZnO. The anomalous Hall effect data indicate that the carriers in the AZO are spin-polarized according to the direction of the applied field at both low temperature and room temperature. NiO/AZO multilayers are therefore a promising candidate for spintronic applications demanding a room-temperature semiconductor.

3:18PM D31.00003 Magnetic Exchange Interactions in Long Range Ordered Diluted Organometallic Semiconductors, NAVIEN RAWAT, LANE MANNING, MADALINA FURIS, University of Vermont — Exchange interactions in diluted organometallic crystalline thin films of Phthalocyanines made of a mixture of organo-soluble derivatives of metal-free (H₂Pc) molecule and MnPc is investigated. The tuning of optical and magnetic properties in organometallics is driven by their emergence in optoelectronic applications involving flexible electronics. Thin films with metal to metal-free Pc ratios ranging from 1: 1 to 1:10 were fabricated using solution processing that produces macroscopic grains. In the case of Mn-Pc, our previous measurements showed enhanced hybridization of ligand π-electronic states with the Mn 3d-orbitals as well as indirect exchange interaction similar to that of RKKY type exchange. The evolution of Zeeman splitting of specific MCD-active states resulted in enhanced effective π-electrons g-factors, analogous to diluted magnetic semiconductors (DMS) systems. Recent Variable temperature Magnetic Circular Dichroism (VTMH-MCD) measurements has now revealed that the exchange interaction is Antiferromagnetic. Recent MCD data for mixed derivatives will be presented along with their temperature dependence that further probes this exchange interaction.

3:30PM D31.00004 ABSTRACT WITHDRAWN —

3:42PM D31.00005 Strong Spin-Exchange Interactions in Magnetically Doped Colloidal Nanocrystals, WILLIAM RICE, WENYONG LIU, THOMAS BAKER, GEN CHEN, JEFFREY PIETRYGA, VICTOR KLIMOV, SCOTT CROOKER, Los Alamos National Lab — Using magnetic circular dichroism, magneto-photoluminescence, and time-resolved Faraday rotation measurements, we study the spin-exchange interactions between excitons and embedded magnetic ions in Mn-doped colloidal nanocrystals. In contrast to undoped nanocrystals, the Mn-doped nanocrystals show giant Zeeman splittings of the nanocrystal conduction and valence bands and a very rapid dephasing of the optically created excitons (two orders of magnitude faster than undoped CdSe). Although the exciton spin coherence is short (less than 10 ps), the spin−d exchange interaction between the exciton and Mn moments induces a long-lived precession of the Mn²⁺ paramagnetic moments that persists out to nanosecond timescales. We study this induced Mn precession as a function of nanocrystal size, Mn doping density, temperature, and magnetic field.

3:54PM D31.00006 Driven magnetic patterns in quantum dots, ALEX MATOS-ABIAIGUE, JAMES PIENTKA, JONG E. HAN, IGOR ZUTIC, University at Buffalo-SUNY — We theoretically investigate the response of magnetic impurities in a quantum dot driven by a dc current. A bias voltage applied between the leads attached to the quantum dot drives the current. In addition, an external gate is used to tune the energy levels of the dot. The steady state magnetic configuration and current are self-consistently determined by using the non-equilibrium Green function formalism. The results reveal the emergence of different magnetization patterns in dependence on the bias and gate voltages for various sets of system parameters (number of magnetic impurities, tunneling coupling between dot and leads, and size of the dot). Under certain conditions and as the result of correlations between current and local magnetization, signatures of magnetic patterns formation can be observed in the I-V characteristics of the quantum dot. This allows for the design and characterization of magnetic patterns in quantum dots by electrical means.

4:06PM D31.00007 Ground State Properties of Magnetic Quantum Dots with Multiple Occupancies, JAMES PIENTKA, Saint Bonaventure University, IGOR ZUTIC, JONG HAN, University at Buffalo — Semiconductor quantum dots doped with magnetic impurities provide an intriguing opportunity to explore the interplay of confinement, Coulomb and exchange interactions [1,2]. Using exact diagonalization we study the ground state properties of a magnetic quantum dot with multiple occupancies. We show that the ground state not only depends on the orientation of the carrier and impurity spins, but is also very sensitive to the position of the magnetic impurities in the quantum dot. Our results reveal magnetic frustration and strongly correlated states, qualitatively different from the Fermi liquid behavior. [1] J. M. Pietkia R. Oszwaldowski, A. G. Petukhov, J. E. Han, and I. Zutic, Phys. Rev. B 86, 161403(R) (2012).[2] R. Oszwaldowski, P. Stano, A. G. Petukhov, and I. Zutic, Phys. Rev. B 86, 201408(R)(2012).

1Supported by DOE-BES, US ONR, and NSF-DMR.
4:18PM D31.00008 Hole States and Magnetic Anisotropy of a Quantum Dot^{1} DAN REDERTH, HARI CHAPAGAIN, RAFAL OSZWALDOWSKI, SDSMT Physics, A.G. PETUKHOV, NASA Ames Research Center — In the era of spin-based advanced semiconductor materials^{1}, spin can be used for the control of quantum devices based on quantum dots (QDs)^{2}. To facilitate the control of the electronic and magnetic properties, magnetic ions can be incorporated in the QDs. We study the properties of such a magnetic II-VI QD charged with one hole. To account for the complex structure of valence band, we propose a method based on the Luttinger-Kohn Hamiltonian. With a robust numerical algorithm suitable for any QD geometry, magnetic properties can be incorporated in the QDs. We study the interplay of quantum confinement and magnetic anisotropy of a flat QD. We go beyond the virtual crystal approximation^{3}, our model also allows for position-dependent direction of magnetization. We discuss the differences between our and previous results, as well as the effects of temperature (mean-field approximation), and of the spin-orbit split-off band. We also discuss possible fluctuations of magnetization in QDs. Supported by DOE DE-SC00004890. 


^{2} DoE

4:30PM D31.00009 Nanostructured lithium oxide-hematite magnetic semiconductor^{1} MONICA SORESCU, BASILII BUSHUNOW, Duquesne University, LUCIAN DIAMANDESCU, FELICIA TOLEA, MIHAELA VALEANU, National Institute of Materials Physics Bucharest, TIANHONG XU, Duquesne University — The study aims at exploring the formation of magnetic oxide semiconductors at the nanoscale, which is of crucial importance for catalysis, sensing and electrochemical applications. xLi2O-(1-x)alpha-Fe2O3 nanoparticles systems were successfully synthesized by mechanochemical activation of Li2O and alpha-Fe2O3 mixtures for 0.12 hours of ball milling time. X-ray powder diffraction (XRD), Mossbauer spectroscopy and magnetic measurements were used to study the phase evolution. Rietveld refinement of the XRD patterns yielded the values of the particle size as function of composition and milling times. The Mossbauer studies showed that the spectrum of the mechanochemically activated composites evolved from a sextet for hematite to sextets and a doublet upon duration of the milling process with lithium oxide. Magnetic measurements recorded at 5 K to room temperature (RT) in an applied magnetic field of 50,000 Oe showed that the magnetization of the milled samples is larger at low temperatures than at RT and increases with decreasing particle size. Zero field cooling measurements made possible the determination of the blocking temperatures of the specimens as function of ball milling time and evidenced the occurrence of superparamagnetism in the studied samples.

^{1} NSF-DMR-0854794

4:42PM D31.00010 ABSTRACT WITHDRAWN —

4:54PM D31.00011 Onset of spin polarization degeneracy in quantum wires ALFREDO SANCHEZ, JEAN-PIERRE LEBURTON, Univ of Illinois - Urbana — We report on the emergence of complex spin-polarized regimes arising from electron-electron interactions in quantum wires by using a three-dimensional unrestricted Hartree-Fock approach. We predict three distinct spin-polarized configurations in the presence of a magnetic field, two of which appear only above a concentration threshold. In the limit of vanishing magnetic fields, the electron system evolves into a pair of symmetric and degenerate regimes, indicating spontaneous spin polarization. The value of the concentration threshold and the energy of the polarized states all depend on the transverse dimensions of the wire. In particular, spontaneous spin polarization is suppressed if the wire cross section is highly asymmetric. Our investigations on spin-related effects are of significant relevance for spintronics applications and for the study of the 0.7 conductance anomaly in semiconductor quantum point contacts.

5:06PM D31.00012 π–d Electron Coupling in Excited State in Organic-Magnetic Nanocomposites, MINGXING LI, Univ of Tennessee, Knoxville, MIN WANG, University of Massachusetts, LEI HE, YU-CHE HSIAO, QING LIU, HENGXING XU, Univ of Tennessee, Knoxville, LONG Y. CHIANG, University of Massachusetts, LOON-SENG TAN, AUGUSTINE URBAS, Wright-Patterson Air Force Base, BIN HU, Univ of Tennessee, Knoxville — The coupling between π electron in organic semiconducting materials and d electron in ferromagnetic materials presents an important mechanism, namely π-d electron coupling, to develop magneto-optical and magneto-electronic properties. The π-d electron coupling has been heavily studied in ground state. This presentation reports the π-d electron coupling in excited state by combining intramolecular charge-transfer dipoles in semiconducting π electron system with spin dipoles from surface-modified magnetic nanoparticles based on organic-magnetic nanocomposites. Our magneto-dielectric studies show that the excited state has a much stronger π-d electron coupling, as compared to ground state, under photoexcitation. We further study the coupling mechanism by analyzing the line-shape of magneto-dielectric response. We find that increasing the Coulomb interactions between electrical dipoles and spin dipoles causes a line-shape narrowing. On contrast, increasing the spin interactions between them leads to a line-shape broadening. As a result, we conclude that the long-range Coulomb interactions and short-range spin interactions are responsible for realizing strong π-d electron coupling in excited state in organic-magnetic nanocomposites.

5:18PM D31.00013 First-Principles study of tris(8-hydroxyquinoline)iron(III) molecules: A promising spin filter material^{1}, WEI JIANG, MIAO ZOU, ZHENHUI LIU, DALI SUN, Z. VALY VARDENY, FENG LIU, University of Utah, FENG LIU’S GROUP TEAM, Z. VALY. VARDENY’S GROUP TEAM — Using first-principles calculations, we have systematically investigated the structural, electronic, and magnetic properties of face-meridional tris (8-hydroxyquinoline)iron(III) (Feq_{3}) molecules, solvent-free Feq_{3} crystals and thin films. Our calculation results show that both Feq_{3} isomers have a high spin state of 5 \mu_B as the ground state when an on-site Hubbard-U term is included to treat the highly localized Fe 3d electrons, in agreement with experiment, while the standard DFT calculations produce a low spin Fe state of 1 \mu_B. Furthermore, the freestanding Feq_{3} films are found to be paramagnetic, but become Ferromagnetic (FM) within each layer when deposited on a NiFe substrate. This is induced by a strong anti-ferromagnetic (AFM) coupling between the first molecular layer and FM substrate. Also, an AFM coupling is found between the molecular layers. These findings suggest that Feq_{3} molecular films may serve as a promising spin filter material in spintronic devices.

^{1} This work is supported by National Science Foundation-Materials Research, Science & Engineering Center (NSF-MRSEC grant # DMR-1121252).

Monday, March 2, 2015 2:30PM - 5:18PM —
Session D32 GMAG DMP: Focus Session: Density Functional Theory of Bulk Complex Oxides
207B - Antonio Cammarata, Czech Technical University, Prague
2:30PM D32.00001 First-principles study of transport in SrTiO3
BURAK HIMMETOGLU, ANDERSON JANOTTI, HARTWIG PEELAERS, AUDRIUS ALKAUSKAS, CHRIS G. VAN DE WALL. University of California Santa Barbara — As a wide-band-gap semiconductor, SrTiO3 has attracted great interest for electronic device applications. While high electron mobilities of around 30,000 cm2 V−1 s−1 have been observed at low temperatures [1], room temperature mobilities are only on the order of a few cm2 V−1 s−1. These low mobilities pose a significant limitation for electronic device applications. In our work, we investigate the transport properties of n-doped SrTiO3 using first-principles calculations. We compute scattering of electrons with longitudinal optical modes in order to determine the scattering rates for the three conduction bands of SrTiO3. These scattering rates are invoked in Boltzmann transport integrals to calculate room-temperature transport coefficients. Our results indicate the strong impact of longitudinal optical phonon scattering as the main mechanism that leads to small electron mobilities at room temperature. In addition, our analysis provides valuable insights into designing high-mobility and high-thermopower materials, based on band-structure and strain engineering. Work supported by ONR and NSF. [1] J. Son, P. Moetakef, B. Jalan, O. Bierwagen, N. J. Wright, R. Engel-Herbert, and S. Stemmer, Nat. Mater. 9, 482 (2010)

2:42PM D32.00002 Many body effects on the formal charge state of 3d - Transition Metal Doped BaTiO3
SUBHASISH MANDAL, Department of Applied Physics, Yale University, New Haven, Connecticut & Geophysical Laboratory, Carnegie Institution of Washington, Washington D. C, R.E. COHEN, Geophysical Laboratory, Carnegie Institution of Washington, Washington D.C. USA & Dept of Earth Sciences, University College London, London, U.K, K. HAULE, Department of Physics, Rutgers University, Picataway, New Jersey, USA — Using density functional theory in combination with dynamical mean field theory in Mn doped BaTiO3, we find a different charge state and 3d - orbital occupations than obtained from either DFT or DFT+U. We find that the explicit treatment of many-body effects induced by the Hund’s rule coupling in Mn shows a donor charge state of Mn2+, instead of usual acceptor charge state of Mn4+ as is found in both DFT and DFT+U. The differences in electron density reveal that charge transfer due to strong Hubbard interactions is not sufficient to describe the electron correlations in transition metal doped ferroelectrics.

2:54PM D32.00003 Pressure induced iron spin state changes in MgGeO3 Perovskite and Post-perovskite
KANCHAN SARKAR, GAURAV SHUKLA, MEHMET TOPSAKAL, RENATA WENTZCOVITCH, University of Minnesota Twin cities — MgGeO3-perovskite is a low pressure analog of MgSiO3-perovskite, the main Earth forming phase, and is used to shed light on several phenomena that occur in MgSiO3, particularly the post-perovskite transition. As such, experimental investigations of spin state changes in Fe-bearing MgGeO3 might help to clarify some aspects of this phenomenon in MgSiO3. Using DFT+U calculations, we have investigated pressure induced spin state changes in Fe2+ and Fe3+ in MgGeO3 perovskite and post-perovskite and their effect on the post-perovskite transition. We uncover a direct relationship between average Fe-O bond-lengths and spin transition pressures in all cases. The effect of iron on the post-perovskite transitions in these phases can also be related to the average Fe-O bond lengths.

3:06PM D32.00004 ABSTRACT WITHDRAWN

3:42PM D32.00005 Oxygen vacancy induced localized state in rutile TiO2
DONGHAN SHIN, CHUNGWEI LIN, ALEXANDER A. DEMKOV, Univ of Texas, Austin — Titanium dioxide (TiO2) is as a promising material for several applications including photocatalysis, solar cells, spintronics and memory devices. Oxygen vacancies (OV) act as active sites for water dissociation and induce ferromagnetism in the bulk. Using density functional theory (DFT) and model Hamiltonian analysis, we investigate the localized states induced by an OV in rutile TiO2. We identify two classes of localized states: a hybrid and polaron states. The hybrid state is caused by the orbital overlap between three Ti atoms next to a vacancy and is mainly driven from the Ti eg orbitals. The polaron state is caused by the local lattice distortion and is mainly composed of one particular t2g orbital from a single Ti atom. The first principles calculation shows that the polaron state is energetically favored, and the tight-binding analysis reveals the underlying connection between the bulk band structure and the orbital character of the polaron. Their respective spin moments are deduced from the on-site electron correlation.

3:54PM D32.00006 The Correlation between Structure, Electronic Structure, and Shift Current in Visible-Light Ferroelectrics from First Principles
FENGONG WANG, STEVE YOUNG, FAN ZHENG, ILYA GRINBERG, ANDREW RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323, USA, SOLAR TEAM — Shift current, as a dominant mechanism of the bulk photovoltaic effect (BPVE), remains not well understood, especially in terms of its connection to material’s structure and electronic structure. This holds especially for the recently designed and demonstrated visible-light ferroelectric photovoltaics, Pb(Ni,Ti)O3−δ and (K,Ba)(Ni,Nb)O3−δ, that have great structural and electronic tunabilities. Here, we study the BPVE of the visible-light-absorbing ferroelectrics by calculating shift current from first principles. The effects of phase, lattice distortion, oxygen vacancy, cation arrangement, composition, and strain on BPVE are systematically studied. The wavefunction nature of the contributing electronic states dictates the eventual shift current yield, which can be significantly affected by the change of the O vacancy location, cation arrangement, and strain. Consequently, under broad spectrum illumination, the total current can be greatly enhanced by reducing the cancellation of counter propagating currents and by increasing the shift vector magnitude. This not only is helpful for understanding other photovoltaic mechanisms that relate to the motion of the photocurrent carriers, but also provides guidelines for the design of the photovoltaic converters.

4:06PM D32.00007 ABSTRACT WITHDRAWN

4:18PM D32.00008 First-Principles Physics of Nanocheckerboard Formation in ZnMnGaO Spinels
MORDECHAI KORNBLUTH, CHRIS MARIANETTI, Columbia University — Using first-principles calculations, we present the physics behind spinel nanocheckerboards in ZnMn4Ga2−xO4. Previously, experiments discovered a group of Mn-based spinels that spontaneously phase-separate into nanocheckerboards. We analyze their origin in the Jahn-Teller (JT) effect, which couples local atomic distortions to an electronic degeneracy (here, the eg manifold of the Mn d-orbital). Using density functional theory, we show that the interaction between cubic Mn-poor and tetragonal Mn-rich regions causes phase separation, but diffusion prevents the thermodynamic ground state of bulk separation. We demonstrate that the energetics and geometry mandate a nanocheckerboard configuration.
4:30PM D32.00009 A DFT+DMFT study of Orbital Physics in a Spin Orbital Lattice Coupled 2\(p\) Electron Mott System: KO\(_2\)  
MINJAE KIM, B.I. MIN, Department of Physics, Pohang University of Science and Technology, DEPARTMENT OF PHYSICS, POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY TEAM — We have investigated the temperature \(T\) - dependent orbital physics in a typical spin-orbital-lattice coupled 2\(p\) electron Mott system KO\(_2\), based on the electronic structures obtained by the dynamical mean-field theory as well as the density functional theory. KO\(_2\) consists of K\(^+\) cations and O\(_2^-\) molecule anions, and there are three electrons in the fourfold degenerate pi anti-bonding orbital of O\(_2^-\) anions. Hence, the orbital degeneracy occurs in a O\(_2^-\) anion with a magnetic moment. We have shown that KO\(_2\) exhibits the orbital fluctuation phenomenon at high \(T\) due to the degenerate pi anti-bonding orbital. Upon cooling, this orbital fluctuation is suppressed by the Jahn-Teller (JT) type crystal field with lowering of the crystal structure symmetry, and then the ferro-orbital (FO) ordering emerges at low \(T\). This FO ordering is compatible with the experimental antiferromagnetic spin order at low \(T\) in KO\(_2\). We suggest that the suppression of the orbital fluctuation in KO\(_2\) upon cooling is similar that in 3d transition-metal oxides such as LaVO\(_3\).

4:42PM D32.00010 Quantum Monte Carlo simulations of Ti4O7 Magnéli phase, ANOUAR BENALI, Argonne Natl Lab, LUKE SHULENBURGER, Sandia National Laboratories, JARON KROGEL, Oak Ridge National Laboratory, XIAOLIANG ZHONG, Argonne National Laboratory, PAUL KENT, Oak Ridge National Laboratory, OLLE HEINONEN, Argonne National Laboratory — Ti4O7 is ubiquitous in Ti-oxides. It has been extensively studied, both experimentally and theoretically in the past decades using multiple levels of theories, resulting in multiple diverse results. The latest DFT+SCF methods and state of the art HSE06 hybrid functionals even propose a new anti-ferromagnetic state at low temperature. Using Quantum Monte Carlo (QMC), as implemented in the QMCPACK simulation package, we investigated the electronic and magnetic properties of Ti4O7 at low (120K) and high (298K) temperatures and at different magnetic states. This research used resources of the Argonne Leadership Computing Facility at Argonne National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357. L.S, J.K and P.K were supported through Predictive Theory and Modeling for Materials and Chemical Science program by the Office of Basic Energy Sciences (BES), Department of Energy (DOE) Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

4:54PM D32.00011 Systematics of spin crossovers across the RECoO3 family\(^1\), MEHMET TOPSAKAL, CHRIS LEIGHTON, RENATA WENTZCOVITCH, Univ of Minn - Minneapolis — We have investigated structural and electronic properties of rare-earth cobaltites (RECoO3) using ab initio DFT + U calculations. A structurally consistent and self-consistent Hubbard U treatment is shown to be essential for the proper description of strongly correlated cobalt-d electrons. We successfully capture the experimentally observed structural variations and explain the trend in the spin transition temperature in cobalt across the RE series. We believe that Hubbard U values presented in this study will allow further predictive studies of RE cobaltites.

\(^1\) NSF/EAR 1319361, NSF/MRSEC DMR-0819885

5:06PM D32.00012 Spin-orbit effects in iridates via electronic structure calculations: effects of tension and dimensionality\(^1\), VICTOR PARDO, Universidade Santiago de Compostela, JOSE L. LADO, International Iberian Nanotechnology Laboratory — Ab initio calculations have been performed in 5d\(^5\)-electron-based oxides in the large spin-orbit coupling limit. Our work tries to analyze the effects of strain and dimensionality in the electronic structure properties of iridates with 1\(r^{4+}: 5d^5\) electronic configuration in order to understand the different set of properties these materials present: they can be either metals or insulators, e.g. We focus on studying how close to the fully ionic 1\(r_{eff}=1/2\) limit the system is by analyzing the 1\(L_z/S_z\) ratio. We observe that it varies continuously as a function of strain or pressure, changing drastically with relatively small variations. We also analyze what effects on the band structure accompany this variation. In order to do this, we needed to include a full non-collinearity in the calculation of spin-orbit interaction. We have explored SrIrO\(_3\), S\(_2\)IrO\(_4\), S\(_3\)IrO\(_2\)\(_2\), thin films of SrIrO\(_3\) so as to analyze the dimensionality effects and the structural implications.

\(^1\) We acknowledge support of the MINECO through the Ramon y Cajal Program, Xunta de Galicia through project no. EM2013/037 and the EU through the Marie Curie ITN “Spinograph”.

Monday, March 2, 2015 2:30PM - 3:54PM – Session D33 GPC DFD: Focus Session: The Physics of Climate II 208 - Juan Restrepo, Oregon State University

2:30PM D33.00001 Scattering and Absorption of E&M radiation by small particles-applications to study impact of biomass aerosols on climate\(^1\), SOLOMON BILILIGN, North Carolina A&T State University, Department of Physics, SUJEEET SINGH, MARC FIDDLER, DAMON SMITH, North Carolina A&T State University — The phenomena of scattering, absorption, and emission of light and other electromagnetic radiation by small particles are central to many science and engineering disciplines. Absorption of solar radiation by black carbon aerosols has a significant impact on the atmospheric energy distribution and hydrologic processes. By intercepting incoming solar radiation before it reaches the surface, aerosols heat the atmosphere and, in turn, cool the surface. The magnitude of the atmospheric forcing induced by anthropogenic absorbing aerosols, mainly black carbon (BC) emitted from biomass burning and combustion processes has been suggested to be comparable to the atmospheric forcing by all greenhouse gases (GHGs). Despite the global abundance of biomass burning for cooking, forests clearing for agriculture and wild fires, the optical properties of these aerosols have not been characterized at wide range of wavelengths. Our laboratory uses a combination of Cavity ring down spectroscopy and integrating nephelometry to measure optical properties of (extinction, absorption and scattering coefficients) of biomass aerosols. Preliminary results will be presented.

\(^1\) Supported by the Department of Defense under grant #W911NF-11-1-0188.
2:42PM D33.00002 Observations Determination of Surface Radiative Forcing by CO2 and CH41, WILLIAM COLLINS, Lawrence Berkeley Natl Lab and UC Berkeley, DANIEL FELDMAN, Lawrence Berkeley Natl Lab, JONATHAN GERO, University of Wisconsin-Madison, Space Science and Engineering Center, MARGARET TORN, Lawrence Berkeley Natl Lab and UC Berkeley, ELI MLAWER, Atmospheric and Environmental Research, Inc., TIMOTHY SHIPPERT, Pacific Northwest National Laboratory, Fundamental and Computational Sciences — Earth’s background atmospheric CO2 and CH4 concentrations have been steadily rising due to anthropogenic emissions, and these increases since 1750 have implications for the radiative balance of the Earth’s atmosphere. The physics governing how atmospheric CO2 and CH4, both well-mixed greenhouse gases (WMGHGs), influence atmospheric infrared energy balance, and thus climate, are well established, but the impact of recent atmospheric WMGHG trends on the surface energy balance has not been experimentally confirmed in the field. Using infrared WMGHG absorption bands and controlling for atmospheric temperature and water vapor, spectra from the DOE ARM Program’s Atmospheric Emitted Radiance Interferometers (AERI) yield the first direct observational evidence of the time-series of WMGHG surface radiative forcing directly attributable to recent increases in WMGHGs, in this case between 2000-2010. The time-series shows a secular trend of the radiative forcing from both CO2 and CH4. This data record provides the first comprehensive observational evidence of surface radiative forcing by WMGHGs, confirming theoretical predictions of the atmospheric greenhouse effect.

1 Office of Biological and Environmental Research, Department of Energy

2:54PM D33.00003 Interaction between carbon dioxide and coal: atomic-scale characteristics and electronic structures1, YINCDI LIU, SANWU WANG, Department of Physics and Engineering Physics, The University of Tulsa — Geologic sequestration of CO2 in unmineable coal seams has been suggested to mitigate the effect of the increasing of the atmospheric CO2 concentration on global warming. Extensive experimental studies have been performed for the injection of CO2 into coalbeds. However, the atomic-level mechanism for the interaction between CO2 and coal has not been fully explored. We report first-principles density-functional calculations and ab initio molecular dynamics simulations for the interaction between CO2 and the coal network. In particular, we report results about atomic-scale and electronic properties of the interaction. We also report a comparison with the interaction between CH4 and coal.

1 This research used the supercomputer resources at NERSC, of XSEDE, at TACC, and at the Tandy Supercomputing Center.

3:06PM D33.00004 Polar Oceanography, Arctic Sea Ice and Climate, MARY-LOUISE TIMMERMANS, Yale University — Intensive sampling from oceanographic moorings, shipboard measurements, and drifting autonomous buoy systems has brought new understanding to Arctic freshwater dynamics, ocean heat and mixing processes, circulation and eddies, and atmosphere-ice-ocean interactions. Observations indicate apparently rapid changes in the basin-scale freshwater distribution that have marked effects on Arctic stratification. Recent measurements support the idea that a strengthened stratification limits the vertical flux of deep-ocean heat. All ocean layers exhibit a rich mesoscale eddy field; eddies, with scales comparable to the Rossby Deformation Radius [O(10km)], transport water and heat over long distances and enhance ocean mixing. Measurements further reveal an active submesoscale flow field in the ocean surface layer. These upper-ocean features, having length scales of a few kilometers or less, are dynamically important in that they can impede surface-layer deepening and modify salt, and for they contribute to the surface ocean and adjacent sea-ice cover. This talk will review highlights of recent Arctic Ocean observational studies across a range of temporal and spatial scales, and illustrate advances in our understanding of ocean drivers of sea ice and climate change.

3:42PM D33.00005 Study of Aerosol Chemical Composition Based on Aerosol Optical Properties1, AUSTIN BERRY, RUDRA ARYAL, Eckerd College — We investigated the variation of aerosol absorption optical properties obtained from the CIMEL Sun-Photometer measurements over three years (2012-2014) at three AERONET sites GSFC; MD Science_Center and Tudor Hill, Bermuda. These sites were chosen based on the availability of data and locations that can receive different types of aerosols from land and ocean. These absorption properties, mainly the aerosol absorption angstrom exponent, were analyzed to examine the corresponding aerosol chemical composition. We observed that the retrieved aerosol absorption angstrom exponents on the two sites, GSFC and MD Science_Center, are near 1 (the theoretical value for black carbon) and with low single scattering albedo values during summer seasons indicating presence of black carbon. Strong variability of aerosol absorption properties were observed over Tudor Hill and will be analyzed based on the air mass embedded from ocean side and land side. We will also present the seasonal variability of these properties based on long-range air mass sources at these three sites.

1 Brent Holben, NASA GSFC, AERONET, Jon Rodriguez

Monday, March 2, 2015 2:30PM - 5:18PM –
Session D34 GSOFT: Gels and Complex Fluids 210A - George Thurston, Rochester Institute of Technology

2:30PM D34.00001 Diffusion of polyelectrolytes in polyelectrolyte gels, ANAND RAHALKAR, MURUGAPPAN MUTHUKUMAR, University of Massachusetts — Using dynamic light scattering, we have investigated the diffusion coefficient of sodium poly(styrene sulfonate) in a matrix of poly(acrylamide-co-acrylate) gels. The diffusion coefficient of the probe polyelectrolyte exhibits a crossover behavior from a particle-diffusion to entropic-barrier dominated diffusion, as the molecular weight is increased. The effect of electrostatics, by varying the charge density of the matrix, on probe diffusion constant will be presented.

2:42PM D34.00002 The origin of and conditions for clustering in fluids with competing interactions, RYAN JADRICH, JONATHAN BOLLINGER, THOMAS TRUSKETT, University of Texas at Austin — Fluids with competing short-range attractions and long-range repulsions exhibit a rich phase behavior characterized by intermediate range order (IRO), as quantified via the static structure factor. This phase behavior includes cluster formation depending upon density-controlled packing effects and the magnitude and range of the attractive and repulsive interactions. Such model systems mimic (to zeroth order) screened, charge-stabilized, aqueous colloidal dispersions of, e.g., proteins. We employ molecular dynamics simulations and integral equation theory to elucidate a more fundamental microscopic explanation for IRO-driven clustering. A simple criterion is identified that indicates when dynamic, amorphous clustering emerges in a polydisperse system, namely when the Ornstein-Zernike thermal correlation length in the system exceeds the repulsive potential tail range. Remarkably, this criterion also appears tightly correlated to crystalline cluster formation in a monodisperse system. Our new gauge is compared to another phenomenological condition for clustering which is when the IRO peak magnitude exceeds ∼ 2.7. Ramifications of crystalline versus amorphous clustering are discussed and potential ways of using our new measure in experiment are put forward.
2:54PM D34.00003 A single parameter description of aggregate morphologies in two-dimensions\footnote{This work was supported by the OIST Graduate University with subsidy funding from the Cabinet Office, Government of Japan} . TAMOGHNA DAS, MAHESH BANDI, OIST Graduate University — A morphological hierarchy of two-dimensional aggregates has been studied using molecular dynamics. Particulate aggregates resulting from the competition between short-range attraction and long-range repulsion show a transition from non-compact to compact to percolated ‘gel’ structures as the competition varies at a constant temperature and density. A three-dimensional (3D) parameter space controlling the competition is mapped to a single dimensionless parameter \( \Lambda \). A unique relation between the reduced second virial coefficient \( B_2^* \), computed for a large set of points in the 3D parameter space, and \( \Lambda \) provides strong support for the proposed description. The observed morphologies were further quantified using an entropic measure \( S_2 \) of positional information. A simple scaling relation between \( S_2 \) and \( \Lambda \) shows the promise of describing the static structures of aggregates in terms of geometry alone.

3:06PM D34.00004 Dynamics across the morphological transition in two-dimensional aggregates\footnote{This work was supported by the OIST Graduate University with subsidy funding from the Cabinet Office, Government of Japan} . MAHESH BANDI, TAMOGHNA DAS, OIST Graduate University — Microscopic dynamics of two-dimensional aggregates have been studied by analysing simulated particle trajectories generated by molecular dynamics. Tuning the competition between the short-range attraction and long-range repulsion in a particulate system at fixed temperature and density results in a continuous non-compact to compact morphological transition. The finite-size aggregates, obtained by very slow cooling, show long-time sub-diffusive behaviour irrespective of their morphologies. By analysing the relative displacement fluctuations of particles with respect to their nearest neighbours, non-compact aggregates can be attributed to bonding between particles while caging is found to be responsible for compact clusters. These dynamical mechanisms are further illustrated by the self-displacement fluctuation of particles which show a continuous change from power-law to exponential behaviour across the non-compact to compact transition.

3:18PM D34.00005 1- and 2-particle Micro rheology of Hyaluronic Acid \footnote{NSF IGERT Fellowship Award No. 0801471} . AUSTIN SAGAN, SARAH KEARNS, DAVID ROSS, MOUNITA DAS, GEORGE THURSTON, SCOTT FRANKLIN, Rochester Inst of Tech — Hyaluronic acid (also called HA or Hyaluronan) is a high molecular weight polysaccharide ubiquitous in the extracellular matrix of soft tissue such as cartilage, skin, the eye’s vitreous gel and synovial fluid. It has been shown to play an important role in mechanotransduction, cell migration and proliferation, and in tissue morphodynamics. We present a confocal micro rheology study of hyaluronic acid of varying concentrations. The mean square displacement (MSD) of sub-micron colloidal tracer particles is tracked in two dimensions and shows a transition from diffusive motion at low concentrations to small-time trapping by the protein network as the concentration increases. Correlations between particle motion can be used to determine an effective mean-squared displacement which deviates from the single-particle MSD as the fluid becomes less homogenous. The real and effective mean-squared displacements are used to probe the local and space-averaged frequency dependent rheological properties of the fluid as the concentration changes.

3:30PM D34.00006 A Rate-Dependent Shear Transformation Zone Model of Shear Band Formation During Flow\footnote{This work was supported by the OIST Graduate University with subsidy funding from the Cabinet Office, Government of Japan} . ADAM R. HINKLE, MICHAEL L. FALK, Johns Hopkins University — Recent shear-experiments of carbopol gels have revealed the formation of a transient shear band before reaching the steady-state characterized by homogeneous flow. Analysis of this phenomenon using a rate-dependent effective temperature in the shear transformation zone (STZ) theory reveals that the observed fluidization proceeds via two distinct processes: A shear band initiates and broadens via disordering at the interface of the band. This is accompanied by spatially homogeneous fluidization outside of the shear band where the disorder of the gel grows uniformly. Experimental data are used to parameterize the STZ theory, and direct, quantitative comparison is made to measurements of the structural evolution of the gel.

3:42PM D34.00007 Effect of short range hydrodynamic on bimodal colloidal gel systems , ARMAR BOROMAND, SAFA JAMALI, JOAO MAIA, Case Western Reserve University — Colloidal Gels and disordered arrested systems has been studied extensively during the past decades. Although they have found their place in multiple industries such as cosmetic, food and so on, their physical principals are still far beyond being understood. The interplay between different types of interactions from quantum scale, Van der Waals interaction, to short range interactions, depletion interaction, and long range interactions such as electrostatic double layer makes this systems challenging from simulation point of view. Many authors have implemented different simulation techniques such as molecular dynamics (MD) and Browninan dynamics (BD) to capture better picture during phase separation of colloidal system with short range attractive force. However, BD is not capable to include multi-body hydrodynamic interaction and MD is limited by the computational resources and is limited to short time and length scales. In this presentation we used Core-modified dissipative particle dynamics (CM-DPD) with modified depletion potential, as a coarse-grain model, to address the gel formation process in short ranged-attractive colloidal suspensions. Due to the possibility to include and separate short and long ranged-hydrodynamic forces in this method we studied the effect of each of those forces on the final morphology and report one of the controversial question in this field on the effect of hydrodynamics on the cluster formation process on bimodal, soft-hard colloidal mixtures.

3:54PM D34.00008 Transient yield in reversible colloidal gels: a micro-mechanical perspective. LILIAN JOHNSON, Cornell University, BENJAMIN LANDRUM, WILLIAM RUSSEL, Princeton University, ROSEANNA ZIA, Cornell University — We study the nonlinear response rheology of colloidal gels via large-scale dynamic simulation, with a view toward understanding the micro-mechanical origins of the transition from solid-like to liquid-like behavior during flow startup, and post-cessation relaxation. Such materials often exhibit an overshoot in the stress response during startup, but the underlying microstructural origin of this behavior remains unclear. The gels studied here comprise Browninan particles interacting via hard-sphere repulsion and short-range attraction of strength of \( O(\xi T) \) that leads to formation of a bi-continuous network. The relatively weak bonds allow the network to restructure over time; our recent work defines the structural evolution and dynamics of such coarsening, and its impact on linear-response rheology. Here we investigate the role of particle attractions and evolving structure on the nonlinear response of the gel. Upon startup of an imposed strain rate, the transition from rest to steady flow is characterized by one or more “overshoots” in the shear stress. Experimental studies, in which the overshoots depend on gel age, strain rate, volume fraction, and attraction strength, suggest that the underlying microstructural origin is a two-step process of cage breaking and bond breaking. However, our detailed studies of the microstructural evolution during startup challenge this view. We present a new model of stress development, relaxation, and memory in reversible colloidal gels in which the ongoing age-coarsening process plays a qualitatively new role.
4:06PM D34.00009 Delayed yield in reversible colloidal gels: a micro-mechanical perspective. ROSEANNA N. ZIA, Cornell University, BENJAMIN J. LANDRUM, Cornell University and Princeton University, WILLIAM B. RUSSEL, Princeton University — We study via dynamic simulation the nonlinear response of a reversible colloidal gel undergoing deformation under applied stress, with a view toward elucidating mechanisms of macroscopic yield at the level of particle dynamics. Under shear, such gels may flow then regain solidlike behavior upon removal of the stress. The transition from solidlike to liquidlike behavior is a yielding process that is not instantaneous but rather occurs after a finite delay. The delay length decreases as stress increases, but the underlying microstructural origin is not clear. Recent experiments reveal two regimes, suggesting multiple yield mechanisms. Theories advanced to link gel structure to rheology aim to predict the ultimate state of a gel under an applied load. While these hypothesize a competition between bond breakage and reconnection rates, no such particle-scale dynamics have been directly observed, and it is not clear these theories reconcile with ongoing structural evolution. To study these behaviors, we conduct large-scale dynamic simulation to model structural evolution and particle transport in colloidal gels subjected to a step stress. A range of volume fraction, attraction strength, and stress is studied, with detailed connection between macroscopic response, microstructure, and particle dynamics.

4:18PM D34.00010 Using dissipative particle dynamics to model micromechanics of responsive hydrogels1. ALEXANDER ALEXEEV, SVETOSLAV NIKOLOV, ALBERTO FERNANDEZ DE LAS NIEVES, Georgia Institute of Technology — The ability of responsive hydrogels to undergo complex and reversible shape transformations in response to external stimuli such as temperature, magnetic/electric fields, pH levels, and light intensity has made them the material of choice for tissue scaffolding, drug delivery, bio-adhesive, bio-sensing, and micro-sorting applications. The complex micromechanics and kinetics of these responsive networks however, currently hinders developments in the aforementioned areas. In order to better understand the mechanical properties of these systems and how they change during the volume transition we have developed a dissipative particle dynamics (DPD) model for responsive polymer networks. We use this model to examine the impact of the Flory-Huggins parameter on the bulk and shear modul. In this fashion we evaluate how environmental factors can affect the micromechanical properties of these networks.

4:30PM D34.00011 Separation and concentration of protein and microgel dispersions, RAFAEL ROA, GERHARD NAE GELE, Forschungszentrum Juelich — Membrane ultrafiltration is a pressure driven process where Brownian particles, such as small colloids or nanoparticles, are concentrated. This process is highly important for the separation and enrichement of protein and microgel dispersions, where convective-diffusive particle transport determines the permeate flux. The efficiency of the separation process is thus strongly dependent on particle hydrodynamic structure and boundary conditions, membrane properties, and particle interactions. We calculate the concentration polarization layer and the permeate flux at different operating conditions for cross-flow ultrafiltration of BSA proteins and for non-ionic and microgel dispersions. We show that the proper specification of the concentration dependent dispersion transport properties and the inclusion of microgel permeability have a significant effect on the filtration behavior on concentrated systems.

4:42PM D34.00012 Relaxation Mode Analysis and Scale-Dependent Energy Landscape Statistics in Liquids, ZHIKUN CAI, YANG ZHANG, Univ of Illinois - Urbana — In contrast to the prevailing focus on short-lived classical phonon modes in liquids, we propose a classical treatment of the relaxation modes in liquids under a framework analogous to the normal mode analysis in solids. Our relaxation mode analysis is built upon the experimentally measurable two-point density-density correlation function (e.g. using quasi-elastic and inelastic scattering experiments). We show in the Laplace-inverted relaxation frequency z-domain, the eigen relaxation modes are readily decoupled. From here, important statistics of the scale-dependent activation energy in the energy landscape as well as the scale-dependent relaxation time distribution function can be obtained. We first demonstrate this approach in the case of supercooled liquids when dynamic heterogeneity emerges in the landscape-influenced regime. And then we show, using this framework, we are able to extract the scale-dependent energy landscape statistics from neutron scattering measurements.

5:44PM D34.00013 Gelation and glass transition of particles with short-range attraction induced by adsorbing microgel1. GUANGCUI YUAN, JUNJUAN LUO, CHARLES C. HAN, Institute of Chemistry, Chinese Academy of Sciences — Mixed suspensions of large hard polystyrene microsphere and small poly(N-isopropylacrylamide) microgel is used as model systems to investigate the static and viscoelastic properties of suspensions which go through liquid to gel and to glass transitions. The microgels cause short-range attraction between microspheres through bridging and depletion mechanism whose strength can be tuned by the microgel concentration. Baxter’s sticky hard-sphere model is used to extract the effective inter-microsphere interaction introduced by bridging or depletion of microgels despite the fact that the physical mechanisms of bridging attraction and depletion attraction are different at a molecular level. A new state diagram of gelation and even of glass transition was constructed by taking the bridges as a short-ranged attractive interaction. With the help of the well-defined bridging bonds, some controversies regarding to the interference between two origins for ergodic to non-ergodic transition in condensed system, i.e. cage effect and bond effect, were clarified.

5:06PM D34.00014 Osmotic Pressure in Ionic Microgel Dispersions, ALAN R. DENTON, QIYUN TANG, Dept. of Physics, North Dakota State University — Microgels are microscopic gel particles, typically 10-1000 nm in size, that are swollen by a solvent. Hollow microgels (microcapsules) can encapsulate cargo, such as dye molecules or drugs, in their solvent-filled cavities. Their sensitive response to environmental conditions (e.g., temperature, pH) and influence on flow properties suit microgels to widespread applications in the chemical, pharmaceutical, food, and consumer care industries. When dispersed in water, polyelectrolyte gels become charged through dissociation of counterions. The electrostatic contribution to the osmotic pressure inside an ionic microgel and the electrostatic contribution to the osmotic pressure. Within a coarse-grained one-component model, we further chart the limits of the cell model for salty dispersions.

1Support from NSF CAREER Award (DMR-1255288) is gratefully acknowledged.

2This work is supported by the National Basic Research Program of China (973 Program, 2012CB821503).

3This work was supported by the National Science Foundation under Grant No. DMR-1106331.

Monday, March 2, 2015 2:30PM - 5:30PM – Session D36 DCOMP: Invited Session: Materials for Energy: Predicting the Properties of Solid/Electrolyte Interfaces from First Principles 211 - Giulia Galli, University of Chicago
2:30PM D36.00001 Electronic properties of semiconductor-water interfaces: Predictions from \textit{ab-initio} molecular dynamics and many-body perturbation theory\textsuperscript{1}. TUAN ANH PHAM, Lawrence Livermore National Laboratory — Photoelectrochemical cells offer a promising avenue for hydrogen production from water and sunlight. The efficiency of these devices depends on the electronic structure of the interface between the photoelectrode and liquid water, including the alignment between the semiconductor band edges and the water redox potential. In this talk, we will present the results of first principles calculations of semiconductor-water interfaces that are obtained with a combination of density functional theory (DFT)-based molecular dynamics simulations and many-body perturbation theory (MBPT). First, we will discuss the development of an MBPT approach that is aimed at improving the efficiency and accuracy of existing methodologies while still being applicable to complex heterogeneous interfaces consisting of hundreds of atoms \cite{5,6}. We will then present studies of the electronic structure of liquid water and aqueous solutions using MBPT, which represent an essential step in establishing a quantitative framework for computing the energy alignment at semiconductor-water interfaces \cite{4,5-5}. Finally, using a combination of DFT-based molecular dynamics simulations and MBPT, we will describe the relationship between interfacial structure, electronic properties of semiconductors and their reactivity in aqueous solutions through a number of examples, including functionalized Si surfaces \cite{6} and GaP/InP surfaces in contact with liquid water.

\textsuperscript{1}T.A.P was supported by the U.S. Department of Energy at the Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and by the Lawrence Fellowship Program.

3:06PM D36.00002 First-principles simulations of charge storage at electrochemical interfaces in supercapacitors. BRANDON WOOD, Lawrence Livermore National Laboratory — Supercapacitors store charge via polarization at the electrode-electrolyte interface. Many models of interfacial charge storage focus on the formation of the electric double layer (EDL) in the electrolyte, but it is often assumed that in the electrode, a shift in the Fermi level is the only notable response to interface polarization. In reality, the presence of the interface impacts the fundamental properties of both the electrode and the electrolyte, often in complex and nontrivial ways that are difficult to capture using simple models. I will discuss how including an applied bias potential in \textit{ab initio} first-principles simulations allows one to directly simulate the process of charge storage at the electrode-electrolyte interface, and thereby to unravel the interplay between the electrode and the electrolyte. I will show how these more complex treatments lead to improved descriptions of intrinsic quantum and EDL capacitance contributions in graphene-based supercapacitors, which can be used to suggest engineering strategies for improved electrode materials. I will also discuss how combining theory with in operando X-ray spectroscopy can give insights into nanoscale chemical changes and mesoscale morphological changes in electrodes during charging. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344.

3:42PM D36.00003 Ab initio joint density-functional theory of solvated electrodes, with model and explicit solvation\textsuperscript{1}. TOMAS ARIAS, Cornell University — First-principles guided design of improved electrochemical systems has the potential for great societal impact by making non-fossil-fuel systems economically viable. Potential applications include improvements in fuel-cells, solar-fuel systems ("artificial photosynthesis"), supercapacitors and batteries. Economical fuel-cell systems would enable zero-carbon footprint transportation, solar-fuel systems would directly convert sunlight and water into hydrogen fuel for such fuel-cell vehicles, supercapacitors would enable nearly full recovery of energy lost during vehicle braking thus extending electric vehicle range and acceptance, and economical high-capacity batteries would be central to mitigating the indeterminacy in GaN and SrTiO\textsubscript{3}. MARIVI FERNANDEZ-SERRA, Physics & Astronomy department, Stony Brook University. Stony Brook, NY — No abstract available.

\textsuperscript{1}Supported as a part of the Energy Materials Center at Cornell, an Energy Frontier Research Center funded by DOE/BES (award de-sc0001086) and by the New York State Division of Science, Technology and Innovation (NYSTAR, award 60923).

4:18PM D36.00004 Link between photocatalytic water splitting efficiency and surface acidity in GaN and SrTiO\textsubscript{3}. MARIVI FERNANDEZ-SERRA, Physics & Astronomy department, Stony Brook University. Stony Brook, NY — No abstract available.

oscillations are found to proceed with different phases for the two components of the scattered light. Satisfactory agreement is found between the experimental frequency comb scattering. The spectrum exhibits predicted features such as multiple sidebands when the pulse duration is long enough. In addition, Rabi and second-order correlation function of the scattered light. In particular, the coherently and incoherently scattered light can be distinguished by virtue of the investigated theoretically. By using a high resolution Fabry-Perot interferometer and a stabilized mode-locked laser source we were able to measure the spectrum scattered near-resonantly by a quantum dot under excitation by a periodically-pulsed laser, i.e., a frequency comb. Even though the scattered light spectrum shifts, combined with tunneling of charges from the QD to nearby defects, provide an explanation of the bunching observed in the correlations. Photoluminescence excitation spectra indicate that the QD experiences discrete spectral shifts due to changes in the local charge environment. These spectral charge carriers introduced by a HeNe laser. Second-order correlation measurements show bunching behavior that changes with HeNe laser power. Resonant photoluminescence excitation spectra indicate that the QD experiences discrete spectral shifts due to changes in the local charge environment. These spectral shifts, combined with tunneling of charges from the QD to nearby defects, provide an explanation of the bunching observed in the correlations.

In quantum dots (QDs), optical fields are an attractive medium for qubit manipulation and readout. The entanglement between a QD spin qubit and an emitted photonic qubit allows for the transport of quantum information between distant quantum memories via decoherence resistant photon channels. I will present recent experimental work showing the entanglement between a single electron spin confined to an InAs QD and its spontaneously emitted photon. This entanglement is significant for the further development of quantum information technologies using QDs and forms the foundation of on-chip technologies using photonic crystal pathways. In addition, I will discuss on-going work on teleportation of information from a single photon generated in a spontaneous parametric down conversion (SPDC) process to a QD spin through intermediate interference between the SPDC photon and the dot’s emitted photon. The ability to integrate two quantum information platforms is not only exciting in its own right, but this technique could allow for an entanglement swapping bridge between other matter-qubit (ions, NV centers, etc.) based quantum memories.

This work is funded by NSF, ARO, AFOSR, ONR and DARPA.

**3:06PM D37.00002 ABSTRACT WITHDRAWN**

**3:18PM D37.00003 Photon Statistics of Quantum Dot Resonance Fluorescence under the Influence of a Non-Resonant Laser**. DISHENG CHEN, GARY LANDER, CABOT ZABRISKIE, EDWARD FLAGG, West Virginia University — We study the statistical behavior of resonance fluorescence from self-assembled InAs quantum dots (QDs) as a function of the density of free charge carriers introduced by a HeNe laser. Second-order correlation measurements show bunching behavior that changes with HeNe laser power. Resonant photoluminescence excitation spectra indicate that the QD experiences discrete spectral shifts due to changes in the local charge environment. These spectral shifts, combined with tunneling of charges from the QD to nearby defects, provide an explanation of the bunching observed in the correlations.

**3:30PM D37.00004 Resonance Fluorescence Spectrum from a Quantum Dot Driven by a Periodically-Pulsed Laser**. KUMARSIRI KONTHASINGHE, MANOJ PEIRIS, BENJAMIN PETRAK, University of South Florida, YING YU, ZHICUAN NIU, Chinese Academy of Sciences, ANDREAS MULLER, University of South Florida — We report the measurement of the spectrum of the light scattered near-resonantly by a quantum dot under excitation by a periodically-pulsed laser, i.e., a frequency comb. Even though the scattered light spectrum under monochromatic excitation, the “Mollow triplet”, is well known, the resonance fluorescence spectrum under pulsed excitation has so far only been investigated theoretically. By using a high resolution Fabry-Perot interferometer and a stabilized mode-locked laser source we were able to measure the spectrum and second-order correlation function of the scattered light. In particular, the coherently and incoherently scattered light can be distinguished by virtue of the frequency comb scattering. The spectrum exhibits predicted features such as multiple sidebands when the pulse duration is long enough. In addition, Rabi oscillations are found to proceed with different phases for the two components of the scattered light. Satisfactory agreement is found between the experimental data and simulations when the effect of spectral diffusion is included.

**3:42PM D37.00005 Magneto-photoluminescence study of InAs quantum dots emitting at 1150nm**. LAURA KINNISCHTZKE, YIMING LAI, ANTONIO BADOLATO, NICK VAMIVAKAS, Univ of Rochester — Self-assembled InAs/GaAs quantum dots are frequently designed to emit light in the range of 920-980nm, and the spectroscopic characterization of neutral and charged excitons in this range is well understood. We study the magnetic field dependence of low-temperature photoluminescence from InAs self-assembled quantum dots emitting close to 1 eV (1150 nm). The dots are incorporated into a field-effect device to map the fine structure of charged and neutral excitons using magneto-photoluminescence spectroscopy in the Faraday geometry up to 7 Tesla. Previously developed models of Coulomb blockade and fine structure in InAs/GaAs QDs can be extended to measure the effective g-factor of the exciton complexes in these lower-energy quantum dots.

We acknowledge support from NSF grant no. DMR-1309734.

**3:54PM D37.00006 Dynamic nuclear polarization in self-assembled quantum dot by quadrupole effect**. BAO LIU, PING WANG, WEN YANG, Beijing Computational Science Research Center — We apply the recently developed theory of dynamic nuclear polarization to analyze a new nuclear polarization mechanism assisted by quadrupole interaction. This mechanism was proposed to explain a series of experimental observations in a self-assembled quantum dot. We find that although the steady state nuclear polarization agrees with previous works, the rate at which the nuclear spins are polarized is smaller by two orders of magnitude.
4:06PM D37.00007 Long-range two-qubit gate between nuclear spins in diamond mediated via an optical cavity . ADRIAN AUPER, GUIDO BURKARD, Department of Physics, University of Konstanz, Germany — Nitrogen-vacancy (NV) centers in diamond represent a promising possibility for a solid-state based realization of a qubit due to their excellent electron- and nuclear-spin coherence properties. Single-qubit gates for the nitrogen nuclear spin have been implemented [1]. Here, we extend an earlier proposal [2] for cavity-mediated coupling between NV electron spins and develop a scheme to implement a universal two-qubit gate between $^{14}$N or $^{15}$N nuclear spins. By virtually exciting a single NV center with an external laser field, a photon can be scattered into a surrounding cavity; we show that this process depends on the spin state of the nitrogen nucleus. For the two-qubit gate, we consider two NV centers coupled to a common cavity mode and each being excited individually. Virtual cavity excitation can then mediate an effective interaction between the NV nuclear spin qubits, generating a controlled-Z gate. Operation times for the gate implementation are found to be below 100 nanoseconds, which is orders of magnitude faster than the decoherence time of nuclear spin qubits in diamond.


4:18PM D37.00008 Quantum error correction with nuclear spins in diamond . TIM HUGO TAMINIAU, QuTech, Delft University of Technology, JULIA CRAMER, M. A. ROL, NORBERT KALB, Kavli Institute of Nanoscience, Delft University of Technology, V. V. DOBROVITSKI, Ames Laboratory and Iowa State University, RONALD HANSON, Kavli Institute of Nanoscience, Delft University of Technology — Quantum error correction is essential for large-scale quantum information processing. By encoding a quantum state in an entangled state of multiple qubits errors can be detected and corrected without obtaining information about the encoded state [1,2]. In this talk I will present quantum error correction based on spins in diamond. We used the electron spin of a nitrogen-vacancy centre to selectively initialize, control and read out multiple carbon-13 nuclear spins in the surrounding spin bath [3]. With these spin we implemented a three-qubit quantum-error-correction protocol and demonstrated the robustness of the encoded state against applied errors [1]. Furthermore, I will discuss how working at cryogenic temperatures will make it possible to realize error correction based on projective multi-qubit parity measurements [4], as envisioned in most modern error correction codes.


4:30PM D37.00009 The spin state depolarization induced by charge state conversion of Nitrogen Vacancy center in diamond . XIANGDONG CHEN, Univ of Sci & Tech of China, CHANGLING ZOU TEAM, LEIMING ZHOU TEAM, FANGWEN SUN TEAM — The negatively charged nitrogen vacancy center (NV$^-$) in diamond possesses the optically polarized electron spin state, which enables it to be used for quantum computation and metrology. In this work, we showed the depolarization of NV$^-$ electron spin state induced by charge state conversion. Both the polarization and depolarization of spin state exist during the two-photon charge state conversion process. The fidelity of NV$^-$ spin state initialization is decreased with the laser power. Due to the charge state conversion induced spin state depolarization, the fluorescence intensity of NV center shows a decrease with high laser power. Our work provide the information to further understand the photon induced charge state conversion, and can help to optimize the application based on NV center.

4:42PM D37.00010 ABSTRACT MOVED TO L14.00013 –


5:06PM D37.00012 Control of multi-qubit nodes for diamond quantum networks . JULIA CRAMER, M. ADRIAAN ROL, NORBERT KALB, Kavli Institute of Nanoscience Delft, VIATCHESSLAV V. DOBROVITSKI, Ames Laboratory and Iowa State University, RONALD HANSON, TIM H. TAMINIAU, Kavli Institute of Nanoscience Delft — Quantum networks consisting of multiple connected nodes enable distributed quantum computation and secure quantum communication. Such networks require multi-qubit quantum registers that can be remotely linked. In this work we demonstrate initialization and control of multiple qubits in a nitrogen-vacancy (NV) node in diamond. We use the NV electron spin as an ancillary qubit to detect individual weakly coupled nuclear carbon-13 spins and construct high-fidelity quantum gates [1]. With these gates we show initialization, control and entanglement of multiple nuclear spins. Combined with projective measurements of the NV electron spin [2] and long-range entanglement through optical channels [3] at cryogenic temperatures, this work paves the way for communication between distant quantum nodes via ancillary qubits while preserving complex entangled states in quantum memories within the nodes.


5:18PM D37.00013 Quantum theory of nuclear spin dynamics in optically pumped diamond nitrogen-vacancy center . PING WANG, WEN YANG, Beijing Computational Science Research Center, Beijing 100084, China — We develop a microscopic theory for a variety of nuclear spin dynamics such as dephasing, relaxation, squeezing, and narrowing due to the hyperfine interaction with an optically pumped nitrogen vacancy center. The first-order result justifies the nonlinear Hamiltonian for nuclear spin squeezing [M. S. Rudner et al., Phys. Rev. Lett. 107, 206806 (2011)]. The second-order result provides a reasonable explanation to the experimentally observed 13C nuclear spin bath narrowing [E. Togan et al., Nature 478, 497 (2011)].
2:30PM D38.00001 Optimal spectrum estimation of density operators with alkaline-earth atoms , ALEXEY GORSHKOV, Joint Quantum Institute — The eigenspectrum $\vec{p} = (p_1, p_2, \ldots, p_n)$ of the density operator $\rho$ describing the state of a quantum system can be used to characterize the entanglement of this system with its environment. In the seminal paper [Phys. Rev. A 64, 052311 (2001)], Keyl and Werner present the optimal measurement scheme for inferring $\vec{p}$ given $n$ copies of an unknown state $\rho$. Since this measurement uses a highly entangled basis over the full joint state $\rho^n$ of all copies, it should naively be extremely difficult to implement in practice. In this talk, we give a simple experimental protocol to carry out the Keyl-Werner measurement for $\rho$ on the nuclear spin degrees of freedom of $n$ alkaline-earth atoms using standard Ramsey spectroscopy techniques.

3:06PM D38.00002 Testing Clauser-Horne-Shimony-Holt inequalities with observables with arbitrary spectrum , ANDREAS KETTERER, Laboratoire Matériaux et Phénomènes Quantiques, Sorbonne Paris Cité, Université Paris Diderot, CNRS UMR 7162, 75013 Paris, France — We report the measurement of the two-photon spectrum of the light scattered near-resonantly by a single InAs semiconductor quantum dot exposed to a monochromatic laser. In contrast to the ordinary (one-dimensional) one-photon spectrum, the two-photon spectrum represents the probability of emitting two photons with two different colors. It is obtained experimentally using a pair of frequency-tunable filters in a modified Hanbury-Brown and Twiss setup. We analyze the resulting two-dimensional maps for different parameters including the Rabi frequency, the laser detuning, and the filter bandwidth. We find excellent agreement with the theory of Del Valle et al. In particular, our measurements reveal the interferences of different decay paths to yield overall antibunched photon statistics while the individual filtered pathways may exhibit photon bunching, photon anti-bunching or near-Poisson statistics. We further evidence how the radiative cascade can proceed via virtual intermediate states giving rise to transitions previously termed “leapfrog transitions”. Highly nonclassical physics are seen, which can violate well-known classical inequalities such as the Cauchy-Schwarz inequality or Bells inequalities.

3:18PM D38.00003 Violation of Classical Inequalities in the Light Scattered by a Quantum Dot 1, MANOJ PEIRIS, BEN PETRAK, KUMARASIRI KONTHASINGHE, University of South Florida, YING YU, ZHICHAU NIIU, Chinese Academy of Sciences, ANDREAS MULLER, University of South Florida — We report the measurement of the two-photon spectrum of the light scattered near-resonantly by a single InAs semiconductor quantum dot exposed to a monochromatic laser. In contrast to the ordinary (one-dimensional) one-photon spectrum, the two-photon spectrum represents the probability of emitting two photons with two different colors. It is obtained experimentally using a pair of frequency-tunable filters in a modified Hanbury-Brown and Twiss setup. We analyze the resulting two-dimensional maps for different parameters including the Rabi frequency, the laser detuning, and the filter bandwidth. We find excellent agreement with the theory of Del Valle et al. In particular, our measurements reveal the interferences of different decay paths to yield overall antibunched photon statistics while the individual filtered pathways may exhibit photon bunching, photon anti-bunching or near-Poisson statistics. We further evidence how the radiative cascade can proceed via virtual intermediate states giving rise to transitions previously termed “leapfrog transitions”. Highly nonclassical physics are seen, which can violate well-known classical inequalities such as the Cauchy-Schwarz inequality or Bells inequalities.

1 NSF grant No. 1254324

3:30PM D38.00004 Classical Model for Measurements of an Entanglement Witness 1, BRIAN LA COUR, E.C. GEORGE SUDARSHAN, The University of Texas at Austin — We describe a classical model that may serve as an analog for joint and local measurements of an entanglement witness. The analogous experimental procedure and data analysis protocol of the model follow those of a previous experiment to measure an entanglement witness with polarized photons prepared in a mixed state [M. Barbieri et al., Phys. Rev. Lett. 91, 227901 (2003)]. Numerical simulations show excellent agreement with both experimental results and quantum mechanical predictions.

1 This work was supported by the Office of Naval Research under Grant No. N00014-14-1-0023 and an Internal Research and Development grant from Applied Research Laboratories, The University of Texas at Austin.

3:42PM D38.00005 Real-time adaptive quantum measurements on a single spin in diamond for sensing and quantum information protocols, MACHIEL BLOK, CRISTIAN BONATO, RONALD HANSON, Delft Univ of Tech — Real-time feedback based on quantum measurements is a crucial ingredient for many proposed quantum information and sensing technologies. Implementation requires high-fidelity measurements as well as fast electronics that perform the control operation. A single electron spin, associated with the Nitrogen-Vacancy defect in diamond, forms an excellent test bed for real-time feedback protocols, since it can be read out with high fidelity in a single shot using optical transitions and maintain coherences for long times. Here we demonstrate an adaptive phase estimation protocol that senses DC magnetic fields with very high precision. The magnetic field is measured with a Ramsey interferometry sequence which is repeated many times. When adjusting the parameters of the Ramsey sequence in real time based on the outcome of previous measurements, the sensitivity of our magnetometer shows scaling close to the fundamental Heisenberg limit ($\sim 1/N$) as the number of measurements $N$ is increased.

3:54PM D38.00006 Joint estimation of phase and phase diffusion for quantum metrology, MIHAI VIDRIGHIN, Imperial College London, GAIA DONATI, MARCO GENONI, XIAN-MIN JIN, STEVEN KOLTHAMMER, MYUNSHIK KIM, ANIMESH DATTA, MARCO BARBIERI, IAN WALMSLEY, Oxford University — Phase estimation, at the heart of many quantum metrology and communication schemes, is affected by noise. We have investigated joint estimation of a phase and the amplitude of phase diffusion. The motivation is that the two parameters are not independent in first order. Using a single chiral molecule in a condensed phase environment, with low photon fluxes, we show that our protocol can outperform standard phase estimation, can work at the Heisenberg limit, and does not need adaptive phase control. We also prove by numerical simulations that our method holds for general states at small diffusion amplitudes.

4:06PM D38.00007 Noise-resilient quantum metrology for single-molecule spectroscopy with low light levels, FELIPE HERRERA, ALAN ASPURU-GUZIK, Department of Chemistry and Chemical Biology, Harvard University — Continuous observation of biological processes over long timescales exceeding seconds is challenging using standard fluorescence techniques due to technical issues such as photodamage. Current photonic technology can be exploited to overcome these challenges while preserving sensitivity at the single molecule level. We show that using a simple quantum metrology scheme involving periodic driving for optical state preparation, it is possible to perform spectroscopy of a single chiral molecule in a condensed phase environment, with low photon fluxes. We show that for certain non-classical optical probes and measurement settings, it is possible to exceed the standard quantum limit of precision for a range of driving parameters, even in the presence of high transmission losses due to background absorption. We propose the expected scheme with fluorescence spectroscopy for single molecule detection, and discuss possible applications of quantum metrology in systems biology.

1 Now at Department of Physics, Universidad de Santiago de Chile.
4:18PM D38.00008 Quantum Computation and Quantum Metrology based on Single Electron Spin in Diamond, JIANGFENG DU, University of Science and Technology of China — It is of great challenge to perform the accurate controlling the electron spin qubits in realistic system, due to the noises aroused from the noisy spin bath and the driving field. Firstly, we adopted dynamically corrected gates to realize robust and high-fidelity quantum gates. In this work, the quantum gate’s performance was pushed to T1 limit [PRL 2014, 112, 050503]. Then, a new Rabi Oscillations (ROs) resulting from Landau-Zener (LZ) transitions is observed useful to suppress the fluctuations of the driving field [PRL 2014, 112, 010503]. Besides, quantum error correction is experimentally employed to overcome the noise effect in diamonds [Nature 2014, 506, 204-207]. Precise quantum control and effectively supressing noise of the environment are of great importance for quantum metrology. We succeeded in sensing and atomic-scale analysis of single nuclear spin clusters in diamond at room temperature [Nature Physics 2014, 10, 21-25], and also have succeed to detect a few nuclear spins with single spin sensitivity [Nature Comm., 2014, 4:4703].

4:30PM D38.00009 High-Sensitivity Temperature Sensing Using an Implanted Single Nitrogen-Vacancy Center Array in Diamond\(^1\), GUANZHONG WANG, JUNFENG WANG, Department of Physics, University of Science and Technology of China, ADVANCED THINFILM LABORATORY, UNIVERSITY OF SCIENCE AND TECHNOLOGY OF CHINA TEAM — We present a high-sensitivity temperature detection using an implanted single Nitrogen-Vacancy center array in diamond. The high-order Thermal Carr–Purcell–Meiboom–Gill (TCPMG) method was performed on the implanted single nitrogen vacancy (NV) center in diamond in a static magnetic field. We demonstrated that under small detunings for the two driving microwave frequencies, the oscillation frequency of the induced fluorescence of the NV center equals approximately to the average of the detunings of the two driving fields. On basis of the conclusion, the zero-field splitting D for the NV center and the corresponding temperature could be determined. The experiment showed that the coherence time for the high-order TCMG was effectively extended, particularly up to 108 µs for TCMG-8, about 14 times of the value 7.7 µs for thermal Ramsey method. This coherence time corresponded to a thermal sensitivity of 10.1 mK/Hz\(^{1/2}\). We also detected the temperature distribution on the surface of a diamond chip by using the implanted NV center array with the TCMG-3. Our approach implies the feasibility for using implanted NV centers in high-quality diamonds to detect temperatures with high-sensitivity and nanoscale resolution.

\(^1\)This work was supported by the National Basic Research Program of China (2013CB921800, 2011CB921400) and the Natural Science Foundation of China (Grant Nos. 11374280, 50772110).

4:42PM D38.00010 Nitrogen Vacancy centers in diamond as \(\theta^2\) sensors\(^1\), SHONALI DHINGRA, BRIAN D’URSO, University of Pittsburgh — Nitrogen-vacancy (NV) centers are naturally occurring defects in diamond, which feature an electronic spin with well-defined quantum behavior, including long quantum coherence times and optical addressability. In this work, we show how to align an external magnetic field to the direction of the internally-defined spin axis of the NV center. We further show that this capability can be explored to use an NV center as a \(\theta^2\) sensor in presence of this external magnetic field. The sensitivity of this sensor is shown to increase very rapidly with the external magnetic field, diverging as the external field approaches a value pre-defined by the NV center parameters. We show that the measured sensitivity has excellent agreement with the theoretical predictions. These results show that NV centers may be useful for coupling to torsional nanomechanical oscillators (NMO), to make quantum non-demolition measurements of the number states of the NMO.

3DARPA Young Faculty Award

4:54PM D38.00011 Optimal sensing at the nanoscale with diamond nitrogen vacancy center\(^1\), WEN YANG, PING WANG, Beijing Computational Science Research Center — Diamond nitrogen-vacancy center is a leading platform for ultra-precise sensing at the nanoscale. The sensing is essentially a parameter estimation problem: (1) Encoding the unknown parameters into the NV state; (2) Readout the NV state from the fluorescence; (3) Process the data to infer the unknown parameters; (4) Adaptation of (1)-(3) based on the updated knowledge about the unknown parameters. Recently, dynamical decoupling and adaptive measurement have significantly improved the sensitivity and dynamic range by improving steps (1) and (4), respectively. However, a full optimization of all the steps remains lacking, e.g., the widely used approach to step (3) based on averaging the data from repeated fluorescence measurements or from single-shot fluorescence binarized into 0 and 1 is suboptimal. Here we apply quantum metrology techniques, developed in optical phase estimation, to construct a general framework for optimal sensing using the NV center, incorporating the finite detection efficiency and decoherence. It can be readily applied to various sensing tasks, such as dc/ac magnetometry, noise spectroscopy, and single-molecular NMR. For illustration, we demonstrate significant sensitivity improvement in tracking a time-varying magnetic field with the NV center.

\(^1\)This work was supported by NSFC (Grant No. 11274036 and No. 11322542) and the MOST (Grant No. 2014CB848700).

5:06PM D38.00012 ABSTRACT WITHDRAWN

5:18PM D38.00013 Tensor network approach to quantum feedback dynamics, ARNE GRIMSMO, Département de Physique, Université de Sherbrooke — In this talk I consider the problem of a quantum system coupled to a bosonic reservoir creating a coherent feedback loop. Since the system can be strongly correlated with the in-loop field, this is in general a highly non-Markovian quantum problem where no perturbative approach can be expected to work well. I will present the first practical approach to model this type of dynamics for general quantum systems and large delay times. Borrowing ideas from the intersection of condensed matter and quantum information theory, I will show that a formal dynamical solution can be found as the continuum limit of a tensor network, much like the recently introduced continuous matrix product states for one-dimensional field theories. This gives rise to a practical and efficient integration scheme in discrete time, which is numerically exact as the time-step goes to zero. Besides opening the possibility to study a new regime of quantum feedback control, this is also a novel application of tensor network techniques that could pave the way for a new approach to non-Markovian quantum dynamics in a broader context as well.

Monday, March 2, 2015 2:30PM - 5:30PM  —  Session D39 GQI: Superconducting Circuits: Decoherence II 213AB - Robert McDermott, University of Wisconsin-Madison

2:30PM D39.00001 Al/AlOx/Al Josephson junctions fabricated without double-angle evaporation, KYLE SUNDQVIST, PRANAV SHARMA, MICHAEL BABB, JAE WOO SUH, H. RUSTY HARRIS, Texas A&M University — Superconducting circuits are a common means to produce quantum-mechanically coherent structures. It is possible to produce superconducting circuits which may sustain and even amplify coherent states of microwaves close to the quantum limit. To this end, work is underway at Texas A&M University to locally implement Josephson junctions in our research. We have developed our own process flow for Josephson junction fabrication. This technique does not rely on the commonly used Dolan-bridge double-angle evaporation technique, and is easily incorporated into the process flow of other solid-state devices at the AggieFab fabrication facility.
2:42PM D39.00002 Dependence of transmon qubit relaxation rate on cavity photon population\(^1\). S.O. MUNDHADA, S. SHANKAR, Y. LIU, M. HATRIDGE, A. NARLA, K.M. SLIWA, S.M. GIRVIN, M.H. DEVORET, Department of Applied Physics, Yale University — In circuit QED experiments, a qubit is dispersively coupled to a cavity such that the cavity frequency depends on the qubit state. This dispersive shift enables quantum non-demolition readout of the qubit by exciting the cavity with a microwave pulse and detecting the phase shift of the reflected signal. However, this cavity excitation has been observed in experiments to increase the qubit relaxation rate, hence demolishing the qubit state and limiting the maximum measurement strength. Here we experimentally study this effect in a transmon qubit coupled to a three-dimensional superconducting cavity. We also explore alternate qubit circuits designed to mitigate this demodulation effect.

\(^1\)Work supported by: IARPA, ARO, and NSF

2:54PM D39.00003 Quasiparticles and vortices in superconducting microwave resonators\(^1\). IBRAHIM NSANZINEZA, B.L.T. PLOURDE, Syracuse University — Nowhere in quantum systems has the role of quasiparticles and vortex interactions been as critical as in superconducting microwave resonators. Here we present results of Monte Carlo simulations on a 1D XY spin model that shows how vortices can trap quasiparticles and lead to a reduction in the quasiparticle loss. We will discuss experiments involving the controlled trapping of vortices for reducing quasiparticle densities as well as the use of normal metal quasiparticle traps in superconducting resonators. In our measurements, quasiparticles are generated either by stray pair-breaking radiation or by direct tunnel-junction injection.

\(^1\)We acknowledge support from the NSF under Grant No. DMR-1105197

3:06PM D39.00004 Quantifying Surface Loss Induced by Anti-Vortex Hole Arrays in Planar Superconducting Circuits for Quantum Computation. B. CHIARO, A. MEGRANT, A. DUNSWORTH, Z. CHEN, B. CAMPBELL, I.-C. HOI, J. KELLY, C. NEILL, P. J. J. O’MALLEY, C. QUINTANA, A. VAINSENCHER, J. WENNER, T. WHITE, UC Santa Barbara, R. BAREND, Y. CHEN, A. FOWLER, E. JEFFREY, J. MUTUS, P. ROUSHAN, D. SANK, Google, Santa Barbara, A. N. CLELAND, UC Santa Barbara, J. M. CAMPBELL, I.-C. HOI, J. KELLY, C. NEILL, P. J. J. O’MALLEY, C. QUINTANA, A. VAINSENCHER, J. WENNER, T. WHITE, UC Santa Barbara, R. BAREND, Y. CHEN, A. FOWLER, E. JEFFREY, J. MUTUS, P. ROUSHAN, D. SANK, Google, Santa Barbara — Two important dissipation sources in superconducting circuits operated at low power are surface loss from two level systems (TLS) and magnetic vortex loss. By patterning the superconducting electrodes with an array of holes, it is possible to reduce or eliminate loss due to magnetic vortices. However, since the highest levels of coherence in planar superconducting circuits have been achieved by improving the electrode-substrate interface, it is natural to expect that adding hole arrays to the electrodes may cause excess surface loss. We present simulations predicting the excess loss magnitude to be < 10% for typical ground plane hole arrays, but for extreme cases of hole size or placement the loss may be much greater. We confirm the simulation result with measurements of high quality factor resonators ($Q_i > 10^6$) with and without the hole patterns.

3:18PM D39.00005 $1/f^{α}$ noise in interacting spin systems: a real space RG approach. KARTIEK AGARWAL, Harvard University, IVAR MARTIN, Los Alamos National Laboratory, EUGENE DEMLER, Harvard University — Localized paramagnetic electrons are believed to be the cause of magnetic flux noise that plagues superconducting qubits, but how such interacting spins generate frequency dependent noise of the form $1/f^{α}$ is not well understood. We describe a novel real space RG procedure that is equipped to calculate directly various dynamical quantities in a strongly disordered Heisenberg spin system (in arbitrary dimensions), including the ‘noise’ from such systems. In 1-D, we find that the RG procedure describes a fairly temperature-independent noise with a power law $α < 1$ that varies smoothly depending on the disorder strength, relative concentration of Ferro-Anti-Ferro bonds and temperature. The dynamic structure factor (of spin-spin correlations) inherits this power law while displaying a crossover to a related power at higher frequencies. In 2-D, the RG results in dynamics that are diffusive at high temperatures but remain anomalous at lower temperatures. A possible connection of the phenomena of $1/f$ noise and Many-Body Localization is also discussed.

3:30PM D39.00006 Flux noise in SQUIDs: Electron versus nuclear spins\(^1\). ROGERIO DE SOUSA, STEPHANIE LAFOREST, University of Victoria, BC — Superconducting Quantum Interference Devices (SQUIDs) are limited by intrinsic flux noise whose origin is unknown. We develop a method to accurately calculate the flux produced by spin impurities in realistic superconducting thin film wires, and show that the flux produced by each spin is much larger than anticipated by former calculations. Remarkably, the total flux noise power due to electron spins at the thin side surface of the wires is found to be of similar magnitude as the one due to electrons at the wide top surface of the wires. In addition, flux noise due to lattice nuclear spins in the bulk of the wires is found to be a sizable fraction of the total noise for some SQUID geometries. We discuss the relative importance of electron and nuclear spin species in determining the total noise power, and propose strategies to design SQUIDs with lower flux noise.

\(^1\)We acknowledge support from the Canadian agency NSERC through its Discovery and Engage programs.

3:42PM D39.00007 Adsorbed Oxygen Molecules as a Possible Source of Flux Noise in SQUIDs\(^1\). CHUNTAI SHI, Univ of California - Irvine, HUI WANG\(^2\), Fudan University, China, JUN HU, CLARE YU, RUQIAN WU\(^3\), Univ of California - Irvine — One of the dominant source of flux noise in SQUIDs is flux noise which has been attributed to mysterious fluctuating magnetic pins on the surface. We propose that the spins producing flux noise could be adsorbed O\(_2\) molecules that have a magnetic moment of about 2 $\mu_B$. Using density functional calculations, we studied O\(_2\) molecules adsorbed on a sapphire surface. We find that the barrier for spin rotation is small enough to allow almost free spin reorientation due to thermal excitations at low temperatures. Monte Carlo simulations of a 2D XY spin model yields $1/f$ noise where $f$ is frequency.

\(^1\)This work was supported by 1000 Talent Program of China through Fudan University. Work at UCI was supported by DOE-BES (Grant No. DE-FG02-05ER46237) and the Army Research Office (Grant No. W911NF-10-1-0494).

\(^2\)University of California-Irvine

\(^3\)Fudan University, China

3:54PM D39.00008 Adsorbed Oxygen Molecules as a Source of Flux Noise in SQUIDs\(^1\). HUI WANG, ZHE WANG, Department of Physics, Fudan University, Shanghai 200433, China, JUN HU, CHUNTAI SHI, CLARE C. YU, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA 92697-4575, USA, DEPARTMENT OF PHYSICS, FUDAN UNIVERSITY, SHANGHAI 200433, CHINA COLLABORATION, DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF CALIFORNIA, IRVINE, CA 92697-4575, USA COLLABORATION — A major obstacle for using superconducting quantum interference devices (SQUIDs) as qubits is the flux noise generated by fluctuating magnetic pins on the surface of SQUIDs. Using density functional theory (DFT) calculations, we investigated O\(_2\) adsorbates and various vacancies on an $\alpha$-alumina surface as spin candidates. Their spectroscopic features are directly compared to experimental data using the x-ray magnetic circular dichroism. The calculated magnetic anisotropy energy for the spin of O\(_2\) to rotate within a plane perpendicular to the axis of the O-O bond is only about 12 mK ($\sim 1 \mu$eV) so we believe that O\(_2\) molecules are the main source of flux noise in Al SQUIDs.

\(^1\)Work at Fudan was supported by the 1000-Talent funds. Work at UCI was supported by DOE-BES (Grant No. DE-FG02-05ER46237) and by NERSC for computing time.
We have measured the power loss and 1/f permittivity noise of deposited dielectrics at microwave frequencies over a range of millikelvin temperatures. The results will be compared to recent strong-interaction theories. We explain the high frequency (f = 1-10 GHz) Ohmic flux noise observed in SQUIDs and superconducting qubits.

1/f noise, and weakly coupled high frequency ohmic or subohmic noise. Noise components with frequencies higher than the qubit tunneling element result in excitation-relaxation dynamics of the qubit. At the same time the low frequency noise (with frequency lower than the qubit tunneling splitting) causes strong modulation of the level splitting between the ground and excited states. We show that the combined effect of the low and high frequency components of the noise results in the qubit freezing in the excited state with a sizable probability. This mechanism may set an upper bound on the quantum annealing computation time.

Magnetic adsorbates on the surfaces of superconducting thin films. We present the results of SQUID-based susceptibility and noise measurements that are part of an ongoing effort to reduce surface spin density and flux noise by improving the vacuum environment of the superconducting device.

Noise results in the qubit freezing in the excited state with a sizable probability. This mechanism may set an upper bound on the quantum annealing computation time.

In conclusion, we propose routes to improving SQ performance by enhancing or minimizing magnetic ordering of induced spins on Al₂O₃ surface.

We acknowledge support from IARPA under contract W911NF-10-1-0324.
Vertical Phase Separation in Bulk-Heterojunction Polymer Solar Cells

YUEH-LIN LOO, HE WANG, JONGBOK KIM, Princeton University — With soft-contact lamination and delamination, we have elucidated whether and how vertical phase separation of active layers affects solar cell performance. We constructed conventional bulk-heterojunction solar cells comprising P3HT, PCPDTBT, PCBM, and a wetting layer, devices with P3HT exhibit only a marginal drop in its current compared to devices without a P3HT wetting layer. We ascribe this difference in active layer prior to cathode deposition. While devices with PCPDTBT and T1 exhibit drastically reduced current compared to devices without the additional fullerene derivatives. To exaggerate the influence of vertical phase separation, we laminated in each case a thin layer of electron donor on the bulk-heterojunction electron acceptor interface within the molecular structure facilitates studies of charge transfer processes, where we can systematically modulate the chemical structure and energetics to perturb exciton dissociation and charge recombination.

Impacts

Monday, March 2, 2015 2:30PM - 5:30PM –
Session D41 DPOLY: Focus Session: Polymers for Solar Energy Conversion - Morphological Impacts 214A - Bryan Boudouris, Purdue University

Laboratory — Weak intermolecular interactions and disorder at junctions of different organic materials limit the performance and stability of organic interfaces and hence the applicability of organic semiconductors to electronic devices. Our approach has focused on utilizing block copolymer architectures — where critical interfaces are controlled and stabilized by covalent bonds — to provide the hierarchical structure needed for high-performance organic electronics from self-assembled soft materials. For example, we have demonstrated control of donor-acceptor heterojunctions through microphase-separated conjugated block copolymers to achieve 3% power conversion efficiencies in non-fullerene photovoltaics. Characterization through X-ray scattering and electron microscopy reveals that the efficient performance of block copolymer solar cells is due to self-assembly into mesoscale lamellar morphologies with primarily face-on crystallite orientations. Furthermore, incorporating the donor-acceptor interface within the molecular structure facilitates studies of charge transfer processes, where we can systematically modulate the chemical structure and energetics to perturb exciton dissociation and charge recombination.

Computational Description of Donor-Acceptor pi-Conjugated Materials for Organic Photovoltaics Applications

JEAN-LUC BREDAS, King Abdullah University — This presentation will focus on the following topics, related to organic solar cell applications: 1) We will describe our recent work on the electronic structure and local morphology of donor-acceptor interfaces in bulk-heterojunction solar cells. 2) We will discuss how we can evaluate the polarization effects, which play a critical role in the charge-separation process at donor-acceptor interfaces in organic solar cells. 3) Finally, we will describe the peculiarities of the electronic structure of a new pi-conjugated polymer with very high hole mobilities over 20 cm²/Vs.

New Insight into Morphology of High Performance BHJ Photovoltaics Using High Resolution AFM

FENG LIU, Lawrence Berkeley National Lab, DONG WANG, KEN NAKAJIMA, Tohoku University, THOMAS RUSSELL, Lawrence Berkeley National Lab, THOMAS RUSSELL COLLABORATION — Direct imaging of the bulk BHJ thin film morphology in OPV is essential to understand device function and optimize efficiency. While transmission electron tomography provides a 3D, real-space image of the morphology, quantifying the structure is not possible. Here we used high-resolution atomic force microscopy in the tapping and nano-mechanical modes to investigate the BHJ active layer morphology which, when combined with Ar ion etching, provided unique insights with unparalleled spatial resolution. PCBM was seen to form a network that interpenetrated into the fibrillar network of the hole-conducting polymer, both being imbedded in a mixture of the two components. The free surface was found to be enriched with polymer crystals having a face-on orientation, and the morphology at the anode interface was markedly different.

Creating Efficient Quasi-3D Transport Pathways With Crossed-Chain Polymer Interfaces

CHRISTOPHER TAKACS, MICHAEL BRADY, NEIL TREAT, MICHAEL CHABINCY, Univ of California - Santa Barbara — While our understanding of the local molecular packing in many well-performing polymer semiconductors has improved, many open questions regarding the molecular level details of long-range connectivity and the best strategies for optimizing electronic functionality remain. Here we focus on the possible benefits of epitaxy in polymer semiconductors for improving nano-scale connectivity, a concept particularly useful for systems where charge-transport is expected to be highly anisotropic. The periodic crossing of the non-parallel chains at the crystal-crystal interfaces may enable efficient coupling across grain-boundaries and increase the effective dimensionality of the charge transport processes. Using a combination of high-resolution transmission electron microscopy, statistical analysis of the electron micrographs, and a variety of molecular simulation methods, we will demonstrate that such epitaxy relationships can be predicted and observed in a variety of well-performing polymer semiconductors. The results suggest that further engineering of epitaxy may lead to substantial advances in both control of self-assembly and electronic performance.

Small Molecule Bulk Heterojunction: Impact of two thermodynamically stable morphologies on the efficiency of organic photovoltaics devices

NURADHIKA HERATH, VALERIA LAUTER, JIM BROWNING, ILIA IVANOV, JONG KEUM, KAI XIAO, JIAHUA ZHU, Oak Ridge National Laboratory, SANJIB DAS, GONG GU, University of Tennessee Knoxville — Structural characteristics of device active layers play a critical role in charge generation, separation and transport in organic photovoltaics (OPVs). Here we report on morphology and structure control of p-DTS(FBTTh₂)₂:PC₇₀BM films by means of thermal annealing and solvent additive processing. Depth-sensitive neutron reflectometry and X-ray diffraction are employed to characterize the thin film structures, and are correlated to the device performance. The neutron reflectometry results reveal that p-DTS(FBTTh₂)₂:PC₇₀BM films fabricated with 1,8-diiodooctane (DIO) reproducibly exhibit a 3-sublayer morphology similar to thermally annealed films without DIO. Moreover, DIO promotes the formation of a large population of p-DTS(FBTTh₂)₂ nanocrystals leading to a device efficiency (PCE) of 5.9 %. The thermally annealing generate p-DTS(FBTTh₂)₂ crystallites one order of magnitude larger than those formed with the DIO. Our results provide direct evidence that delicate size control of crystal domains closer to the optimum exciton diffusion length is as important as a high crystallinity of charge transport layers.

This research was conducted at Spallation Neutron Source and at the Center for Nanophase Materials Sciences, which is sponsored at ORNL by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.
4:06PM D41.00007 Morphology and performance of organic photovoltaics containing a small-molecule acceptor. KATHRYN O'HARA, University of California, Santa Barbara, DAVID OSTROWSKI, University of Colorado Boulder, CHRISTOPHER TAKACS, University of California, Santa Barbara, LUNS. KOLDEMER, Colorado School of Mines, SEAN SHAHEEN, University of Colorado Boulder, ALAN SELLINGER, Colorado School of Mines, MICHAEL CHABINYC, University of California, Santa Barbara — Fullerenes are derivatives that are widely used as acceptor materials in organic photovoltaics (OPVs). However, they have a high cost, low absorption in the visible range and limited synthetic variability compared to small molecule alternatives, which generally underperform PCBM, but it is unclear if the reason is morphological or due to the electronic structure of the acceptor. A promising fullerene alternative, HPI-BT, is blended with P3HT to achieve a power conversion efficiency (PCE) of 2.1%, which is lower than for fullerene OPVs (10%), but an understanding of the morphology could improve the efficiency of future small-molecule based devices. The active layer microstructure is probed complimentary techniques of atomic force microscopy (AFM), grazing incidence wide angle x-ray scattering (GIWAXS), and scanning transmission electron microscopy (STEM). STEM indicates that HPI-BT crystals are buried in the film upon casting and AFM shows they grow to the film surface upon annealing. GIWAXS reveals the acceptor is crystalline, which should improve charge transport, but film texturing suggests that crystals nucleate off the substrate, cover the anode and ultimately limit cell performance.

4:18PM D41.00008 Direct internuclear distance measurements of P3HT/PCBM interfaces in bulk heterojunction thin films using $^{13}$C $^2$H REDOR NMR. RYAN NIEUWENDAAL, DEAN DELONGHAMP, NIST, ALEX SIEVAL, Solene BV, J.C. HUMMELEN, University of Groningen, MARTIN HEENEY, ZHUHONG FEI, Imperial College — Robust structure/function relationships are generally lacking in organic photovoltaic (OPV) thin film active layers. Structural complexity has contributed to a lack of performance predictability, so there exists a need for measurement tools that can unveil fine details of the bulk heterojunction (BHJ) thin film structure. Optical methods, microscopy (AFM, TEM), and scattering techniques are useful for coarse morphological assessment, but their lack of sub-nm spatial resolution has obscured perhaps the most pertinent morphological quality of the BHJ: the donor/acceptor interface. In this contribution, I will discuss the results of solid state NMR measurements performed in our laboratory to characterize the donor/acceptor interface. $^{13}$C $^2$H REDOR experiments on isotopically-enriched thin film blends of P3HT and PCBM are used to determine distances between nuclei in the donor molecules ($^2$H on P3HT main chain) and acceptor molecules ($^{13}$C-enriched C$_{60}$ cage). Experiments are performed on ~ 100 nm thin film samples utilizing casting recipes that are typical for fabricating real OPV devices.

4:30PM D41.00009 ABSTRACT WITHDRAWN

4:42PM D41.00010 Two-Dimensional Effects on Lateral Organic Bulk Heterojunction Devices. KELLY LIANG, ERIC DANIELSON, Univ of Texas, Austin, ZIEN OOI, Agency for Science, Technology and Research, ANANTH DODABALAPUR, Univ of Texas, Austin — For moderately thick (50 nm) lateral organic bulk heterojunction (OBHJ) photovoltaic devices, a one-dimensional space charge limited current model with electric field independent mobility accurately simulates key device metrics, like photocurrents, mobilities, and bimolecular recombination coefficients. However, as the thickness of these lateral organic devices approaches thinner and thicker limits, two-dimensional effects greatly influence device characteristics, and a one-dimensional approximation is no longer sufficient. Both the two-dimensional electric field spreading in the OBHJ semiconductor and the electric field dependent mobility of the material system need to be considered in these devices. Introducing a geometric prefactor—dependent on the thickness of the organic semiconductor, to the one-dimensional space charge limited model accounts and adjusts for the two-dimensional effects. Using this modified and more accurate model, we further examined the photoconduction and photovoltaic gain in lateral OBHJ devices and reaffirmed that high gains originate from contact injection rather than bulk photoconduction.

4:54PM D41.00011 High-Performance All-Polymer Solar Cells Based on Face-on Stacked Polymer Blends with Low Interfacial Tension.BUMJOON KIM, HYUNBUM KANG, CHANGYEON LEE, TAESU KIM, KAIST — We report highly-efficient all-polymer solar cells with power conversion efficiencies of over 4.5% by highly-intermixed blends of poly[4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b]-dithiophene-3-fluorothieno[3,4-b]thiophene-2-carboxylate] (PTB7-Th) donor and poly[(N,N′-bis(2-octyldodecyl)-naphthalene-1,4,5,8-bis(dicarboximide)-2,6-diyl]-alt-5,5-(2,2′-bithiophene)] (P[NDI2OD-T2]) acceptor polymers. The low interfacial tension and the face-on π–π stackings of the all-polymer blends afforded desired nanophase morphology, which facilitates efficient charge transport from active layer to each electrode. In addition, the incorporation of 1,8-diiodooctane additives was able to tune the degree of crystallinity and orientation of P[NDI2OD-T2] acceptors, resulting in remarkable enhancement of electron mobility, external quantum efficiency and $J_{SC}$ values.

5:06PM D41.00012 All-polymer photovoltaics: Correlating Efficiency and Morphology. YAN JIN, University of Cincinnati, JONG K, KEUM, KUNLUN HONG, JAMES F. BROWNING, GREGORY S. SMITH, Oak Ridge National Laboratory, VIKRAM K. KUPPA, University of Cincinnati, OAK RIDGE NATIONAL LABORATORY COLLABORATION — We have recently demonstrated how the efficiency of devices fabricated from a blend of the polymers P3HT and F8BT increases three-fold by incorporating pristine graphene into the active layer. The fundamental mechanisms underlying this enhancement are investigated, and are shown to arise from improvements in both charge transport and morphology. We investigate the structure via small angle neutron scattering (SANS) studies of the deuterated-P3HT/F8BT system with and without graphene. SANS reveals the existence of disk-like P3HT crystallites distributed in an amorphous miscible blend of P3HT and F8BT. P3HT crystallinity was enhanced upon graphene addition, resulting in larger crystallites and a higher degree of ordering. These structural changes are accompanied by better charge transport, resulting in a peak improvement of over 200% in the short-circuit current of the devices. Results on cell characterization and recombination mechanisms are also reported, and indicate means of addressing fundamental problems in OPV systems.

5:18PM D41.00013 Role of Molecular Linker on Charge Separation and Photovoltaic Performance in All-Conjugated Block Copolymers. JORGE WU MOK, YEN-HAO LIN, KENDALL SMITH, RAFAEL VERDUGO, Rice Univ — Recent studies have demonstrated the potential of all-conjugated donor–acceptor block copolymer for organic photovoltaics, but it remains unclear how molecular structure, morphology, and electronic properties of conjugated block copolymers influence performance. Here, we study the role of chemical linker between donor and acceptor polymers on photovoltaic performance and optoelectronic properties. Two poly[(3-heptylthiophene)-poly(2,7-diyl-alt-[4,7-bis(thiophen-5-yl)]-2,1,3-benzothiadiazole)-2,2′-diyl-(9,9-diocetyfluorene)] (P3HT-PTBTF) donor–acceptor block copolymers which differ only in the chemistry of linking group are studied through device measurements, GIIXS, and steady-state and time-resolved absorbance and photoluminescence. Device studies show that power conversion efficiencies decrease by one order of magnitude by changing the linking group. X-ray analysis shows that the morphology is virtually identical in both samples, as expected. Transient absorption measurements reveal charge separation in block copolymers which contain a wide bandgap monomer at the donor–acceptor interface, but charge separation is suppressed when donor and acceptor blocks are directly linked without this spacer present. This work demonstrates that the linking group chemistry influences charge separation in all-conjugated block copolymer systems, and also suggests that all-conjugated block copolymers can be used as model systems for the donor-acceptor interface in bulk heterojunction blends. 

1 Oak Ridge National Laboratory
and application of metrology methods to BCPs a critical area. In particular, methods for determining the real space structure of the BCP DSA films are needed.

DOVER, CHRISTOPHER LIMAN, NIST - Natl Inst of Stds & Tech, JUAN DE PABLO, University of Chicago, JOSEPH KLINE, NIST - Natl Inst of Stds & Tech

Self-Assembly Thin Films using Inverse Genetic Algorithms

A key obstacle, however, is inducing the resulting structures to align perpendicularly, rather than parallel, to the substrate. In this talk, we present our simulation results relating to some strategies which have been pursued by experimentalists to overcome the above goal. One part of this talk will focus on the self-assembly of block copolymers on a homogeneously patterned surface. The second part of this talk will focus on the case of inhomogeneously patterned surfaces and identify the interplay between pattern width and the surface free energies in dependencies on grafting density, relative chain length between the free and grafted polymers, and blockiness of the random copolymer chains. The second part of this talk will focus on the case of inhomogeneously patterned surfaces and identify the interplay between pattern width and the surface free energies in dependencies on grafting density, relative chain length between the free and grafted polymers, and blockiness of the random copolymer chains.

3:06PM D42.00004 Self-Assembly of Diblock Copolymers on Modified and Patterned Surfaces

VENKAT GANESAN, University of Texas at Austin — The self assembly of diblock copolymer thin films into lamellar and cylindrical structures has been proposed as a method of creating small patterns in polymer thin films for electronic materials applications. A key obstacle, however, is inducing the resulting structures to align perpendicularly, rather than parallel, to the substrate. In this talk, we present our simulation results relating to some strategies which have been pursued by experimentalists to overcome the above goal. One part of this talk will focus on the self-assembly of block copolymers on a homogeneously patterned surface. The second part of this talk will focus on the case of inhomogeneously patterned surfaces and identify the interplay between pattern width and the surface free energies in dependencies on grafting density, relative chain length between the free and grafted polymers, and blockiness of the random copolymer chains. The second part of this talk will focus on the case of inhomogeneously patterned surfaces and identify the interplay between pattern width and the surface free energies in dependencies on grafting density, relative chain length between the free and grafted polymers, and blockiness of the random copolymer chains. The second part of this talk will focus on the case of inhomogeneously patterned surfaces and identify the interplay between pattern width and the surface free energies in dependencies on grafting density, relative chain length between the free and grafted polymers, and blockiness of the random copolymer chains. The second part of this talk will focus on the case of inhomogeneously patterned surfaces and identify the interplay between pattern width and the surface free energies in dependencies on grafting density, relative chain length between the free and grafted polymers, and blockiness of the random copolymer chains.

3:42PM D42.00005 Optimizing the Morphology Characterization of Block Copolymer Directed Self-Assembly Thin Films using Inverse Genetic Algorithms

ADAM HANNON, DANIEL SUNDAY, DONALD WINDOVER, CHRISTOPHER LIMAN, NIST - Natl Inst of Stds & Tech, JUAN DE PABLO, University of Chicago, JOSEPH KLINE, NIST - Natl Inst of Stds & Tech — Block copolymer (BCP) directed self-assembly (DSA) is one of the leading candidate methods for nanopatterning transfer needed in the next generation of integrated circuit and memory storage devices. Much research has gone into precisely controlling the morphology of BCP thin films, making the development and application of metrology methods to BCPs a critical area. In particular, methods for determining the real space structure of the BCP DSA films are needed. Recently, resonant soft X-ray scattering experiments have shown promise as such a method by inversely calculating the real space structure from the scattered intensity profile [Sunday et. al. ACS Nano 2014, 8 (8), 8426-8437]. These inverse methods are limited in application by their computation speed. Here we present recent work in using genetic algorithms to determine the real space structure of PS-PMAA thin films. The calculated results are compared with the structure found in self-consistent field theory simulations using boundary conditions analogous to the experimental DSA templates.

3:54PM D42.00006 Instantaneous Formation of Block Copolymer Patterns via Solvo-Thermal Casting Process

HYUN JUNG WOO, JONGSANG WOO, JUNE HUH, JOONA BANG, Department of Chemical and Biological Engineering, Korea Univ. — A self-assembly of block copolymer (BCPs) exhibits one of the most promising alternative methods for the next-generation lithography. Many semiconductor companies have explored the possibility of implementing this process in actual chip process, whereas the critical challenges such as feature size control, defect density, and long processing time need to be overcome. Regarding the BCP process, the formation of BCP patterns usually requires long processing time via thermal or solvent annealing. Herein we developed a simple processing method to promote a microphase separation of BCPs using solvo-thermal spin casting process. Spin casting has a very similar mechanism to solvent vapor annealing but its short processing time prevents BCP chains from reaching equilibrium morphology. To maximize the chain mobility, we employed a high boiling point solvent and also applied the heat during spin casting. As a result, a well ordered BCP patterns were obtained within less than 5 min via solvo-thermal casting process without further additional annealing step.
4:06PM D42.00007 Cyclic Solvent Vapor Annealing for Rapid, Robust Vertical Orientation of Features in BCP Thin Films. SEAN PARADISO, KRIS DELANEY, GLENN FREDRICKSON. Univ of California - Santa Barbara — Methods for reliably controlling block copolymer self assembly have seen much attention over the past decade as new applications for nanostructured thin films emerge in the fields of nanopatterning and lithography. While solvent assisted annealing techniques are established as flexible and simple methods for achieving long range order, solvent annealing alone exhibits a very weak thermodynamic driving force for vertically orienting domains with respect to the free surface. To address the desire for oriented features, we have investigated a cyclic solvent vapor annealing (CSVVA) approach that combines the mobility benefits of solvent annealing with selective stress-confined domains. It has been shown that structures oriented parallel to the free surface as the film is repeatedly swollen with solvent and dried. Using dynamical self-consistent field theory (DSCFT) calculations, we establish the conditions under which the method significantly outperforms both static and cyclic thermal annealing and implicate the orientation selection as a consequence of the swelling/deswelling process. Our results suggest that CSVVA may prove to be a potent method for the rapid formation of highly ordered, vertically oriented features in block copolymer thin films.

4:18PM D42.00008 Decoupling Substrate Surface Interactions in Block Polymer Thin Film Self-Assembly. CAMERON SHELTON, THOMAS EPPS, University of Delaware — Understanding the impact of the major factors that affect block polymer (BP) thin film self-assembly is necessary to control nanostructure ordering, orientation, and defect density. In this work, we systematically studied the influence of the substrate surface energy, one of the most significant parameters directing self-assembly, on wetting behavior, through-film interactions, and substrate surface field propagation. Notably, we determined the applicability of decoupled surface energy components (dispersive and polar interactions) as opposed to total surface energy, using a suite of chlorosilane monolayers and UV-ozone degradation to create a library of total, dispersive, and polar surface energy effects. Our results could complement literature that indicated repulsive total surface energy interactions are the dominant forces at the substrate-polymer interface, whereas attractive decoupled surface energy interactions become significant past the contacting layer. This work represents a thorough analysis of a vital force affecting BP self-assembly as well as a blueprint for the generalized design of substrate surfaces that achieve target BP nanostructure orientations for nanolithography, templating, and nanoporous membrane applications.

4:30PM D42.00009 A Block Copolymer Self-Assembly Approach for 3D Nanoconfined Dopants in Semiconductors. BHOOSHAN POPERE, BORIS RUSS, WILLIAM CHANG, University of California, Berkeley, ANDREW HEITSCH, The Dow Chemical Company, Midland, MI, PETER TREFONAS, Dow Electronic Materials, Marlboro, MA, RACHEL SEGALMAN, University of California, Santa Barbara — Continuous shrinking of electronic circuits presents a new challenge to demonstrate reliable, uniform nanoscale doping. Directed self-assembly (DSA) of block copolymers (BCP) has proved critical in meeting the technology nodes by enabling excellent pitch control for lithography. Yet, controlling the 3D dopant distribution remains a fundamental design challenge. To this end, we have utilized BCP self-assembly in a novel approach to confine dopants to nanoscopic domains within a semiconductor. The periodic nature of these domains affords precise control over the dosage and spatial positions of dopant atoms. Dopant incorporation within the block copolymer domains via hydrogen bonding eliminates the need for tailored synthesis, making the approach highly modular. Rapid thermal annealing (RTA) effectively drives the dopants into the underlying substrate, thus confining them to within 10-20 nm in all dimensions. Additionally, the size, pitch, dopant dosage and the junction depth can be independently varied for a wide range of dopants. Compositional and electronic measurements indicate that the domains are indeed discrete and nanoconfined. Our approach, thereby, enables a facile method for controlled nanoscopic doping in semiconductors.

4:42PM D42.00010 Defect motion and annihilation in block copolymer thin films1. MARCUS MUELLER, WEIHUA LI, Georg-August University, Institute for Theoretical Physics, Goettingen, Germany — Using self-consistent field theory and computer simulation of a soft, coarse-grained particle model we study defect motion and annihilation in thin films of lamella-forming block copolymers on neutral and chemically patterned substrates. By virtue of the strain-field mediated interactions, dislocation defects with opposite orientation move towards each other. This motion depends both on the thermodynamic, strain-field mediated driving force and the single-chain dynamics that is required to alter the morphology and reduce the distance between the defect cores. This interplay results in a qualitative dependence of the time evolution on the topology of the defect morphology. Upon collision of the defects, they either spontaneously annihilate or form a metastable, tight defect pair. In the latter case, a free-energy barrier has to be overcome to finally produce a defect-free structure. Computing the minimum free-energy path within self-consistent field theory we investigate the dependence of the free-energy barriers of defect motion and annihilation on incompatibility, strength of the chemical surface pattern, and defect morphology.

4:54PM D42.00011 Accelerating the search for globally stable block polymer microphases using genetic algorithms1. CAROL TSAI, KRIS DELANEY, GLENN FREDRICKSON. UC Santa Barbara — The diverse array of block copolymer (BCP) applications is possible because in the melt state, various morphologies that are periodic structures on the nanoscale emerge depending on the particular composition and architecture of the BCPs used. However, knowing which compositional parameters to use to obtain materials with desired properties is a Herculean task: there is an enormous parameter space to search. Furthermore, the problem is exacerbated by the fact that even at a fixed set of compositional parameters, it is difficult to determine the globally stable morphology and low-lying metastable states that will emerge, as complications arise from a rough free-energy landscape. A significant result could be a more efficient and economic screening for the desired microphasology. In this way, the search for optimal microphasology would be reduced to a series of computer simulations, something that can be done on a large scale. This work builds off of previous methods used in conjunction with local optimizations performed by SCFT.

5:06PM D42.00012 Kinetic Aspects of Defect Annihilation in Block Copolymer Thin Films on Patterned Substrates. SU-MI HUR, University of Chicago, PAULINA RINCON-DELGADILLO, IMEC, VIKRAM THAPAR, Cornell University, ABELARDO RAMÍREZ-HERNÁNDEZ, Argonne National Lab., GURDAMAN KHAIRA, PAUL NEALEY, University of Chicago, MARCUS MÜLLER, Institut fur Theoretische Physik, JUAN DE PABLO, University of Chicago — Although there has been significant progress on understanding various aspects of directed self-assembly of block copolymers at equilibrium, important challenges remain regarding the development of materials and processes leading to a perfect, defect-free assembly. We present minimum free-energy pathway calculations for annihilation of dislocation defects in block copolymer thin films using the string method combined with a Theoretically Informed Coarse-Grained (TICG) simulation approach. Our results demonstrate the importance of kinetics in the elimination of defects, where an extraordinarily large thermodynamic driving force is not necessarily sufficient for defect removal. The kinetic path follows a complex three-dimensional morphological changes; the corresponding transition states often consist of a very slight connection between edge dislocation and the neighboring nanodomains. A systematic analysis of the transition states provides useful insights into the possible rate-determining mechanisms for defect motion. We also explore the dependency of the kinetic-energy barriers on the defect type and position, and on processing conditions such as the type of chemical pattern or the strength of the segregation force between the blocks.

Monday, 23, 2015 2:30PM - 5:30PM – Session D43 DPOLY: Focus Session: Self Assembled Block Copolymers and Soft Nanoparticles in Solution 1 214C - Sangwoo Lee, Rensselaer Polytechnic Institute
2:30PM D43.00001 Exotic nanoparticles with block copolymer design and solution construction with kinetic control, DARRIN POCHAN, University of Delaware — Kinetic pathways and temporal stabilities of different micelles and nanoscale aggregates have been used to construct exotic nanoparticles in solution. Due to low chain exchange dynamics between block copolymeric micelles and solvent, global thermodynamic equilibrium is extremely difficult, if not impossible, to achieve in block copolymer assembly. However, by taking advantage of this slow kinetic behavior of polymeric micelles in solution, one can purposely produce multicompartiment nanoparticles and multilength nanoparticles by forcing different block copolymers to reside in the same nanoscale structure through kinetic processing. While kinetically trapped in common nanostructures, local phase separation can occur producing compartments. This compartmentalization can be used within common micelle geometries to make complex spheres and cylinders or can be used to make new nanostructures such as multigometry aggregates (e.g. hybrid cylinder-sphere aggregates, disk-cylinder nanoparticles). Furthermore, new interparticle nanomaterials can be created with hierarchical solution construction methods.

2:42PM D43.00002 Corona contraction and polyelectrolyte complexation of polybasic micelles in buffered aqueous solution, JENNIFER LAASER, YAMING JIANG, THERESA REINEKE, TIMOTHY LODGE, University of Minnesota — We investigate the pH- and ion strength-induced contraction of polycationic micelles with a polystyrene core and poly(dimethylaminoethyl methacrylate) corona in buffered aqueous solutions, and report on complexation of these micelles with poly(styrene sulfonate) under varying ion strength conditions. We find that in monoprotic buffers, the micelle corona behaves as a salted osmotic brush, as has been observed for other block polyelectrolyte micelle systems in unbuffered solutions. In polyprotic buffers, however, we find that concentration of the charged buffer species in the micelle corona shifts the buffer dissociation equilibrium farther toward multivalent species than in the bulk, resulting in an anomalously high degree of corona contraction. In our complexation experiments, we observe two distinct size distributions that evolve on timescales of days to weeks at physiologically relevant ion concentrations, which may have implications for the design of gene- and drug-delivery vehicles using these types of interpolyelectrolyte complexes.

2:54PM D43.00003 Predicting the Solution Morphology of a Sulfonated Block Copolymer in Binary Solvent Mixtures, PHILIP GRIFFIN, GRACE SALMON, JAMIE FORD, KAREN WINEY, University of Pennsylvania — The physicochemical properties of solvent-casted block copolymer films are highly dependent on the microscopic morphology of the solutions from which they are cast. In order to achieve macroscopically homogeneous polymer solutions, binary or higher-degree solvent mixtures are often required, which introduces additional complexity in understanding the molecular level interactions that control block copolymer self-assembly in solution. Using small angle x-ray scattering, we have explored the solution morphology in ternary blends of a sulfonated pentablock copolymer in select binary solvent mixtures over a range of solvent compositions and polymer concentrations. We have found that the solution morphologies in these ternary blends depend strongly on the composition of the solvent mixture. Furthermore, we demonstrate that the solvent-composition-dependent morphologies can be accurately predicted by quantifying the polymer/solvent interactions using Hansen solubility parameters. These studies are an important step toward developing a complete and predictive understanding of the solution morphology of complex polymer/solvent mixtures.

3:06PM D43.00004 Structure of block copolymer micelles in the presence of co-solvents, MEGAN ROBERTSON, SHU WANG, KIM MAI LE, University of Houston, RACHELE PIEMONTE, LOUIS MADSEN, Virginia Tech — Amphiphilic block copolymer micelles in water are under broad exploration for drug delivery applications due to their high loading capacity and targeted drug delivery. We aim to understand the kinetic and thermodynamic processes that underlie the self-assembly of diblock copolymer micelle systems. The present work focuses on diblock copolymers containing poly(ethylene oxide) (a hydrophilic polymer) and polycaprolactone (a hydrophobic polymer), which spontaneously self-assemble into spherical micelles in water. Addition of a common good solvent (a co-solvent) for both of the constituting blocks, such as tetrahydrofuran (THF), reduces the interfacial tension at the core-corona interface. We are currently investigating the effect of this phenomenon on the micelle structural properties, using scattering experiments and nuclear magnetic resonance. We have characterized the hydrodynamic radius, core radius, corona thickness, aggregation number, degree of swelling of the micelle core with the co-solvent, and unimer (free chain) concentration, as a function of the co-solvent concentration. Fundamental knowledge from these studies will inform design of drug delivery systems by allowing us to tailor micelle properties for optimal cargo loading.

3:18PM D43.00005 Solvents effect on the structure of pentablock ionic polymers: A SANS study, MANJULA SENENAYAKE, THUSITHA ETAMPAWALA, SIDATH WIJESINGHE, NARESHT OSTI, Clemson University, LILIN HE, Oak Ridge National Laboratory, DVORA PERAHIA, Clemson University — Solution structure of ionic co-polymers is critical to their processing. The difference of the interactions between blocks with the solvent results in a rich phase diagram. Here, solutions of ABCBA symmetric ionic pentablock copolymer consisting of t-butyl polystyrene end blocks, hydrogenated isoprene inner blocks and randomly and selectively sulfoanted polystyrene as middle block, was studied by small angle neutron scattering (SANS). Specifically the impact of adding 1-propanol, a polar solvent to a cyclohexane-heptane solution was investigated. This polar solvent is associating ionizable block and it’s expected to modify the packing of the polymer. Our results shows upon addition of 1-propanol, the spherical micelles transfer into worm like object. This transformation requires the break up of the ionic clusters formed by this polymer. These changes are in line with rheology measurements of Dr. Robert Weiss who has shown that propanol unlocks ionic clusters in polystyrene sulfonate.

3:30PM D43.00006 Reversible, All-Aqueous Assembly of Hydrogen-Bonded Polymersomes, YUHAO WANG, SVETLANA SUKHISHVILI, Department of Chemistry, Chemical Biology and Biomedical Engineering, Stevens Institute of Technology, Hoboken, New Jersey 07030 — We report on supra-micron-sized polymersomes formed through single-step, all-aqueous assembly of hydrogen-bonded amphiphilic polymers. The hollow morphology of these assemblies was revealed by transmission electron microscopy (TEM), cryogenic scanning electron microscopy (cryo-SEM) and confocal laser scanning microscopy (CLSM). Stable in acidic media, these polymersomes could be dissolved by exposure to basic pH values. Importantly, the diameter of assembled hollow structures could be controlled in a wide range from 30 nm to 1 µm by the molecular weight of hydrogen-bonding polymers. We will discuss key quantitative aspects of these assemblies, including kinetics of hollow structure formation, time evolution of polymersome size, and the role of polymer molecular weight on membrane thickness and bending rigidity. We believe that our approach demonstrates an efficient and versatile way to rationally design nanocounters for drug delivery, catalysis and personal care applications.

1 This work was supported by the Innovation & Entrepreneurship doctoral fellowship from Stevens Institute of Technology.
Aqueous Self-Assembly of Non-Ionic Bottlebrush Block Copolymer Surfactants with Tunable Molecular Shapes\(^1\). JAVID RZAYEV. University at Buffalo, SUNY — Polymer amphiphiles provide a robust and versatile platform for the fabrication of nanostructured soft matter. In this research, we explore a new class of polymer surfactants based on comb-like bottlebrush architecture as highly tunable molecular building blocks for aqueous self-assembly. Excluded volume interactions between densely grafted polymer side chains in the bottlebrush architecture are alleviated by backbone stretching, which leads to the formation of shape-persistent cylindrical macromolecules whose molecular dimensions can be precisely tailored during chemical synthesis. Amphiphilic bottlebrush block copolymers containing hydrophobic poly(lactide) (PLA) and hydrophilic poly(oligoethylene oxide methacrylate) (PEO) side chains of various lengths were synthesized by a combination of controlled radical and ring-opening polymerizations. In dilute aqueous solutions, bottlebrush surfactants rapidly assembled into spherical, cylindrical and bilayer aggregates, as visualized by cryogenic transmission electron microscopy (cryo-TEM). Depending on the compositional side chain asymmetry, the formation of spherical micelles with different sizes and dispersities was observed.

The molecular shape-dependent assembly was analyzed with help of a packing parameter \(p\) computed from the molecular composition data akin to small molecule surfactants, with most uniform spherical aggregates observed for bottlebrush amphiphiles with \(p\) close to 0.3. The formation of highly uniform micelles and the presence of a rich morphological diagram with relatively narrow compositional windows was attributed to the lack of conformational freedom in bottlebrush surfactants. Similarly, the unusual formation of cylindrical micelles with long aspect ratios was attributed to their inability to stabilize morphological defects, such as Y-junctions, with large deviations from mean curvature.

Financial support for this work was provided by the National Science Foundation (DMR-1409467).

4:18PM D43.00008 Phase Transfer of Polystyrene-b-poly(ethylene oxide) Polymersomes from a Hydrophobic Ionic Liquid to Water. SOONYONG SO, TIMOTHY LODGE. Univ of Minn - Minneapolis — The phase transfer of molecules and supramolecular assemblies from one phase to the other in a biphasic system is desirable for various applications such as catalysis, separation, and delivery. Herein, we describe the phase transfer of polystyrene-b-poly(ethylene oxide) (PS-PEO) polymersomes from a hydrophobic ionic liquid, 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([EMIM][TFSI]), into water. The phase transfer behavior of PS-PEO polymersomes was studied systematically by varying the molecular weight of PS and the PEO volume fraction of the PS-PEO. We demonstrate a general boundary for the phase transfer in terms of a reduced tethering density for PEO, which is independent of the molecular weight of the hydrophobic PS. The tethering density can be increased by increasing the block length of PEO and the size of the polymersomes, and the increased tethering density induces the phase transfer. This phase transfer were also analyzed thermodynamically with the free energy difference of the polymersomes in [EMIM][TFSI] and water. Higher grafting density can reduce the interfacial tension between PS and water, and leads the polymersomes to transfer from [EMIM][TFSI] to water at room temperature.

4:30PM D43.00009 Micellization and Gelation of Water Soluble Thermo-and Light-sensitive Block Copolymer Investigated by SANS. LILIN HE, Oak Ridge National Laboratory, BIN HU, BIN ZHAO, The University of Tennessee, Knoxville — Here we present an extensive small-angle neutron scattering (SANS) characterization of micellization and gelation of PEO-b-P(TEGA-co-NBA) in deuterated water in a wide range of temperatures and concentrations before and after the removal of o-nitrobenzyl group by UV irradiation. Scattering data analysis indicated that unimers predominated in the solutions at low temperatures and concentrations. The polymer self-assembled into micelles with the P(TEGA-co-NBA) block packed into the core and PEO forming the corona layer. A core-shell model was used to fit SANS data and obtain sizes and scattering length densities. Structural parameters such as the aggregation numbers, the radius of gyration of the chains in the shell region, the number of water molecules to the lack of conformational freedom in bottlebrush surfactants. Similarly, the unusual formation of cylindrical micelles with long aspect ratios was attributed to their inability to stabilize morphological defects, such as Y-junctions, with large deviations from mean curvature.

Monday, March 2, 2015 2:30PM - 5:30PM — Session D44 GSNP GSOFT: Invited Session: Mechanical Metamaterials 214D - Pedro Reis, Massachusetts Institute of Technology
both discrete and continuous Rouse chains. Direct and forward-flux simulations of Rouse chains of different lengths. A good agreement between the analytical calculations and simulations was achieved for the transition processes. Helfand proposed that the arm in the tube can be represented as a harmonic spring with an applied thermal tension such that the arm-end feels an entropic tension due to arm-retraction in which the star arms explore new configurations by withdrawing along their tubes and stretching out towards a new direction. Pearson and co-workers have shown that for a single star polymer in a melt of extremely long linear chains, the stress of star polymer relaxes within a time scale of the Rouse mode relaxation time [et al., 2004].

1 This research was done in collaboration with Zachary Nicolaou, and was supported by the National Science Foundation and the Alfred P. Sloan Foundation.

4:18 PM D44.00004 Performance through Deformation and Instability, KATIA BERTOLDI, SEAS, Harvard University — Materials capable of undergo large deformations like elastomers and gels are ubiquitous in daily life and nature. An exciting field of engineering is emerging that uses these compliant materials to design active devices, such as actuators, adaptive optical systems and self-regulating fluidics. Compliant structures may significantly change their architecture in response to diverse stimuli. When excessive deformation is applied, they may eventually become unstable. Traditionally, mechanical instabilities have been viewed as an inconvenience, with research focusing on how to avoid them. Here, I will demonstrate that these instabilities can be exploited to design materials with novel, switchable functionalities. The abrupt changes introduced into the architecture of soft materials by instabilities will be used to change their shape in a sudden, but controlled manner. Possible and exciting applications include materials with unusual properties such negative Poisson’s ratio, phononic crystals with tunable low-frequency acoustic band gaps and reversible encapsulation systems.

4:54 PM D44.00005 Programmable and Frustrated Mechanical Metamaterials, MARTIN VAN HECKE, Huigens-Kamerlingh Onnes Lab, Leiden University, the Netherlands, and FOM-Institute Amolf, Amsterdam, the Netherlands — Most metamaterials to data consist of periodic lattices of unit cells that work together in harmony. Here we demonstrate how frustration leads to new functionality. First we discuss 2D mechanical metamaterials whose response to uniaxial compression can be programmed by lateral confinement, allowing monotonic, nonmonotonic, and hysteretic behavior. These functionalities arise from a broken rotational symmetry which causes a highly nonlinear competition between two mutually incompatible modes of deformation. Second we show how to create non-periodic 3D metamaterials, leading to a wealth of novel functionalities, including mechanical pattern recognition. By perturbing the stacking order in these materials we incorporate frustration which leads to multistable behavior.

Monday, March 2, 2015 2:30PM - 5:18PM –

Session D45 DPOLY: Polymer Melts & Solutions II 216AB - Muzhou Wang, National Institute of Standards and Technology

2:30PM D45.00001 From form to feel: using origami design principles to shape mechanics, CHRISTIAN SANTANGELO, University of Massachusetts — No abstract available.

3:06PM D44.00002 Mechanical metamaterials for cloaking, MARTIN WEGENER, Karlsruhe Institute of Technology — We review our experiments on mechanical metamaterials for cloaking. This includes two-dimensional graded laminate elastic metamaterials for broadband cloaking of flexural waves in thin plates, three-dimensional pentamode metamaterials and modifications thereof, e.g., for three-dimensional core-shell cloaks, and direct coordinate transformations of discrete hexagonal lattices. We suspect that the latter mimic inhomogeneous and anisotropic Cossatot metamaterial distributions. Polymer structures with sub-micrometer feature sizes are fabricated by galvo-scanner dip-in three-dimensional direct-laser-writing optical lithography, macroscopic structures by a commercially available three-dimensional printer.

3:42PM D44.00003 Mechanical Metamaterials with Negative Compressibility Transitions, ADILSON MOTTER, Northwestern University — When tensioned, ordinary materials expand along the direction of the applied force. In this presentation, I will explore network concepts to design metamaterials exhibiting negative compressibility transitions, during which the material undergoes contraction when tensioned (or expansion when pressured). Such transitions, which are forbidden in thermodynamic equilibrium, are possible during the decay of metastable, super-strained states. I will introduce a statistical physics theory for negative compressibility transitions, derive a first-principles model to predict these transitions, and present a validation of the model using molecular dynamics simulations. Aside from its immediate mechanical implications, our theory points to a wealth of analogous inverted responses, such as inverted susceptibility or heat-capacity transitions, allowed when considering realistic scales. References: Z.G. Nicolaou and A.E. Motter, J. Stat. Phys. 151(6), 1102 (2013); Z.G. Nicolaou and A.E. Motter, Nature Materials 11, 608 (2012).

3:54PM D44.00004 Visco-elasticity of bottlebrush polymer melts: Pushing the lower limit of the entanglement modulus, WILLIAM DANIEL, Univ of NC - Chapel Hill, JOANNA BURDYNASKA, Carnegie Mellon University, ANDREY DOBRYNIN, Univ of Conn, KRZYSZTOF MATYJASZEWSKI, Carnegie Mellon University, MICHAEL RUBINSTEIN, SERGEI SHEIKO, Univ of NC - Chapel Hill, MATERIALS INTERDISCIPLINARY RESEARCH TEAM @ UNC CHAPEL HILL TEAM — Without swelling in a solvent, it is challenging to obtain materials with a modulus below 1 GPa, which is dictated by chain entanglements. Here we analyze the densely grafted molecular brush architecture to create solvent-free neat polymer melts and elastomers with plateau moduli down to hundred Pa. Such materials are theorized to behave as linear chains with rescaled dimensions of the entanglement strand due to the increase in both width and persistence length of polymer bottlebrushes. This simple rescaling leads to a prediction that entanglement modulus decreases with the degree of polymerization (DP) of the sidechains to the -1.5 power. Experimental evidence gives a remarkably close power of -1.38 ± 0.05 with moduli in the hundreds of Pascals for long sidechains with DP≈100. The experimental data have been fit using a combination of the Rouse relaxation and double reputation models lending further evidence that bottlebrush polymer behave as linear polymers with large entanglement weights and longer persistence lengths. With the addition of crystallizable block it will be possible to control the crosslinking density and design ultrasoft shape-memory materials for use in mechanically sensitive applications.

4:24PM D45.00002 First-Passage Time in Entangled Star Polymers Melts, JING CAO, JIAN ZHU, ZUOWEI WANG, ALEXEI LIKHTMAN, Univ of Reading — For a single star polymer in a melt of extremely long linear chains, the stress of star polymer relaxes by arm-retraction in which the star arms explore new configurations by withdrawing along their tubes and stretching out towards a new direction. Pearson and Helfand proposed that the arm in the tube can be represented as a harmonic spring with an applied thermal tension such that the arm-end feels an entropic force if it fluctuates away from its equilibrium position. We have investigated the first-passage(FP) time of the destruction of tube segments by representing the arm as a one-dimensional Rouse chain. In contrast, we found that the disengagement of a tube segment is getting faster with more Rouse modes added in, which means the FP problem can be modelled by a multi-dimensional multi-Schrödinger’s problem. We found a new way of solving the multi-dimensional FP problem by projecting the problem along the most probable trajectory termed “minimal action trajectory” and correcting it by entropy term. In addition, we performed direct and forward-flux simulations of Rouse chains of different lengths. A good agreement between the analytical calculations and simulations was achieved for both discrete and continuous Rouse chains.
2:54PM D45.00003 Simplified tube models for entangled supramolecular polymers \(^1\) — VICTOR BOUDARA, DANIEL READ, University of Leeds — This presentation describes current efforts investigating non-linear rheology of entangled, supramolecular polymeric materials. We describe two recently developed models: 1) We have developed a simplified model for the rheology of entangled telechelic star polymers. This is based on a pre-averaged orientation tensor, a stretch equation, and stretch-dependent probability of detachment of the sticker. In both linear and non-linear regimes, we produce maps of the whole parameter space, indicating the parameter values for which qualitative changes in response to flow are predicted. Results in the linear rheology regime are consistent with previous more detailed models (van Ruijweke et al. Macromolecules, 43, 4401-4411, 2010) and are in qualitative agreement with experimental data. 2) Using the same modelling framework, we investigate entangled linear polymers with stickers along the backbone. We use a set of coupled equations to describe the stretch between each stickers, and use equations similar to our star model for attachment/detachment of the sticky groups. This model is applicable to industrial polymers such as entangled thermoplastic elastomers, or functionalised model linear polymers.

\(^1\)The work leading to these results has received funding from the People Programme (Marie Curie Actions) of the European Union’s Seventh Framework Programme (FP7/2007-2013) under REA grant agreement no. 607937 (SUPOLEN)

3:06PM D45.00004 Fingerprinting the Non-linear Response of Three Arm Star Polystyrene by Mechanical Spectral Hole Burning, Lissajous-Bowditch Loops, and Fourier Transform Rheology \(^2\) — ZHIYUAN QIAN, GREGORY B. MCKENNA, Texas Tech Univ — It is well known that large amplitude oscillatory shear (LAOS) has become a powerful tool to fingerprint the nonlinear response of polymers and other complex fluids. In a recent work, Nabila and McKenna [J. Rheol. 58(1), 43-62, 2014] used the mechanical spectral hole burning (MSHB) which was developed in their labs, along with Lissajous-Bowditch (LB) curves and Fourier transform rheology (FTR) methods to characterize the nonlinearity of linear polystyrene solutions. They observed a linear relationship between the horizontal hole intensity and the square of pump strain amplitude. The similar quadratic dependence was found for the third harmonics from FTR. However, the origins are not same for these two signatures. In the current work, the nonlinearity of polymers with more complicated molecular structure, such as three arm star polystyrene, will be studied by these three methods. The concentration dependence of the fingerprinting will also be discussed.

\(^2\)The authors are thankful to the American Chemical Society, Petroleum Research Fund 53205-ND7, for the support of this project.

3:18PM D45.00005 Breakup dynamics of Non-Newtonian droplets in microfluidic devices: From necking to Rupture — POUYAN BOUKANY, SHAURYA SACHDEV, Delft University of Technology — It has been shown that addition of small amounts of polymers to a Newtonian fluid can exhibit non-Newtonian behavior in extensional flows. For instance, polymeric fluids produce strong filament thinning called necking when subjected to extensional flows. Coiled polymeric chains are expected to be stretched in this exponential necking regime. These stretched long chains induce elastic stress that resist the capillary forces trying to break the filament apart. Still, the molecular picture behind filament thinning and rupture of polymeric threads in extensional flow conditions is unknown. In this work, we study breakup and filament thinning of micro-droplets containing polymeric suspensions by using micro-fluidic devices. To reveal the underlying mechanism of thinning and rupture of polymeric filament, conformation of DNA suspensions were visualized in different flow conditions. Experiments have been done on both dilute and concentrated polymeric solutions. These new results allow us to explain the molecular mechanism behind filament thinning and flow instabilities in strong extensional flows of polymeric fluids.


3:30PM D45.00006 Polymer relaxation and stretching dynamics in semi-dilute DNA solutions: a single molecule study \(^1\) — KAI-WEN HSIAO, Graduate student at University of Illinois at Urbana Champaign, CHRISTOPHER BROCKMAN, Intel, CHARLES SCHROEDER, Associate professor at University of Illinois at Urbana Champaign — In this work, we study polymer relaxation and stretching dynamics in semi-dilute DNA solutions using single molecule techniques. Using this approach, we uncover a unique scaling relation for longest polymer relaxation time that falls in the crossover regime described by semi-flexible polymer solutions, which is distinct from truly flexible polymer chains. In addition, we performed a series of step-strain experiments on single polymers in semi-dilute solutions in planar extensional flow using an automated microfluidic trap. In this way, we are able to precisely control the flow strength and the amount of strain applied to single polymer chains, thereby enabling direct observation of the full stretching and relaxation process in semi-dilute solutions during transient start-up and flow cessation. Interestingly, we observe polymer individualism in the conformation of single chains in semi-dilute solutions, which to our knowledge has not yet been observed. In addition, we observe the relaxation data can be explained by a multi-exponential decay process after flow cessation in semi-dilute solutions. Overall, our work reports key advances in non-dilute polymer systems from a molecular perspective via direct observation of dynamics in strong flows.

\(^1\)DOW fellowship

3:42PM D45.00007 Optical Nanodozers — AHMED KHORSHID, WALTER REISNER, McGill University, TAKAHIRO SAKAUE, Kyushu University — Experiment, simulation and scaling analytics are converging on a comprehensive picture regarding the equilibrium behaviour of nanochannel confined semiflexible, self-avoiding chains. Yet, strongly non-equilibrium behaviour of confined polymers is largely unexplored from either an experimental or theoretical point of view. Combining optical trapping and nanofluidics, we have developed a “nandozer” assay for quantifying confined polymer dynamics. An optical trap is used to slide a nanosphere at a fixed velocity along a nanochannel. The trapped bead acts as a permeable gasket, letting fluid escape but preventing the polymer from passing. As the sliding bead comes in contact with a nanochannel extended DNA, the molecule is dynamically compressed, undergoing transient dynamics characterized by a traveling concentration “shockwave” before reaching a final steady state with a ramp-like concentration profile. Remarkably, these strongly nonequilibrium measurements can be quantified via a simple nonlinear convective-diffusion formalism and yield insights into the local blob statistics, allowing us to conclude that the compressed nanochannel confined chain exhibits mean-field behaviour.

3:54PM D45.00008 Shear and normal forces in charged polymer brushes — QI LIAO, Chinese Academy of Sci (CAS), MICHAEL RUBINSTEIN, Department of Chemistry, University of North Carolina, Chapel Hill, 27599 NC, USA — We present the results of molecular dynamics simulations of steady shear between a pair of opposing charged polymer brushes in the osmotic-brush regime and compare the results with predictions of scaling models. Using the monomer and counterion density profiles, we have verified different regimes in the diagram of states of compressed polyelectrolyte brushes predicted by the scaling model of Zhuлина et al [Macromolecules, 2014]. Our simulation results for the normal forces of compressed polyelectrolyte brushes are in excellent agreement with predictions of the scaling model. However, our results for the dependence of the shear forces on the separation between brushes are only in qualitative agreement with the predictions of the scaling model. The dependence of the interpenetration length on the separation of polyelectrolyte brushes exhibits a maximum instead of the plateau predicted by the scaling model for the partially interpenetrated brushes. Our simulation results confirm that our implicit solvent simulations of polyelectrolyte brushes that ignore hydrodynamic interaction are in agreement with the scaling predictions that include hydrodynamic interaction because of screening of hydrodynamic interaction and long range electrostatic interactions on the correlation length scale.
A Molecular Mechanism of viscoelasticity in aligned polyethylene

A. Hamad, H. Hasan, T.D. Swinburne, M. Kawaija, Department of Physics, Imperial College London, London SW7 2AZ, S. Del-Rossa, L. Ianniucci, Department of Aeronautics, Imperial College London, London SW7 2AZ — The key observed property of aligned polyethylene is its viscoelastic behaviour, which is traditionally fitted with Maxwell models [1]. Although these empirical models are successful at reproducing the mechanical response of the material, they fail to capture the underlying molecular mechanisms that lead to the observed viscoelastic behaviour. We explain the observed viscoelastic behaviour in terms of the formation, interaction and movement of solitons, and relate these molecular mechanisms to the semi-crystalline microstructure of the material. Using Molecular Dynamics we demonstrate the following results: (a) The formation of solitons from interfaces between crystalline and amorphous regions (b) The transfer of tensile load between molecular chains (c) the pile-up of solitons in a molecular chain that allows the concentration of stress at particular points (d) The disassociation of solitons into π-twistons at 300K.


European Science Research Council (EPSRC)

Electrostatics effects on normal load capacity of two like-charge hydrogels

Aykut Erbas, Jos Zwanikken, Monica Olivera de la Cruz, Northwestern University, OLVERA DE LA CRUZ TEAM — In mammalian joints, an effective lubrication mechanism is maintained under extremely high pressures due to charged polymeric structures coating the surfaces of the relatively moving tissues. Equally low frictional forces are also observed experimentally in the shear motion of polyelectrolyte gel and brush bilayers. The lubrication capabilities of these systems are attributed to either a polymer-free zone, separating the bilayers or hydration layers that can dissolve polymeric segments. Previous hypothesis have stated that the separation zone should decrease the polymer-polymer physical contact, and hence, result in only viscous friction of the liquid filling this layer. In this study, we use extensive Molecular Dynamics simulations and analytical tools, we investigate the separation zone under compression at high electrostatic strengths. We show that Coulomb interactions significantly change the thickness of the separation zone, as well as the normal pressure that a hydrogel bilayer can support upon control-strains deformation. We observe that under high pressures the separation zone completely disappears. As a result, the number of polymer-polymer contacts increases. We speculate that the frictional forces between polymer segments can reduce the efficiency of the lubrication.

Hierarchical assembly of block copolymer micelles into reversible networks: MC simulations

Zilu Wang, Physics Department and Institute of Materials Science, University of Connecticut, Elena Dormidonova, Institute of Materials Science, University of Connecticut — The rapid development of nanoscience has considerably expanded the range of building blocks for complex self-assembled nanostructure formation, which show great potential for numerous advanced applications. We apply Monte Carlo simulations to gain understanding of molecular mechanism of self-assembly of nanostructures formed by diblock copolymer micelles interconnected by means of metal-ligand complexation. These systems exhibit interesting chemical and mechanical stimuli-responsive behavior and possess two levels of self-assembly: 1) self-assembly of diblock copolymers into micelles and 2) reversible inter-micelle bridging by coordination bonding between metal ions and ligands attached to the coronas of nanoparticles, which is responsible for the network viscoelastic properties. Using MC simulations we investigate the effect of metal-ligand complexation on diblock-copolymer micelle formation and vice versa. We analyze the extent of intra- and inter-micelle loops and bridges formed by metal-ligand complexion in relation to the degree of crosslinking and elastic properties of the network. The effect of polymer concentration, hydrophilic block length, metal to oligomer ratio and type of complexation (2:1 or 3:1) on equilibrium properties of reversible networks will be discussed.


217A - Andre Schleife, University of Illinois-Urbana
2:30PM D46.00001 Achieving High Performance Perovskite Solar Cells. YANG YANG, University of California, Los Angeles — Recently, metal halide perovskite based solar cell with the characteristics of rather low raw materials cost, great potential for simple process and scalable production, and extreme high power conversion efficiency (PCE), have been highlighted as one of the most competitive technologies for next generation thin film photovoltaic (PV). In UCLA, we have realized an efficient pathway to achieve high performance perovskite solar cells, where the findings are beneficial to this unique materials/devices system. Our recent progress lies in perovskite film formation, defect passivation, transport materials design, interface engineering with respect to high performance solar cell, as well as the exploration of its applications beyond photovoltaics. These achievements include: 1) development of vapor assisted solution process (VASP) and moisture assisted solution process, which produces perovskite film with improved conformity, high crystallinity, reduced recombination rate, and the resulting high performance; 2) examination of the defects property of perovskite materials, and demonstration of a self-induced passivation approach to reduce carrier recombination; 3) interface engineering based on design of the carrier transport materials and the electrodes, in combination with high quality perovskite film, which delivers 15 ~ 20% PCEs; 4) a novel integration of bulk heterojunction to perovskite solar cell to achieve better light harvest; 5) fabrication of inverted solar cell device with high efficiency and flexibility and 6) exploration the application of perovskite materials to photodetector. Further development in film, device architecture, and interfaces will lead to continuous improved perovskite solar cells and other organic-inorganic hybrid optoelectronics.

3:06PM D46.00002 Modeling organohalide perovskites for photovoltaic applications: From materials to interfaces†. FILIPPO DE ANGELIS, Computational Laboratory for Hybrid/Organic Photovoltaics, CNR-ISTM, Perugia — The field of hybrid/organic photovoltaics has been revolutionized in 2012 by the first reports of solid-state solar cells based on organohalide perovskites, now topping at 20% efficiency. First-principles modeling has been widely applied to the dye-sensitized solar cells field, and more recently to perovskite-based solar cells. The computational design and screening of new materials has played a major role in advancing the DSCs field. Suitable modeling strategies may also offer a view of the crucial heterointerfaces ruling the device operational mechanism. I will illustrate how simulation tools can be employed in the emerging field of perovskite solar cells. The performance of the proposed simulation toolbox along with the fundamental modeling strategies are presented using selected examples of relevant materials and interfaces. The main issue with hybrid perovskite modeling is to be able to accurately describe their structural, electronic and optical features. These materials show a degree of short range disorder, due to the presence of mobile organic cations embedded within the inorganic matrix, requiring to average their properties over a molecular dynamics trajectory. Due to the presence of heavy atoms (e.g. Sn and Pb) their electronic structure must take into account spin-orbit coupling (SOC) in an effective way, possibly including GW corrections. The proposed SOC-GW method constitutes the basis for tuning the materials electronic and optical properties, rationalizing experimental trends. Modeling charge generation in perovskite-sensitized TiO₂ interfaces is then approached based on a SOC-DFT scheme, describing alignment of energy levels in a qualitatively correct fashion. The role of interfacial chemistry on the device performance is finally discussed.

3:42PM D46.00003 Interface Energetics in Organo-Metallic Halide Perovskite-based Photo-voltaic Cells. PHILIP SCHULZ, National Renewable Energy Laboratory — In my presentation I will talk about the most recent findings on the electronic structure of methylammonium lead tri-halide (MAPbX₃, X=I, Br) perovskite films and their interfaces to adjacent transport layers. Intricate knowledge of the electronic alignment at the contact interfaces in perovskite solar cells is essential for the understanding of the working principle as well as improving design and thus performance of respective devices. In our studies we employ ultra-violet, X-ray and inverse photoemission spectroscopy (UPS, XPS, IPES) to directly determine valence and conduction band offsets. In this way we are able to report a direct measurement of the electronic band gap as well as ionization energy and electron affinity found for perovskite surfaces. Furthermore, our findings indicate that the electronic energy level alignment of adjacent organic hole transport layers, such as spiro-MeOTAD, can limit the maximum attainable open circuit voltage (V_{oc}) in solar cells if the highest occupied molecular orbital of the hole transport material is not well aligned to the valence band maximum of the perovskite layer. Using better suited hole transporters, like CBP, values for V_{oc} larger than 1.5 V could be achieved in the case of MAPbBr₃ based devices. More recently, inverted perovskite solar cells based on nickel oxide bottom anodes have been reported to yield viable power conversion efficiencies and stability. We find that the interface between the p-doped NIO surface and the MAPbI₃ layer on top lead to p-type perovskite film while the same material deposited on TiO₂ in the conventional cell geometry turns out to be n-type. A further investigation of a C₆₀ layer deposited on top of p-type perovskite films reveals an ideal alignment between the lowest unoccupied molecular orbital of the organic electron transport materials and the conduction band minimum of the perovskite film underneath. These results explain why the inverted solar cell structure could achieve similar successes as the conventional structure and highlight the versatility of perovskite sub-cells in potential tandem cell architectures.

4:18PM D46.00004 Impact of Atomic Structure on Absolute Energy Levels of Methylammonium Lead Iodide Perovskite. JOSHUA CHOI, University of Virginia — There has been a staggeringly rapid increase in the photovoltaic performance of methylammonium lead iodide (MAPbI₃) perovskite - greater than 19 percent solar cell power conversion efficiency has been reported in less than five years since the first report in 2009. Despite the progress in device performance, structure-property relationships in MAPbI₃ are still poorly understood. I will present our recent findings on the impact of changing the Pb-I bond length and Pb-I-Pb bond angle on the electronic structure of MAPbI₃. By using the combination of temperature dependent X-ray scattering, ultraviolet photoelectron spectroscopy, absorbance and PL spectroscopy, we show that the energy levels of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) shift in the same direction as MAPbI₃ goes through tetragonal-to-cubic structural phase transition wherein the rotational angle of PbI₆ octahedra is the order parameter of the transition. Our experimental results are corroborated by density functional theory calculations which show that the lattice expansion and bond angle distortion cause different degree of orbital overlap between the Pb and I atoms and the anti-bonding orbital nature of both HOMO and LUMO results in the same direction of their shift. Moreover, through pair distribution function analysis of X-ray scattering, we discovered that the majority of MAPbI₃ in thin film solar cell layer has highly disordered structure with a coherence range of only 1.4 nm. The nanostructuring correlates with a blueshift of the absorption onset and increases the photoluminescence. Our results underscore the importance of understanding the structure-property relationships in order to improve the device performance of metal-organic perovskites.
4:54PM D46.00005 Electronic structure of hybrid halide perovskite photovoltaic absorbers. MARK VAN SCHILFGAARDE, King’s College London — The performance of organometallic perovskite solar cells has rapidly surpassed those of both traditional dye-sensitized and organic photovoltaics, e.g., solar cells based on CH$_3$NH$_3$PbI$_3$ have recently reached 18% conversion efficiency. We analyze its electronic structure and optical properties within the quasiparticle self-consistent GW approximation (QSGW). Quasiparticle self-consistency is essential for an accurate description of the band structure: bandgaps are much larger than what is predicted by the local density approximation (LDA) or GW based on the LDA. Several characteristics combine to make the electronic structure of this material unusual. First, there is a strong driving force for ferroelectricity, as a consequence the polar organic moiety CH$_3$NH$_3$. The moiety is only weakly coupled to the PbI$_3$ cage; thus it can rotate give rise to ferroelectric domains. This in turn will result in internal junctions that may aid separation of photoexcited electron and hole pairs, and may contribute to the current-voltage hysteresis found in perovskite solar cells. Second, spin orbit modifies both valence band and conduction band dispersions in a very unusual manner: both get split at the R point into two extrema nearby. This can be interpreted in terms of a large Dresselhaus term, which vanishes at R but for small excitations about R varies linearly in k. Conduction bands (Pb 6p character) and valence bands (I 5p) are affected differently; moreover the splittings vary with the orientation of the moiety. We will show how the splittings, and their dependence on the orientation of the moiety through the ferroelectric effect, have important consequences for both electronic transport and the optical properties of this material.

3:30PM D47.00001 The neurobiology of individuality. BENJAMIN DE BIVORT, Harvard University — Individuals often display conspicuously different patterns of behavior, even when they are very closely related genetically. These differences give rise to our sense of individuality, but what is their molecular and neurobiological basis? Individuals that are nominally genetically identical differ at various molecular and neurobiological levels: cell-to-cell variation in somatic genomes, cell-to-cell variation in expression patterns, individual-to-individual variation in neuronal morphology and physiology, and individual-to-individual variation in patterns of brain activity. It is unknown which of these levels is fundamentally causal of behavioral differences. To investigate this problem, we use the fruit fly Drosophila melanogaster, whose genetic toolkit allows the manipulation of each of these mechanistic levels, and whose rapid lifecycle and small size allows for high-throughput automation of behavioral assays. This latter point is crucial; identifying inter-individual behavioral differences requires high sample sizes both within and across individual animals. Automated behavioral characterization is at the heart of our research strategy. In every behavior examined, individual flies have individual behavioral preferences, and we have begun to identify both neural genes and circuits that control the degree of behavioral variability between individuals.

2:30PM D47.00002 Higher throughput high resolution multi-worm tracker. AVELINO JAVER, KEZHI LI, BERTALAN GYENES, ANDRE BROWN, MRC CSC, Imperial College London, BEHAVIOURAL GENOMICS TEAM — We have developed a high throughput imaging system for tracking multiple nematode worms at high resolution. The tracker consists of 6 cameras mounted on a motorized gantry so that up to 48 plates (each with approximately 30 worms) can be imaged without user intervention. To deal with the high data rate of the cameras we use real time processing to find worms and only save the immediately surrounding pixels. The system is also equipped with automatic oxygen and carbon dioxide control for observing stimulus response behaviour. We will describe the design and performance of the new system, some of the challenges of truly high throughput behaviour recording, and report preliminary results on inter-individual variation in behaviour as well as a quantitative analysis of C. elegans response to hypoxia, oxygen reperfusion, and carbon dioxide.

1Supported by EPSRC grant EP/M009602/1

3:18PM D47.00003 Locomotion and drag in wet and dry granular media. DANIEL GOLDMAN, ROBYN KUCKUK, SARAH SHARPE, Georgia Institute of Technology — Many animals move within substrates such as soil and dry sand; the resistive properties of such granular materials (GM) can depend on water content and compaction, but little is known about how such parameters affect locomotion or the relevant physics of drag and penetration. We developed a system to create homogeneous wet GM of varying moisture content and compaction in quantities sufficient to study the burial and subsurface locomotion of the Ocellated skink (C. ocellatus) a desert-generalist lizard. X-ray imaging revealed that in wet and dry GM the lizard slowly buried (~30 seconds) propagating a wave from head to tail, while moving in a start-stop motion. During forward movement, the head oscillated, and the forelimb on the convex side of the body propelled the animal. Although body kinematics (and “slip”) were similar in both substrates, the burial depth was smaller in wet GM. Penetration and drag force experiments on smooth cylinders revealed that wet GM was ~3× more resistive than dry GM, suggesting that during burial the lizard operated near its maximum force producing capability and was thus constrained by environmental properties.

1Supported by the Medical Research Council

3:06PM D47.00002 Higher throughput high resolution multi-worm tracker. AVELINO JAVER, KEZHI LI, BERTALAN GYENES, ANDRE BROWN, MRC CSC, Imperial College London, BEHAVIOURAL GENOMICS TEAM — We have developed a high throughput imaging system for tracking multiple nematode worms at high resolution. The tracker consists of 6 cameras mounted on a motorized gantry so that up to 48 plates (each with approximately 30 worms) can be imaged without user intervention. To deal with the high data rate of the cameras we use real time processing to find worms and only save the immediately surrounding pixels. The system is also equipped with automatic oxygen and carbon dioxide control for observing stimulus response behaviour. We will describe the design and performance of the new system, some of the challenges of truly high throughput behaviour recording, and report preliminary results on inter-individual variation in behaviour as well as a quantitative analysis of C. elegans response to hypoxia, oxygen reperfusion, and carbon dioxide.

1Supported by EPSRC grant EP/M009602/1

3:30PM D47.00004 Physics of Fission and Fusion for the Diagnostics and Monitoring of the Deadliest Illness of Mankind. ARJUN SAXENA, Retired — The physics of fission and fusion has been well known for the past several decades. It has been used primarily for destructive purposes (e.g., nuclear armaments) with both processes. However for peaceful purposes, e.g., generation of energy, only fission has been used, but not yet fusion. It is also well known that the deadliest illness of mankind is the group of illnesses called mental illnesses. A large segment of the world population is afflicted by them causing more loss of human lives, destruction of families, businesses and overall economy than all the other illnesses combined. Despite outstanding advancements in medical research and huge investments, unfortunately no diagnostic techniques have yet been found which can characterize the patient’s mental illness. Consequently, no quantitative monitoring techniques are available to evaluate the efficacy of the various medicines used to treat the patients, and to develop them in the pharmaceutical labs. The purpose of this paper is to apply the constructive aspects of fission and fusion to identify the missing links in the diagnosis and treatment of mental illnesses. Each patient is a unique human being, not a disease or a group of symptoms. This makes it even more difficult to treat the patients suffering from mental illness...
Sparse Coding of Natural Human Motion Yields Eigenmotions Consistent Across People

Across People emergent run-and-tumble sparse activation of “eigenmotion” neurons, and is consistent with data on grasp-type specificity of specialised neurons in the premotor cortex. Our findings suggest the motor system can compose complex movement behaviours out of the spatially and temporally sparse activation of “eigenmotion” neurons, and is consistent with data on grasp-type specificity of specialised neurons in the premotor cortex.

A stochastic model for bacterial dynamics toward point food sources with emergent run-and-tumble. — HOSSEIN JASHNSAZ, TYLER NGUYEN, HORIA PETRACHE, STEVE PRESSE, Indiana University- Purdue University- Indianapolis, STATPHYSBIO TEAM — Despite stark differences in chemotactic signaling networks and flagellar physiology across bacterial species, all bacteria sense their environment through a series of stochastic detection events (“hits”) at their chemoreceptors and bias their random walk on the basis of this information. We present a general statistical model describing how bacteria locate point sources of food on the basis of stochastic event detection, rather than gradient information. We show how model parameters can be directly inferred using maximum likelihood methods from microscopy tracking data. We find that “run-and-tumble” dynamics naturally emerge from our statistical model and recapitulate known results from experiments when we consider bacterial dynamics in well-controlled chemotactrant gradients. However, our model goes beyond reproducing known run-and-tumble statistics. It also makes a number of predictions unique to bacteria tracking point sources. In our model, all parameters are directly inferred from tracking data thus there are no adjustable parameters; detection events by bacteria are assumed stochastic as they occur in nature; and our “top-down” modeling approach is broadly applicable across bacterial species.

Adhesion of D. discoideum on Hydrophobic Substrate

2:30PM D48.00001 Adhesion of D. discoideum on Hydrophobic Substrate

PLOSCARIU, Kansas State University — Adhesion by amoeboid cells, such as D. discoideum, is poorly understood but critical for other behaviors such as phagocytosis and migration. Furthermore, both leucocytes and breast cancer cells employ the amoeboid mode of movement at various points in their life-cycles. Hence, improved knowledge of amoeboid adhesion may lead to be new strategies for controlling other important cellular processes. This study regards adhesion by D. discoideum on silanized glass substrates. Reflection interference contrast microscopy is used in conjunction with other methods to determine the contact angle, cell-medium interfacial energy, and adhesion energy of these cells. The contact angle of individual cells settling under gravity onto a substrate is observed to increase as the size of the contact patch increases. This behavior occurs on slower time-scales than expected for the settling of inert vesicles. The implications of this observation on the nature of the underlying forces will be discussed. 

Energetic modeling and single-molecule verification of dynamic regulation on receptor protein diffusion by actin corals and lipid raft domains receptor

2:42PM D48.00002 Energetic modeling and single-molecule verification of dynamic regulation on receptor protein diffusion by actin corals and lipid raft domains receptor

CHIEN YU LIN, JUNG Y. HUANG, Department of Photonics, Chiao Tung University, LEU-WEI LO, Institute of Biomedical Engineering and Nanomedicine, National Health Research Institutes — To faithfully estimate a signal that varies in both space and time, the optimization strategy used by a live cell is to organize a collection of distributed and mobile receptors into a mobile active clustering. However, living eukaryotic cells are highly heterogeneous and stochastically dynamic. It is therefore important to develop an energetic model based on fundamental laws to verify that the underlying processes are energetically favorable. We developed an energetic model based on the generalized Langevin equation and the Cahn-Hilliard equation to simulate the diffusive behaviors of receptor proteins in the plasma membrane with a hierarchical structure of actin corals, lipid domains, and receptor proteins. Single-molecule tracking data of EGFR acquired on live HeLa cells agrees with the simulation results. We discovered that after ligand binding, EGFR molecules move into lipid nanodomains. The transition rates between different diffusion states of liganded EGFR molecules are regulated by the lipid domains. Our method captures both the sensitivity of single-molecule processes, statistic accuracy of data analysis, and the hierarchical structure of plasma membranes.

Possible Domain Formation In PE/PC Bilayers Containing High Cholesterol

2:54PM D48.00003 Possible Domain Formation In PE/PC Bilayers Containing High Cholesterol

MATTHEW HEIN, FAZLE HUSSAIN, JUYANG HUANG, Texas Tech University — Cholesterol is a significant component of animal cell membranes, and its presence has the effects of not only adding rigidity to the lipid bilayer, but also leading to the formation of lipid domains. Two other lipids of interest are phosphatidylethanolamine (PE), which constitutes about 45 percent of the phospholipids found in human nervous tissues, and phosphatidylcholine (PC), which is found in every cell of the human body. The maximum solubility of cholesterol is the highest molle fraction of cholesterol that the lipid bilayer can retain, at which point cholesterol begins to precipitate out to form cholesterol monohydrate crystals. We have measured the maximum solubility of cholesterol in mixtures of 16:0-18:1PE and 16:0-18:1PC using a new light scattering technique, which utilizes the anisotropic nature of light scattering by cholesterol crystals. This new method is highly accurate and reproducible. Our results show that the maximum solubility of cholesterol increases linearly as a function of the molar ratio POPC/(POPE+POPC), which suggests possible domain formation in mixtures of PE and PC containing maximum amount of cholesterol.
3:06PM D48.00004 Self-Healing of Polymer Networks with Reversible Bonds

Michael Rubinstein,
University of North Carolina at Chapel Hill — Self-healing polymeric materials are systems that after damage can revert to their original state with full or partial recovery of mechanical strength. Using scaling theory we study a simple model of autonomic self-healing of polymer networks. In this model one of the two end monomers of each polymer chain is fixed in space mimicking dangling chains attachment to a polymer network, while the sticky monomer at the other end of each chain can form pairwise reversible bond with the sticky end of another chain. We study the reaction kinetics of reversible bonds in this simple model and analyze the different stages in the self-repair process. The formation of bridges and the recovery of the material strength across the fractured interface during the healing period occur appreciably faster after shorter waiting time, during which the fractured surfaces are kept apart. We observe the slowest formation of bridges for self-adhesion after bringing into contact two bare surfaces with equilibrium (very low) density of open stickers in comparison with self-healing. The primary role of anomalous diffusion in material self-repair for short waiting times is established, while at long waiting times the recovery of bonds across fractured interface is due to hopping diffusion of stickers between different bonded partners. Acceleration in bridge formation for self-healing compared to self-adhesion is due to excess nonequilibrium concentration of open stickers. Full recovery of reversible bonds across fractured interface (formation of bridges) occurs after appreciably longer time than the equilibration time of the concentration of reversible bonds in the bulk. The model is extended to describe enhanced toughness of dual networks with both permanent and reversible cross-links.

1This work was done in collaboration with Drs. Ludwik Leibler, Li-Heng Cai, Evgeny B. Stukalin, N. Arun Kumar and supported by the National Science Foundation.

3:42PM D48.00005 Assembly of transmembrane proteins on oil-water interfaces

Peter Yunker,
Georgia Institute of technology, Harvard University, New England Biolabs, Corey Landry, Louisiana State University, ShaoRong Chong, New England Biolabs, David Weitz, Harvard University — Transmembrane proteins are difficult to handle by aqueous solution-based biochemical and biophysical approaches, due to the hydrophobicity of transmembrane helices. Detergents can solubilize transmembrane proteins; however, surfactant coated transmembrane proteins are not always functional, and purifying detergent coated proteins in a micellar solution can be difficult. Motivated by this problem, we study the self-assembly of transmembrane proteins on oil-water interfaces. We found that the large water-oil interface of oil drops prevents nascent transmembrane proteins from forming non-functional aggregates. The oil provides a hydrophobic environment for the transmembrane helix, allowing the ectodomain to fold into its natural structure and orientation. Further, modulating the strength or valency of hydrophobic interactions between transmembrane proteins results in the self-assembly of spatially clustered, active proteins on the oil-water interface. Thus, hydrophobic interactions can facilitate, rather than inhibit, the assembly of transmembrane proteins.

3:54PM D48.00006 Bio-Inspired Composite Interfaces: Controlling Hydrogel Mechanics via Polymer-Nanoparticle Coordination Bond Dynamics

Niels Holtan-Andersen,
Massachusetts Institute of Technology — In soft nanocomposite materials, the effective interaction between polymer molecules and inorganic nanoparticle surfaces plays a critical role in bulk mechanical properties. However, controlling these interfacial interactions remains a challenge. Inspired by the adhesive chemistry in mussel threads, we present a novel approach to control composite mechanics via polymer-particle interfacial dynamics; by incorporating iron oxide nanoparticles (Fe3O4 NPs) into a catechol-modified polymeric network the resulting hydrogels are crosslinked via reversible coordination bonds at Fe3O4 NP surfaces thereby providing a dynamic gel network with robust self-healing properties. By studying the thermally activated composite network relaxation processes we have found that the polymer-NP binding energy can be controlled by engineering both the organic and inorganic side of the interface.

4:06PM D48.00007 Photo-induced Reshuffling of Covalent Networks for Shape Actuators

Mitchell Anthamatten, Yuan Meng,
University of Rochester, Dept. Chemical Eng. Team — Photo-responsive allyl sulfide linkages within a polymer network can undergo addition fragmentation chain transfer (AFC), in the presence of free radicals, to cause bond reshuffling. This phenomenon is employed to program a single-phase, two-way shape actuator that is thermal-responsive, even without an applied external load. Semicrystalline poly(caprolactone) networks containing allyl sulfide linkages are melted, strained to various elongations (hundreds of percent), and irradiated. Light causes a cascade of AFC events, resulting in rupture of some network strands, configurational relaxation of dangling ends, and reformation of network bonds. After irradiation, the resulting double networks assume a mechanical state-of-ease and chains are under permanent configurational bias; when cooled, they crystallize in a preferred direction leading to fully reversible shape actuation. The mechanism of shape actuation is investigated using a combination of calorimetry and X-ray scattering.

4:18PM D48.00008 TBD

4:54PM D48.00009 Mussel-inspired reversible metal-coordinate bonds as a pathway towards temporal control over the mechanical hierarchy of soft materials

Scott Grindy, Robert Learsch, Niels Holtan-Andersen,
Massachusetts Inst of Tech-MIT — Dynamic, reversible crosslinks have been shown to specifically control the mechanical properties of a wide variety of mechanically tough and resilient biomaterials. Here, we show that reversible histidine-metal ion interactions, long thought to contribute to the strong mechanical properties and self-healing nature of mussel byssal threads, can be used to control and engineer the hierarchical mechanical properties of model polyethylene glycol hydrogels orthogonally from the spatial structure of the material. We delve into the physics underlying these types of materials to properly understand how to explicitly engineer the mechanical properties of tough soft materials by utilizing their temporal hierarchy.

5:06PM D48.00010 Active Dynamic Frictional Probes

Joshua Steimel, Juan Aragones, Alfredo Alexander-Katz,
Massachusetts Inst of Tech-MIT — In biological systems there are a myriad of interactions occurring instantaneously and these interactions can vary drastically in the strength of the interaction, the speed at which this interaction occurs, and the duration of the interaction. When multiple interactions occur any of these factors can determine which particular interaction is dominant. However, currently it is extremely difficult to measure binding affinity, K_on, and K_off rates in a relatively high throughput manner. Here we propose a novel and versatile system that will be able to detect differences in binding affinity of wide range of transient interactions and will be able to extract the relevant time scales of these interactions. Our system will utilize ferromagnetic particles that can be easily functionalized with a receptor of interest and the substrate will be coated in the corresponding ligand. A rotating magnetic field will cause particles, henceforth referred to as rollers, to rotate and this rotational motion will be converted into translational motion via the effective frictional force induced by interaction that is being probed. By measuring the translation of the rollers to a baseline, where only hydrodynamic friction occurs, we can measure the relative strength of the interactions. We can also potentially measure kinetic information by changing the frequency at which the magnetic field rotates, since changing the frequency at which the bead rotates is akin to changing the time allowed for bond formation. We will measure a wide range of interaction including ionic, metal-ion coordination, IgG-Protein A complex, and biotin-streptavidin complex.
5:18PM D48.00011 Magnesium Dependence of the RNA Free Energy Landscape, RYAN HAYES, JEFFREY NOEL, Center for Theoretical Biological Physics, Rice University, ANA MANDIC, Department of Biomedical Engineering, University of Houston, PAUL WHITFORD, Department of Physics, Northeastern University, KARISSA SANBONMATSU, Theoretic Biology and Biophysics, Los Alamos National Labs, UDAYAN MOHANTY, Department of Chemistry, Boston College, JOSE ONUCHIC, Center for Theoretical Biological Physics, Rice University — The RNA free energy landscape is highly sensitive to ionic concentrations, and especially to Mg$^{2+}$, as most RNA tertiary structure will not form in the absence of Mg$^{2+}$. At physiological concentrations, the energy landscape must be smooth and funneled to fold on biological time scales, but changes in ionic concentration may affect the relative stability of alternative states. We perturb a structure-based model, which captures the funneled nature of the energy landscape, to include electrostatic effects. Our model includes explicit Mg$^{2+}$ and screening by implicit KCl. A dynamic model for the local competition between Manning condensed Mg$^{2+}$ and KCl is introduced, which makes the model more broadly applicable and transferable than a previous static model. We use the excess Mg$^{2+}$ ions associated with the RNA (I$^2_{2+}$) to test the model. I$^2_{2+}$ is an ideal metric because it is closely related to the Mg$^{2+}$-RNA interaction free energy, and is easily measurable in both experiment and simulation. The model captures intermediate states of a small pseudoknot missed by models without electrostatics.

5:30PM D48.00012 Exploiting Dynamic Bonds in Polymer-grafted Nanoparticle Networks to Create Mechanomutable, Reconfigurable Composites, ANNA C. BALAZS, MATTHEW J. HAMER, BALAJI V. S. IYER, VICTOR V. YASHIN, University of Pittsburgh — Via a new dynamic, three-dimensional computer model, we simulate the tensile deformation of polymer-grafted nanoparticles (PGNs) that are cross-linked by labile bonds, which can readily rupture and reform. For a range of relatively high strains, the network does not fail, but rather restructures into a stable, ordered structure. Within this network, the reshuffling of the labile bonds enables the formation of this new morphology. The studies reveal that the appropriate combination of stress-responsive hybrid materials and applied stress can yield distinct opportunities to dynamically switch between different structures, and thus, the properties of the material. Thus, the results provide guidelines for designing mechano-responsive hybrid materials that undergo controllable structural transitions through the application of applied forces.

Monday, March 2, 2015 2:30PM - 5:30PM – Session D49 GSOFT DBIO: Focus Session: Active Living Matter I 217D - Vernita Gordon, University of Texas at Austin

2:30PM D49.00001 Rheology of Active Gels, DANIEL CHEN, Department of Physics Brandeis University — Active networks drive a diverse range of critical processes ranging from motility to division in living cells, yet a full picture of their rheological capabilities in non-cellular contexts is still emerging, e.g., How does the rheological response of a network capable of remodeling under internally-generated stresses differ from that of a passive biopolymer network? In order to address this and other basic questions, we have engineered an active gel composed of microtubules, bidirectional kinesin motors, and molecular depletant that self-organizes into a highly dynamic network of active bundles. The network continually remodels itself under ATP-tunable cycles of extension, buckling, fracturing, and self-healing. Using confocal rheometry we have simultaneously characterized the network’s linear and non-linear rheological responses to shear deformation along with its dynamic morphology. We find several surprising and unique material properties for these active gels; most notably, rheological cloaking, the ability of the active gel to drive large-scale fluid mixing over several orders of flow magnitude while maintaining an invariant, solid-like rheological profile and spontaneous flow under confinement, the ability to exert micro-Newton forces to drive persistent directed motion of the rheometer tool. Taken together, these results and others to be discussed highlight the rich stress-structure-dynamics relationships in this class of biologically-derived active gels.

3:06PM D49.00002 Collective dynamics of sperm in viscoelastic fluid, CHIH-KUAN TUNG, Deptment of Biophysical Sciences, City University of Hong Kong — Active networks provide an unlimited path, microtubule loops allow the study of kinesin motility on distances exceeding that offered by a single microtubule. Moreover, the periodicity of the path allows for the comparison of trajectories between laps. Here we study the motility of quantum dot labeled kinesin on microtubule loops. Motility of kinesins over multiple laps is observed and their trajectories are extracted from kymograph using a custom algorithm. Distribution of velocities at given locations do not vary randomly but show a correlation with the presence of obstacles. Possible mechanisms responsible for the long range transport are discussed in the context of available theories.
We also study a related equilibrium model that clarifies the role of orientational fluctuations.

Chiral organization although the interactions are achiral. We elucidate under which conditions these chiral states will emerge and grow to large scales.

We perform large-scale molecular dynamics simulations (up to 

breaking is ubiquitous in biological systems, from DNA to bacterial suspensions. A key unresolved problem is how chiral structures may spontaneously emerge.

The paradigmatic model organism for chemotaxis is E. coli. E. coli has multiple flagella and uses these to swim with a run-and-tumble random walk, biasing its runs towards chemotactant. However, P. aeruginosa has only a single polar flagellum and therefore in a bulk fluid can only go forward and backward (with small changes in angle possible).

We find that the efficiency of P. aeruginosa chemotaxis depends strongly on the initial swimming direction as well as the steepness of the sensed gradient of chemotactant.

The cortical actin cytoskeleton is a quasi 2-D active material in which dynamics are dominated by rapid actin turnover and myosin-driven contractility. Here we present a reconstituted model system that emulates these processes in artificial cell-like compartments. By tuning physical and chemical parameters, we induce a non-equilibrium phase transition. We characterize the local dynamics of these reconstituted cortices by tracking embedded single-walled carbon nanotubes (SWNTs). We create high-resolution maps of the contractile actomyosin flows in a homogenous and during transition to an inhomogeneous steady state. We find evidence that connectivity percolation drives the non-equilibrium phase transition.
compaction that agrees with estimated compaction that we observe directly. This makes their dynamic behavior in restricted geometries very different from that observed in the bulk. Here we analyze the motion of spermatozoids confined to shallow chambers, investigating the nature of the cell trajectories and their accumulation near the side boundaries. Observed cell trajectories are composed of a succession of quasi-circular and quasi-linear segments. This suggests that the cells follow a path of intermittent trappings near the top and down surfaces separated by stretches of quasi-free motion near the center of the gap. Use of microstructured petal-shaped edges limits accumulation near the borders and contributes to increase the concentration in the chamber interior. System stabilization occurs over times of the order of minutes, which agrees well with a theoretical estimate that assumes that the cell mean-square displacement is largely due to the quasi-linear segments. Pure quasi-circular trajectories would require several hours to stabilize. Our estimates also indicate that stabilization proceeds 2.5 times faster in the rosette geometries than in the smooth-edged chambers, which is another practical reason to prefer the former.

5:06PM D49.00012 Shape-Conserved Dynamic Convection in the Process of Astér Formation from a System of Microtubules and Cross-Linked Kinesin Motors. K. KIM, A. SIKORA, WPI-AIMR, Tohoku University, Japan. H. NAKAZAWA, Dept of Biomolecular Engineering, Graduate School of Engineering, Tohoku University, Japan. M. UMETSU, WPI-AIMR/Dept of Biomolecular Engineering, Graduate School of Engineering, Tohoku University, Japan. W. HWANG, Dept of Biomedical Engineering/Materials Science and Engineering, Texas A&M University, USA; School of Computational Sciences, KIAS, Korea. W. TEIZER, WPI-AIMR, Tohoku University, Japan; Dept of Physics and Astronomy/Materials Science and Engineering, Texas A&M University, USA; We report fluorescence microscopy studies of a cellular element-based active system that is composed of rhodamine-labeled microtubules and functionalized kinesin motor proteins, cross-linked via streptavidin-coated quantum dots. The motor proteins organize microtubules into aster-like structures containing core aggregations of the quantum dot-motor protein complexes. The cores result from the dynamic condensation of sub-clusters that are connected to each other randomly. The inter-cluster distance decays exponentially with time during the condensation. Intriguingly, the shape defined by lines connecting the clusters is well conserved while the dynamic process reduces the size. This shape conservation is achieved by a dynamic balance with respect to the distance between sub-clusters. We explain this isomorphic contraction during the aster formation process using a simple mechanistic model.

5:18PM D49.00013 Broken detailed balance in active fluctuations of semiflexible filaments. JANNES GLADROW, Georg-August University of Göttingen, Germany. NIKTA FAKHRI, MIT. FRED C. MACKINTOSH, Vrije Universiteit, Netherlands. CHRISTOPH F. SCHMIDT, Georg-August University of Göttingen, Germany. CHASE P. BROEDERSZ, Princeton University — Non-equilibrium microscopic force generation in cells often results in stochastic steady-state fluctuations. In the cell cytoskeleton, for example, cytoplasmic myosins can drive vigorous conformational fluctuations of actin filaments and microtubules. We here present an analytical and numerical analysis of randomly driven shape fluctuations of semiflexible filaments in a viscoelastic environment. To detect and quantify non-equilibrium dynamics, we focus on the breaking of detailed balance in a conformational phase space subtended by eigenmodes of the beam equation. Molecular dynamics simulations reveal a non-zero circulatory flux in phase space induced by motor activity. Furthermore, we derived an analytical expression of nonequilibrium mode correlations that allows us to predict temporal effects of active molecular motors.

Monday, March 2, 2015 2:30PM - 4:54PM — Session D50 GSOFT GSNP: Focus Session: Dynamic Jamming Fronts and Shear Thickening

2:30PM D50.00001 Shear thickening and S-shaped flow curves. ROMAIN MARI, Levich Institute, CCNY, RYOHEI SETO, Levich Institute, CCNY / Okinawa Institute of Science and Technology. JEFFREY F. MORRIS, MORTON M. DENN, Levich Institute and Department of Chemical Engineering, CCNY — The discontinuous shear thickening (DST) of dense suspensions is a remarkable phenomenon in which the viscosity can increase by several orders of magnitude at a critical shear rate. It follows the phenomenology of a first order transition between two “states” that we have recently identified as Stokes flows with lubricated or frictional contacts, respectively. Here we extend the analogy further and show the existence of a non-monotonic steady state flow curve by means of stress-controlled simulations, analogous to a non-monotonic equation of state. While we associate DST to an S-shape flow curve, at volume fractions above the shear jamming transition the frictional state loses flowability and the flow curve reduces to an arch, permitting the system to flow only at small stresses. Whereas a thermodynamic transition leads to phase separation in the coexistence region, we observe a uniform shear flow all along the transition channel. A stability analysis suggests that uniform shear may be mechanically stable for the small Reynolds numbers and system sizes in a rheometer.

2:42PM D50.00002 Sedimentation of athermal particles in clay suspensions1. XAVIER CLOTET, ARSHAD KUDROLLI, Department of Physics, Clark University — We discuss sedimentation of athermal particles in dense clay suspensions which appear liquid-like to glass-like. These studies are motivated by the physics important to a diverse range of problems including remediation of oil sands after the extraction of hydrocarbons, and formation of filter cakes in bore wells. We approach this problem by first considering collective sedimentation of athermal spherical particles in a viscous liquid in quasi-two dimensional and three dimensional containers. We examine the system using optical and x-ray tomography techniques which gives particle level information besides global information on the evolution of the volume fraction. Unlike sediments in the dilute limit – which can be modeled as isolated particles that sediment with a constant velocity and slow down exponentially as they approach the bottom of the container – we find interaction between the different flow regimes leads to the emergence of a novel behavior during the sedimentation. We find significant avalanching behavior and cooperative motion as the grains collectively settle, and non-exponential increase in settling time. We discuss the effect of stirring caused by the sedimenting particles on their viscosity and consequently the sedimentation rates as a function of particle concentration.

1Supported by Petroleum Research Fund Grant PRF # 54045-ND9.

2:54PM D50.00003 Dynamic jamming fronts in iceberg-choked fjords. IVO PETERS, University of Chicago, JASON AMUNDSON, University of Alaska Southeast, RYAN CASSOTTO, University of New Hampshire, MARK FAHNESTOCK, University of Alaska Fairbanks, KRISTOPHER DARNELL, University of Texas Austin, MARTIN TRUFFER, University of Alaska Fairbanks, WENDY ZHANG, University of Chicago — During summertime at the glacier terminus at Jakobshavn Isbræ, Greenland, calving events are followed by rapid motion in the ice mélange in front of the terminus. Understanding the dynamics of ice mélange is important because it acts as a resisting force to calving events. We analyze this motion using time-lapse photography and terrestrial radar images. Large calving events last for approximately 5 minutes, during which ~ 10^{14} J of potential energy is released. Motion in the ice mélange quickly spreads out over at least 16 km down the fjord, and relaxes in about 1 hour. The ice mélange can be viewed as a dense granular system, which is packed close to the jamming point. A jammed ice mélange resists expansion of the glacier terminus much more strongly and reduces iceberg calving, which may therefore play a significant role in glacier evolution. In our images, we observe dynamic jamming fronts, which propagate one order of magnitude faster than the instantaneous speed of the calving iceberg. From the ratio between the speed of the front and the calving iceberg we calculate a compaction that agrees with estimated compaction that we observe directly.
In oscillatory shear, as the original scattering volume periodically comes back to the original position, we could better study the changes in autocorrelation of silica nanoparticle suspensions in PEG under different shear strain regimes using small angle x-ray scattering (SAXS) and x-ray photon correlation spectroscopy (XPatial dynamics and provide an explanation of why shear thickening becomes weaker in highly viscous solvent.

However, in the real application, high shear strain or rate is applied, where the viscoelastic properties are affected by the microstructural deformation by this modulus. In this regime, their microstructure does not change by shear, and the shear stress linearly responds to the applied strain.

By combining the fluctuation analysis in different regimes, we quantitatively show how the interactions between grains affect the suspension dynamics and provide an explanation of why shear thickening becomes weaker in highly viscous solvent.

For low viscosity suspending liquids, we show that, in the shear thickening regime, shear and normal stresses are highly coupled and exhibit significant fluctuations with time. As shear rate increases, the stress distributions evolve from Gaussian to more complex distributions. By contrast, for highly viscous solvents, stress fluctuations are greatly reduced and only show Gaussian distributions at different shear rates. Moreover, the fluctuation behaviors are associated with various relaxation modes of the system and therefore lead to different scalings of the power spectral density.

3:30PM D50.00007 Dynamics of Concentrated Silica Suspension under Oscillatory Shear Studied by SAXS and XPCS, JONGHUN LEE, XIAO-MIN LIN, ALEC SANDY, SURESH NARAYANAN, Argonne National Laboratory, X-RAY SCIENCE DIVISION TEAM, CENTER FOR NANOMATERIALS TEAM — The viscoelastic properties of complex fluids are often obtained by applying small amplitude oscillatory shear (SAOS). In this regime, their microstructure does not change by shear, and the shear stress linearly responds to the applied strain. However, in the real application, high shear strain or rate is applied, where the viscoelastic properties are affected by the microstructural deformation by this modulus. In this regime, their microstructure does not change by shear, and the shear stress linearly responds to the applied strain.

3:42PM D50.00008 Discontinuous shear thickening for frictional granular particles, MATTHIAS GROB, CLAUS HEUSSINGER, ANNETTE ZIPPELIUS, Institute for Theoretical Physics, Göttingen University — We study the rheology of frictional granular particles with analytical modelling and numerical simulations in two dimensions. We derive a phase diagram with a topology different from the well known Liu-Nagel phase diagram for frictionless particles with a zero stress critical point. In contrast to the frictionless scenario, jamming first occurs at finite stress at a critical packing fraction \( \phi_C \) while a finite yield stress emerges only at \( \phi_\text{y} > \phi_C \). Remarkably, the flow is reentrant and we observe discontinuous shear thickening in the flow curve for \( \phi_\text{r} < \phi_\text{y} \) with \( \phi_\text{y} > \phi_C \). All these features can be rationalized with a simple constitutive equation which contains the frictionless scenario as a limiting case.

3:54PM D50.00009 Material properties of the shear-thickened state in concentrated near-hardsphere colloidal dispersions, NORMAN WAGNER, COLIN CWALINA, Chemical and Biomolecular Engineering, University of Delaware — Reversible shear thickening is common in concentrated dispersions of Brownian hard-spheres at high shear rates. We confirm the existence of a well-defined colloidal shear-thickened state through experimental measurements of the shear stress and the first and second normal stress differences in the shear-thickened state as a function of the particle volume fraction \( \phi \) for a model dispersion of near hard-spheres. The shear stress and normal stress differences are observed to grow linearly with the shear rate in the shear-thickened state and both normal stress differences are observed to be negative. Our experimental results show that the shear-thickened state of colloidal dispersions can be described by three material properties: shear viscosity and first and second normal stress difference coefficients—that are a function of the volume fraction. All three material properties are found to diverge with a power law scaling with the approach to maximum packing, which is found to be 0.54 ± 0.01. We find the magnitude of the relative shear viscosity is greater than the magnitude of the dimensionless second normal stress difference, which is greater than the magnitude of the dimensionless first normal stress difference. These results are consistent with theoretical predictions for shear thickening by hydrocluster formation and quantitatively comparable to Stokesian Dynamics simulations.

4:06PM D50.00009 The reciprocal effect of lubrication and contact forces in shear-thickening of colloidal suspensions, SAFA JAMALI, ARMAN BOROMAND, JOAO MAIA, Case Western Reserve Univ — Recently, the shear-thickening of colloidal suspensions has been attributed to frictional contact forces at high shear rates. This emerging understanding of the contact forces in a suspension has brought back the well-known dilatancy theory which was rather dormant in the past two decades. Here, we study the necessity of short-range hydrodynamics and the correlation between the contact and lubrication forces in shear-thickening suspensions. We use a modified Dissipative Particle Dynamics method that includes squeeze mode lubrication potentials based on the two interacting colloids. The effect of simulation parameters and contact potentials on the rheological response of a suspension is studied. Our results show that although the quality of the shear-thickening behavior (whether DST can be obtained or not) is dominated by the contact potentials, the lubrication force is a prerequisite for any type of shear-thickening to be recovered. Needless to mention that this argument is valid for the high Péclet numbers, as opposed to shear-thinning regime which can be fully reproduced without the need to lubrication or contact potentials.
4:18PM D50.00010 Dynamic jamming under impact in shear thickening suspensions1, SHOMEEK MUKHOPADHYAY, Yale University — Shear thickening fluids such as cornstarch and water show remarkable impact response allowing, for example, a person to run on the surface. We perform constant velocity impact experiments and imaging in shear thickening fluids at velocities lower than 500 mm/s and suspension heights of a few cm. In this regime where inertial effects are insignificant, we find that fronts with a dynamically jammed (DJ) region behind it are generated under impact. When this front and the DJ region reaches the opposite boundary it is able to support large stresses like a solid. These stresses are sufficient to support the weight of a running person. In addition we find a shear thickening transition under impact due to collision of the fronts with the boundary. There is a critical velocity required to generate these impact activated fronts. Using the observations on fronts, DJ region and using energy balance arguments we construct a model to explain the phenomena of running on the surface of cornstarch suspensions. The model shows quantitative agreement with our measurements using high-speed video of running on cornstarch and water suspensions.

1Supported by NSF DMR 1410157

Monday, March 2, 2015 2:30PM - 5:30PM —  Session D51 GQI DCMP: Invited Session: Towards a Scalable Superconducting Quantum Computer  Grand Ballroom C1 - Michel Devoret, Yale University

2:30PM D51.00001 The surface code: processing experimental data, AUSTIN FOWLER, Google — The surface code requires only nearest neighbor interactions and fidelities above approximately 0.99, making it highly compatible with superconducting circuits. In this talk, I review the surface code, and highlight the challenges and available optimizations when classically processing the output of a 9-qubit slice of surface code.

3:06PM D51.00002 Bit-flip error correction with superconducting Xmon qubits, JOHN MARTINIS, UC Santa Barbara and Google Inc. — One of the outstanding challenges of quantum computation has been the realization of scalable qubits with high fidelity for all necessary operations. Here I discuss the design of a linear chain of 9 superconducting Xmon qubits that allows initialization, single and two qubit gates, and fast repetitive and simultaneous measurement with fidelity in the 99%-99.9% range. This performance has allowed us to perform bit-flip error correction with 8 repetition cycles that leads to improved lifetime of the state. The use of error correction based on the surface code enables all errors, both data and measurement, to be corrected to 1st and 2nd order.

3:42PM D51.00003 Detecting arbitrary quantum errors via stabilizer measurements, MATTHIAS STEFFEN, IBM — Fault tolerant quantum computing requires error correction, which relies on the ability to extract information about the error that occurred rather than the states of the data qubits themselves. Stabilizer codes are an attractive solution to this problem in which the parity of the data qubits is measured with the aid of additional ancilla qubits, resulting in the “stabilization” of a specific quantum state. Here, we perform syndrome (or error) extraction and arbitrary error detection by using a 2x2 lattice of superconducting qubits and simultaneous quantum non-demolition stabilizer measurements. In this experiment one of the Bell states is stabilized, and any arbitrary single-qubit bit or phase error can be detected without destroying the stabilized Bell state. This lattice is a representative of a primitive tile for the surface code which is a promising approach towards quantum error correction.

4:18PM D51.00004 Tracking a Quantum Error Syndrome in Real Time: Quantum Jumps of Photon Parity1, ROBERT SCHOELKOPF, Yale University — Dramatic progress has been made in the last decade and a half towards realizing solid-state systems for quantum information processing with superconducting quantum circuits. Artificial atoms (or qubits) based on Josephson junctions have improved their coherence times more than 100,000-fold, have been entangled, and used to perform simple quantum algorithms. The next challenge for the field is demonstrating quantum error correction that actually improves the lifetimes, a necessary step for building more complex systems. I will describe recent experiments with superconducting circuits, where we store quantum information in the form of Schrodinger cat states of a microwave cavity, containing up to 100 photons. Using an ancilla qubit, we then monitor the gradual death of these cats, photon by photon, by observing the first jumps of photon number parity. This represents the first continuous observation of a quantum error syndrome, and may enable new approaches to quantum information based on photonic qubits. The performance of this error-monitoring system and the prospects for reaching “breakeven,” where quantum error correction improves the lifetime of stored information, will be discussed.

1This work performed with many collaborators at Yale University, and supported by the Army Research Office, the Laboratory for Physical Science, and the NSF.

4:54PM D51.00005 Detecting bit-flip errors in a logical qubit using stabilizer measurements, DIEGO RISTE, QuTech and Kavli Institute of Nanoscience, Delft University of Technology — Quantum data is susceptible to decoherence induced by the environment and to control errors. A future-fault-tolerant quantum computer will use quantum error correction (QEC) to actively protect against both. In the smallest QEC codes, the information in one logical qubit is encoded in a two-dimensional subspace of a larger Hilbert space of multiple physical qubits. For each code, a set of non-demolition multi-qubit measurements, termed stabilizers, can discretize and signal physical qubit errors without collapsing the encoded information. Using a 5-qubit superconducting processor, we realize the two parity measurements comprising the stabilizers of the three-qubit repetition code protecting one logical qubit from physical bit-flip errors. We construct these stabilizers as parallelized indirect measurements using ancillary qubits, and evidence their non-demolition character by generating three-qubit entanglement from superposition states. We demonstrate stabilizer-based quantum error detection (QED) by subjecting a logical qubit in any initial state to bit-flip errors on its constituent three physical qubits. Crucially, and in contrast to previous QED implementations, this approach keeps the quantum information encoded at all times, meeting a fundamental requirement for fault tolerance.

Monday, March 2, 2015 2:30PM - 5:42PM —  Session D52 DCMP: Invited Session: DCMP Prize Session  Grand Ballroom C2 - Laura Greene, Universirty of Illinois-Urbana
GPa at T > c. However, metallization of hydrogen is still under debates. As an alternative, hydrogen dominated materials were extensively explored because of their lower materials, College of Physics, Jilin University — Hydrogen was predicted to metalize at high pressures and believed to be a room-temperature superconductor.

Materials, College of Physics, Jilin University — Hydrogen was predicted to metalize at high pressures and believed to be a room-temperature superconductor.

3:06PM D52.00002 Davison-Germer Prize Talk: Structure and Reactivity of Surfaces in Vacuum and Under Ambient Gas Pressures, MIQUEL SALMERON, Materials Science Division of the Lawrence Berkeley National Laboratory — The goal of surface science research is to provide atomic level understanding of the structural and dynamic properties of surfaces, a goal particularly relevant for chemical applications, including catalysis, photochemistry, batteries and fuel cells. With X-ray Photoemission Spectroscopy (XPS) we can determine the composition and electronic structure. With Scanning Tunneling Microscopy (STM) we can image atoms and molecules as they adsorb, diffuse and react on single crystal surfaces. STM uniquely permits to visualize and determine adsorbate-adsorbate interactions by making movies of their motion. I will show how water molecules diffuse, H-bond to each other, and wet the surface forming 2D films. We also imaged how H2 molecules adsorb and dissociate on a Pd surface, and how the movies revealed that a particular arrangement of substrate atoms is required to generate the active sites through fluctuations. To study surfaces in the presence of gases, in the Torr to Atmospheric pressure range, new instrumentation is needed. Over the last years we developed high pressure STM and XPS, which allows us to study surfaces under high coverage of adsorbates in equilibrium with gases near ambient pressures and temperature. I will show how under these conditions the structure of surfaces can be very different from that at low coverage, or even at high coverage but at low temperature. Adsorbates can induce dramatic restructuring of the surface, as I will show in the case of CO on Pt and Cu. Equally important, reactions on catalyst surfaces can now be followed in real time, by measuring composition with XPS, and structure with STM, during the reactions to extract kinetic parameters.

3:42PM D52.00003 Lars Onsager Prize Talk: Flow Equations for Hamiltonians, FRANZ WEGNER, Ruprecht-Karls-University Heidelberg — The equation dH(l) = GH(l) can describe the renormalization group equation for the Hamiltonian/Lagrangian H(l) and the generator G of the group. But it can also describe a Hamiltonian flow for bosons/fermions, which eliminates the off-diagonal matrix elements or (quasi-)particle violating terms by means of unitary transformations dH(l)/dl = [η(l), H(l)]. Typically off-diagonal matrix elements are eliminated for ∆E > l−1/2. The flow equation has been applied to numerous systems (F. Wegner, J. Phys. A: Math. Gen. 39 (2006) 8221, arXiv: cond-mat/0511660; S. Kehrein, The Flow Equation Approach to Many-Particle Systems, Springer 2006), among them to the two-dimensional Hubbard-model, spin-boson models, the Anderson impurity model, QED and QCD. A simple and surprising result (as compared to that by Frohlich) is obtained for the elimination of the electron-phonon interaction yielding an attractive interaction for all energies. (P. Lenz and F. Wegner, Nucl. Phys. B482 (1996) 693; arXiv: cond-mat/9604087)

4:18PM D52.00004 Julius Edgar Lilienfeld Prize Talk: Quantum spintronics: abandoning perfection for new technologies1, DAVID D. AWSCHALOM, Institute for Molecular Engineering, University of Chicago — There is a growing interest in exploiting the quantum properties of electronic and nuclear spins for the manipulation and storage of information in the solid state. Such schemes offer qualitatively new scientific and technological opportunities by leveraging elements of standard electronics to precisely control coherent interactions between electrons, nuclei, and electromagnetic fields. We provide an overview of the field, including a discussion of temporally- and spatially-resolved magneto-optical measurements designed for probing local moment dynamics in electrically and magnetically doped semiconductor nanostructures. These early studies provided a surprising proof-of-concept that quantum spin states can be created and controlled with high-speed optoelectronic techniques. However, as electronic structures approach the atomic scale, small amounts of disorder begin to have outsized negative effects. An intriguing solution to this conundrum is emerging from recent efforts to embrace semiconductor defects themselves as a route towards quantum machines. Individual defects in carbon-based materials possess general trends in connection with reduced dimensions, surprising findings including phonon-mediated pseudogaps, and technology potential.

1Work supported by the AFOSR, ARO, DARPA, NSF, and ONR.

4:54PM D52.00005 Experimental observation of high-temperature superconductivity in H2S at P~150 GPa, M. EREMETS, University of Mainz, Germany — We found that sulfur hydride transforms at P~90 GPa to a superconductor with Tc increasing with pressure to 150 K at approximately 200 GPa. Moreover, we found superconductivity with Tc ~ 190 K in a H2S sample pressurized to P > 150 GPa at T > 220 K. This superconductivity likely associates with the dissociation of H2S, and formation of SHn (n > 2) hydrides. We proved occurrence of superconductivity by the drop of the resistivity at least 50 times lower than the copper resistivity, the decrease of Tc with magnetic field, and the strong isotopic shift of Tc in D2S which evidences a major role of phonons in the superconductivity.

5:18PM D52.00006 High Tc phase of (H3S)2H3 at high pressures, TIAN CUI, State Key Laboratory of Superhard Materials, College of Physics, Jilin University — Hydrogen was predicted to metalize at high pressures and believed to be a room-temperature superconductor. However, metallization of hydrogen is still under debates. As an alternative, hydrogen dominated materials were extensively explored because of their lower metalization pressure. Here I present the high-pressure studies on structures, metalization, and superconductivity of (H3S)2H3 from ab initio calculations [1]. At lower pressures, two phases containing H2 units are stable with P1 (< 37 GPa) and Ccmm (37-111 GPa) symmetries, which are still insulators. Upon further compression, H2 units disappear and two new metallic structures with Im-3m and Im-3m symmetries are reconstructive above 111 GPa and 180 GPa, respectively. Remarkably, the estimated Tc of Im-3m phase at 200 GPa achieves a very high value of 191 ~ 204 K. Moreover, Tc decreases with pressure at an approximate rate of (∂Tc/∂P) of -0.12 K/GPa. Our predicted high Tc and its pressure dependence in Im-3m phase are subsequently verified by recent experiments [2]. Our findings support the conjecture that hydrogen-rich materials are a way to achieve a metallic phase with high Tc at accessible experimental pressures and represent a significant step toward the understanding of high-pressure behavior of metallic hydrogen.


2:30PM D53.00001 Manipulation of magnetic skyrmions with spin-polarized STM. KIRSTEN VON BERGMANN, Department of Physics, University of Hamburg, Germany — Spin textures of ultra-thin magnetic layers exhibit a surprising variety. The loss of inversion symmetry at the interface of magnetic layer and substrate gives rise to the so-called Dzyaloshinskii-Moriya interaction (DMI) which favors non-collinear spin arrangements with unique rotational sense [1]. An ideal tool to investigate such systems down to the atomic scale is spin-polarized scanning tunneling microscopy (SP-STM), which has enabled the discovery spin spirals with unique rotational sense at surfaces [2-4]. Recently, different interface-driven skyrmion lattices have been found, that either exist without external magnetic field [5,6] or are induced by it [7]. A tuning of the magnetic properties can be realized by tiny variations of the electronic structure due to stacking and hybridization of the magnetic layer. Isolated skyrmions can be stabilized in a wide magnetic field range [7] and the high lateral resolution of SP-STM together with its magnetic sensitivity enables a precise characterization of the evolution of size and shape of single skyrmions with field. A comparison to micromagnetic theory yields the material parameters including the DMI which is responsible for skyrmion formation. The writing as well as the deletion of individual skyrmions based on local spin-polarized current injection has been demonstrated [7]. A new mechanism to detect skyrmions using non-spin-polarized currents has been discovered and can be understood based on the mixing of spin-up and spin-down bands. These interface-induced non-collinear magnetic states offer new exciting possibilities to study fundamental physical properties on the atomic-scale and to tailor material properties for spintronic applications.


3:06PM D53.00002 Simulations of skyrmion manipulation in confined geometries. VINCENT CROS, Unit Mixte de Physique CNRS/Thales — No abstract available.

3:42PM D53.00003 Electrical Creation and Manipulation of Magnetic Skyrmion Bubbles. WANJUN JIANG, Materials Science Division, Argonne National Laboratory — Magnetic skyrmions are topologically stable spin textures, which exhibit many fascinating features including an emergent electromagnetic field and efficient manipulation. Nevertheless, until now this has been challenging to achieve at room temperature, which is a bottleneck for technological implementation of skyrmion-based spintronics. Towards this end, room-temperature electric-current creation of skyrmions in two different (metallic and insulating) commonly accessible materials system will be discussed. First, the experimental creation of magnetic skyrmions triggered by an electric current in Ta/CoFeB/TaOx trilayers is demonstrated. The skyrmion generation is enabled by laterally inhomogeneous current-induced spin-orbit torques. This process is analogous to the spontaneous droplet formation in surface-tension driven fluid flows. We establish a novel phase diagram that summarizes the dependence of skyrmion generation on the external magnetic fields, and the strength of in-plane currents. Furthermore, we reveal the efficient manipulation of these skyrmions by electric currents. More importantly, a prototype skyrmion racetrack memory device will be experimentally demonstrated. Secondly, the manipulation of skyrmion bubbles by using spin Hall spin torques in (Pt or W)/(Y,Bi)Fe2O12 (YIG-Bi) bilayers will be discussed. Using MOKE imaging, we have identified a hexagonal lattice of skyrmion bubbles (1.8-μm diameter). Subsequent current pulses through the Pt layer results both in the motion of some of the skyrmions and a reduction in size of others, which is consistent with different wall structures and resultant skyrmion numbers. Furthermore, we observe distinct anomalous Hall signals associated with the underlying magnetization textures, which may indicate topological Hall effects in bilayer.

1Financial support for the work at Argonne came from DOE, Office of Science, BES, Materials Sciences and Engineering Division, work at UCLA was supported by TANMS.

2This work was performed in collaboration with W. Zhang, M. B. Jungfleisch, F. Y. Fradin, J. E. Pearson, O. Heinonen, S. G. E. te Velthuis, and A. Hoffmann (Argonne National Laboratory), P. Upadhyaya, G. Yu, Y. Tserkovnyak, K. L. Wang (UCLA), Q. H. Yang, Q.Y. Wen, and H. W. Zhang (UESTC, China).

4:18PM D53.00004 Creation and Dynamics of Individual Skyrmions in Helimagnets1. JIADONG ZANG, Johns Hopkins Univ — The physics and future applications of magnetic skyrmions in helimagnet have attracted great attentions in the past years. Now the major focus of this field is the ability of creating single skyrmions in a controlled manner, and exploring novel properties of skyrmions as quasi-particles. In this talk, I will introduce our recent work on creating a single skyrmion via electric current or geometric confinement. The time and position of the skyrmion can be accurately controlled. More importantly, the microscopic mechanism is clearly revealed by the analysis of the topological charge, which also explains the topological origin of the skyrmion stability for the first time. The distinct feature of the skyrmion is an emergent gauge field attached to it. The motion of a single skyrmion is realized by coupling this emergent gauge field to electric current or magnon current. I will show that an electric current or temperature gradient can result in a steady motion of a single skyrmion.


1This work was supported in part by the TIPAC, the U.S. Department of Energy, Office of Basic Energy Sciences under Award No. DEFG02-08ER46544, and NSF under ECCS-1408168.
Magnetic skyrmions are topologically protected particle-like spin structures, with a topology characterised by their Skyrmion number. They can arise due to various interactions, including exchange, dipolar and anisotropy energy in the case of bubbles (skyrmion bubbles) and an additional Dzyaloshinskii-Moriya interaction (DMI) in the case of chiral skyrmions. Numerical predictions suggest that they exhibit rich dynamical behaviour governed by their topology, such as the basic gyrotropic and breathing eigenmodes [1,2]. The dynamical experiments are performed on skyrmion bubbles in nanostructures from symmetric CoB/Pt multilayers, tailored for high-frequency dynamics. Asymmetric layers were also fabricated (Co layers in-between 5d-metals) in order to tune the DMI, as expected from recent experiments [4]. Stabilizing chiral skyrmions confined in such nanostructures is highly desirable due to their enhanced stability and smaller size that makes them ideal candidates for integration in recently proposed novel spintronics devices [3]. By investigating the size of magnetic domains in magnetic field cycles, and comparing to micromagnetic simulations, asymmetric multilayers were explored. By performing pump-probe dynamical X-ray imaging on confined skyrmion bubbles the first observation of their basic eigenmode dynamics was demonstrated [5]. In particular, we present picosecond nanoscale imaging data i) of the gyrotropic mode of a single skyrmion bubble in the GHz regime and ii) the breathing-like behaviour of a pair of skyrmionic configurations. The observed dynamics is used to confirm the skyrmion topology and show the existence of an unexpectedly large inertia that is key for describing skyrmion dynamics [1,5]. These results demonstrate new ways for observing skyrmion dynamics and provide a framework for describing their behaviour. The next step is to achieve chiral skyrmion dynamics on a DMI system.

8:00AM F1.00001 Black Phosphorus Boron Nitride Heterostructures, NATHANIEL GILLGREEN, YAFIS BARLAS, YANMENG SHI, JIAWEI YANG, University of California Riverside, TAKASHI TANIGUCHI, National Institute for Materials Science, CHUN NING (JEANIE) LAU, University of California Riverside — There has been significant recent interest in black phosphorus as a candidate for future electronics applications, as it possesses both a layer- and band gap and a relatively high mobility (compared to other 2D candidates). However, black phosphorus' degradation in ambient conditions constitutes a major roadblock in future applications. As a potential solution for this problem we explore the effects of encapsulating black phosphorus between hexagonal boron nitride. We will present the effects of this heterostructure on both the stability and transport properties of thin black phosphorus devices.

8:12AM F1.00002 Electronic Structure and Rashba Spin-Orbit Coupling in Black Phosphorus, ZORAN POPOVIC, JAMSHID MORADI KURDESTANY, SASHI SATPATHY, Department of Physics, University of Missouri, Columbia, MO 65221 — We investigate the electronic structure of black phosphorus using both the first-principles density-functional methods as well as a tight-binding model. The electronic structure in the gap region is described by a tight-binding Hamiltonian keeping the nearest-neighbor hopping and the $p$ orbitals. The calculated bond-centered Wannier functions lead to the bonding picture in terms of the occupation of the $p_x$ bond orbitals along the phosphorous-phosphorous bonds. We find that a symmetry-breaking external electric field introduces a Rashba spin-orbit coupling; however, its magnitude is small, phosphorus being a small-Z atom. The magnitude is enhanced significantly if the phosphorus is replaced by the larger-Z bismuth.

8:24AM F1.00003 Probing Anisotropic Excitonic Wavefunctions in Black Phosphorus using Scanning Tunneling Microscopy, AYELET NOTIS, CARLOS ARGUELLO, ETHAN ROSENTHAL, ABHAY PASUPATHY, Columbia University — Black phosphorus is a layered, van der Waals semiconductor that has several structural similarities to graphite. Ultrathin black phosphorus (phosphorene) is conjectured to have a thickness-tunable band gap and high carrier mobility, making it attractive for electronic and optical applications. Unlike graphene which is a truly planar structure, phosphorene layers have a pronounced c-axis corrugation. This causes the electronic structure to be anisotropic, with different effective masses, carrier velocities and dielectric constants parallel and perpendicular to the direction of the corrugation. This has been predicted to lead to anisotropic wavefunctions for hydrogenic states and excitons in the material. In this talk, we present recent scanning tunneling microscopy and spectroscopy (STM and STS) studies investigating the topographic features and electronic structure of black phosphorus. We show that the primary charge defects are acceptors. By studying the local electronic structure in the vicinity of these defects that create hydrogenic states within the bandgap, we directly probe excitonic wavefunctions and their anisotropy in this material. We will describe spatially-resolved measurements of the bandgap and its inhomogeneity in the presence of defects.

8:36AM F1.00004 Highly Anisotropic and Robust Excitons in Monolayer Black Phosphorus, XIAOMU WANG, Yale Univ, AARON M. JONES, KYLE L. SEYLER, Univ of Washington, VY TRAN, Washington University, YICHEN JIA, Yale Univ, HUAN ZHAO, HAN WANG, Univ of Southern California, LI YANG, Washington University, XIAODONG XU, Univ of Washington, FENGNIAN XIA, Yale Univ — Recently, black phosphorus emerged as a promising new 2D material due to its widely tunable and direct bandgap, high carrier mobility and remarkable in-plane anisotropic electrical, optical and phonon properties. However, current progress is primarily limited to its thin-film form, and its unique properties at the truly 2D quantum confinement have yet to be demonstrated. Here, we reveal highly anisotropic and tightly bound excitons in monolayer black phosphorus using polarization-resolved photoluminescence measurements at room temperature. We show that regardless of the excitation laser polarization, the emitted light from the monolayer is linearly polarized along the light effective mass direction and centers around 1.3 eV, a clear signature of emission from highly anisotropic bright excitons. In addition, photoluminescence excitation spectroscopy suggests a quasiparticle bandgap of 2.2 eV, from which we estimate an exciton binding energy of around 0.9 eV, consistent with theoretical results based on first-principles. The experimental observation of highly anisotropic, bright excitons with exceedingly large binding energy not only opens avenues for the future explorations of many-electron effects in this unusual 2D material, but also suggests a promising future in optoelectronic devices such as on-chip infrared light sources.

8:48AM F1.00005 Anisotropic transient reflection spectrum of Black Phosphorus thin films, SHAOFENG GE, ZHIMING ZHANG, QIU JUN, Peking Univ, JUNKU LIU, China Academy of Space Technology, XUEFENG LIU, QINSHENG WANG, DONG SUN, Peking Univ — We present an experimental investigation on the ultrafast dynamics of the black phosphorus film, which is studied by femtosecond transient reflection spectroscopy. The results show that the transient reflection spectrum is polarization sensitive to both pump and probe laser pulse. The pump polarization has effect on the absorption of photons which determines the magnitude of the signal while the probe polarization has effect on the shape of the signal which indicates it correspond to different dynamics for different probe polarization. Moreover, the temperature dependent and pump power dependent has been performed.

8:00PM EE2.00004 Beating liquid helium: the technologies of cryogen-free superconducting magnets, JOHN BURGOYNE, Oxford Instruments Omicron NanoScience — Cryogen-free superconducting magnets have been available now for almost 15 years, but have only become standard commercial products in more recent years. In this review we will consider the pros and cons of dry design including superconducting wire development and selection, thermal budgeting, and the alternative methods for achieving magnet cooling.

Tuesday, March 3, 2015 8:00AM - 11:00AM – Session F1 DMP: Focus Session: Beyond Graphene - Phosphorene II 001A - Xiaomu Wang, Yale University
9:00AM F1.00006 Tiling Phosphorene, ZHEN ZHU, DAVID TOMANEK, JIE GUAN, Michigan State University — We introduce a scheme to categorize the structure of different layered phosphorene allotropes by mapping their non-planar atomic structure onto a two-color 2D triangular tiling pattern. In the puckered structure of a phosphorene monolayer, we assign atoms in “top” positions to dark tiles and atoms in “bottom” positions to light tiles. Optimum sp² bonding is maintained throughout the structure when each triangular tile is surrounded by the same number N of like-colored tiles, with 0 ≤ N ≤ 2. Our ab initio density functional calculations indicate that both the relative stability and electronic properties depend primarily on the structural index N. The proposed mapping approach may also be applied to phosphorene structures with non-hexagonal rings and 2D quasicrystals with no translational symmetry, which we predict to be nearly as stable as the hexagonal network.

9:12AM F1.00007 Few-Layer Phosphorene and Arsenene Allotropes: A Computational Study, DAVID TOMANEK, ZHEN ZHU, JIE GUAN, Michigan State University — There has been rising interest in layered compounds of group V elements including phosphorus and arsenic 2D semiconductors with a substantial band gap and a high carrier mobility. Our ab initio density functional calculations suggest the existence of multiple sp² bonded phosphorene and arsenene allotropes that are stable as free-standing monolayers. We have found that α-P (black), β-P (blue), γ-P and δ-P allotropes of phosphorus are similarly stable, but display a different electronic structure. The monolayer of grey arsenic has a very similar structure as blue phosphorene and also has a wide band gap. The fundamental band gap of the compounds depends sensitively not only on the allotrope, but also the number of layers, the stacking arrangement, and in-layer strain. The energy penalty to interconnect different allotropes of the same element is unusually low, which becomes particularly valuable in assembling heterostructures with well-defined metallic and semiconducting regions in one contiguous layer.

9:24AM F1.00008 Lattice Stacking Interactions: Comparisons between bilayer graphene and silicene, DAVID CAREY, NATHANAEL ROOME, Univ of Surrey — The stacking arrangement of atoms in elemental 2D materials, such as graphene and silicene, plays a crucial role in determining their structural, electronic, and vibrational properties. The weaker π bonding in silicene results in atomic buckling, and previously we have found linear band dispersion in a low atom buckling geometry with a Fermi velocity about 2/3 that of graphene and electron-phonon matrix elements are about a factor of 25 times smaller than in graphene [1]. Here we investigate the properties of different stacking configurations of bilayer silicene with those of bilayer graphene (BLG). In the case of BLG there are two stable configurations AA and AB stacking, with no atomic buckling present. In the case of bilayer silicene the presence of buckling and the different stacking arrangements results in a range of stable configurations. We calculate the frequencies of the IR and Raman active modes as a means to identify the different bonding and stacking configurations. This approach of fingerprint identification is applicable to other elemental layered materials.

9:36AM F1.00009 SnS₂: An Emerging Layered Metal Dichalcogenide Semiconductor, YUAN HUANG, PETER SUTTER, Center for Functional Nanomaterials, Brookhaven National Laboratory — Layered materials are of interest for new physics and due to their promise for device applications. Recent research has extended from graphene to transition metal dichalcogenides, with a strong focus on MoS₂. Here, we report a comprehensive study of a new group IV metal dichalcogenide, tin disulfide (SnS₂) [1]. Using exfoliated from bulk crystals, we establish the characteristics of single- and few-layer SnS₂ in optical and atomic force microscopy, Raman spectroscopy and transmission electron microscopy. Band structure study show that SnS₂ is an indirect gap semiconductor over the entire thickness range from bulk to a single layer. Ultrathin transistors screened by a liquid gate show promising characteristics, such as on-off current ratios >10⁶, high carrier mobilities (up to 230 cm² V⁻¹ s⁻¹) and near-ideal subthreshold swing. SnS₂ transistors are efficient photodetectors, but similar to other dichalcogenides they show a relatively slow response to pulsed irradiation, likely due to adsorbate-induced long-lived extrinsic trap states.

9:48AM F1.00010 Semiconducting Behavior, Schottky Barriers and Field Effect Transistors in Ultrathin Rhenium Disulfide, CHRIS CORBET, CONNOR MCCHELLAN, AMRITESH RAI, SUSHANT SONDE, EMANUEL TUTUC, SANJAY K. BANERJEE, The University of Texas at Austin — We report the fabrication, characterization, and device characteristics of exfoliated dual-gated ReS₂ Field Effect Transistors (FETs). All devices were created on few-layer crystals isolated using micro-mechanical exfoliation of source material grown by chemical vapor deposition. The devices were fabricated with e-beam evaporated alumina gate dielectric and Cr/Au top-gate. The dual-gated FETs demonstrated current saturation and voltage gain with a subthreshold swing of 148 mV/decade.

9:00AM F1.00011 Rhenium Disulfide Depletion-Load Inverter, CONNOR MCCHELLAN, CHRIS CORBET, AMRITESH RAI, HEMA C.P. MOVVA, EMANUEL TUTUC, SANJAY K. BANERJEE, The University of Texas at Austin — Many semiconducting Transition Metal Dichalcogenides (TMD) materials have been effectively used to create Field-Effect Transistor (FET) devices but have yet to be used in logic designs. We constructed a depletion-load voltage inverter using ultrathin layers of Rhenium Disulfide (ReS₂) as the semiconductor channel. This ReS₂ inverter was fabricated on a single micromechanically-exfoliated flake of ReS₂. Electron beam lithography and physical vapor deposition were used to construct Cr/Au electrical contacts, an Alumina top-gate dielectric, and metal top-gate electrodes. By using both low (Aluminum) and high (Palladium) work-function metals as two separate top-gates on a single ReS₂ flake, we create a dual-gated depletion mode (D-mode) and enhancement mode (E-mode) FETs in series. Both FETs displayed current saturation in the output characteristics as a result of the FET “pinch-off” mechanism and On/Off current ratios of 10⁶. Field-effect mobilities of 23 and 17 cm²V⁻¹s⁻¹ and subthreshold swings of 97 and 551 mV/decade were calculated for the E-mode and D-mode FETs, respectively. With a supply voltage of 1V, at low/ negative input voltages the inverter output was at a high logic state of 900 mV. Conversely with high/positive input voltages, the inverter output was at a low logic state of 500 mV. The inversion of the input signal demonstrates the potential for using ReS₂ in future integrated circuit designs and the versatility of depletion-load logic devices for TMD research.

1Supported by the National Science Foundation Cooperative Agreement #EEC-0832785, titled “NSEC: Center for High-rate Nanomanufacturing.”

2Supported by the National Science Foundation Cooperative Agreement #EEC-0832785, titled “NSEC: Center for High-rate Nanomanufacturing.”

3NRI SWAN Center and the ARL STTR program

10:00AM F1.000111 Rhenium Disulfide Depletion-Load Inverter, CONNOR MCCHELLAN, CHRIS CORBET, AMRITESH RAI, HEMA C.P. MOVVA, EMANUEL TUTUC, SANJAY K. BANERJEE, The University of Texas at Austin — Many semiconducting Transition Metal Dichalcogenides (TMD) materials have been effectively used to create Field-Effect Transistor (FET) devices but have yet to be used in logic designs. We constructed a depletion-load voltage inverter using ultrathin layers of Rhenium Disulfide (ReS₂) as the semiconductor channel. This ReS₂ inverter was fabricated on a single micromechanically-exfoliated flake of ReS₂. Electron beam lithography and physical vapor deposition were used to construct Cr/Au electrical contacts, an Alumina top-gate dielectric, and metal top-gate electrodes. By using both low (Aluminum) and high (Palladium) work-function metals as two separate top-gates on a single ReS₂ flake, we create a dual-gated depletion mode (D-mode) and enhancement mode (E-mode) FETs in series. Both FETs displayed current saturation in the output characteristics as a result of the FET “pinch-off” mechanism and On/Off current ratios of 10⁶. Field-effect mobilities of 23 and 17 cm²V⁻¹s⁻¹ and subthreshold swings of 97 and 551 mV/decade were calculated for the E-mode and D-mode FETs, respectively. With a supply voltage of 1V, at low/ negative input voltages the inverter output was at a high logic state of 900 mV. Conversely with high/positive input voltages, the inverter output was at a low logic state of 500 mV. The inversion of the input signal demonstrates the potential for using ReS₂ in future integrated circuit designs and the versatility of depletion-load logic devices for TMD research.

3NRI SWAN Center and ARL STTR Program

10:12AM F1.00012 ABSTRACT WITHDRAWN —
10:24AM F1.00013 Field effect vs. Hall mobility in back-gated multilayered InSe FETs1, SUKRIT SUCHARITAKUL, NICHOLAS GOBLE, Case Western Reserve University, U. RAJESH KUMAR, RAMAN SANKAR, FANG CHENG CHOU, YIT-TSONG CHEN, National Taiwan University, XUAN GAO, Case Western Reserve University — 2D graphene-like materials, not only are interesting for their exotic transport behavior but also, hold promises for their mechanical robustness and many possibilities in miniaturization. As one material belonging to this category, InSe is not only a promising candidate for optoelectronic devices [1] but also has potential for ultrathin field effect transistor (FET) with high mobility transport [2]. Recent investigation [2] showed that exfoliated InSe FET device on PMMA substrate can yield field effect mobility as high as 1000 cm²/Vs at room temperature. In this work, various substrates such as PMMA, bare SiO₂, patterned SiO₂, and Si₃N₄ were used to fabricate InSe FET devices. Through back gating and Hall measurement, the devices’ field effect mobility and intrinsic Hall mobility were extracted at various temperatures to study the dielectric effect on the material’s intrinsic transport behavior. Overall trend of the devices’ mobility was found to increase as the temperature is reduced due to reduced phonon scattering. The sample’s field effect and Hall mobilities overall over the range of 77-300K fall in the range of 0.5-2.0 × 10⁵ cm²/Vs, better than the transition metal-dichalcogenides.


3X.P.A.G. acknowledges NSF CAREER Award (grant number DMR-1151354).

10:36AM F1.00014 Quasiparticle and Optical Properties of Mono- and Bi-layer SnS2: A First-Principles GW and GW+BSE Study1, MENG WU, DIANA QIU, STEVEN G. LOUIE, Physics Department, UC Berkeley and Lawrence Berkeley National Lab — Unlike most semiconducting transition metal dichalcogenides, SnS₂, another layered metal dichalcogenide, is calculated within density functional theory to be an indirect bandgap semiconductor in both its bulk and monolayer forms. Experimental characterization of mono- and bi-layer SnS₂ has been performed, but the details of its quasiparticle and excitonic properties remain unclear. Thus, we employ ab initio GW and GW+BSE calculations to study the quasiparticle band structure and optical absorption spectrum, respectively, of mono- and bi-layer SnS₂ with spin-orbit coupling included throughout the calculations. We further investigate the character of excitonic states contributing to the optical spectrum.

1This work was supported by NSF Grant No. DMR10-1066184 and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory’s NERSC facility.

10:48AM F1.00015 Thickness-dependent Dielectric Constant of Few-layer In₂Se₃ Nano-flakes , DI WU, Department of Physics, University of Texas at Austin, ALEXANDER PAK, Department of Chemical Engineering, University of Texas at Austin, YINGNAN LIU, XIAOYU WU, YUAN REN, Department of Physics, University of Texas at Austin, YU-HAO TSAI, Department of Chemical Engineering, University of Texas at Austin, MIN LIN, HAILIN PENG, College of Chemistry and Molecular Engineering, Peking University, Beijing China, GYEONG HWANG, Department of Chemical Engineering, University of Texas at Austin, KEJI LAI, Department of Physics, University of Texas at Austin — The dielectric constant or relative permittivity of active materials in electronic devices is a critical parameter for charging and screening effects. For layered two-dimensional (2D) materials, it is of great interest to understand how their dielectric constants depend on dimensionality and the arrangement of crystal lattices. Here we present both experimental and theoretical investigations on the dielectric constant of a few-layer In₂Se₃ nano-flakes grown on mica substrates by van der Waals epitaxy. A nondestructive microwave impedance microscope (MIM) is employed to simultaneously quantify the number of layers and local electrical and optical properties. The measured effective dielectric constant increases monotonically as a function of the thickness and saturates to the bulk value at around 6-8 quintuple layers. The same trend of layer-dependent dielectric constant is also revealed through a density functional theory approach. Our results of the dielectric response are expected to be significant for the applications of layered materials in nano-devices.

Tuesday, March 3, 2015 8:00AM - 11:00AM — Session F2 DMP: Focus Session: Beyond Graphene - Optics in 2D semiconductors II 001B - Sefaattin Tongay, Arizona State University

8:00AM F2.00001 Measurement of the optical dielectric function of transition metal dichalcogenide monolayers: MoS₂, MoSe₂, WS₂ and WSe₂ . ALBERT RIGOSI, YILEI LI, ALEXEY CHERNIKOV, XIAN ZHANG, HEATHER HILL, AREND VAN DER ZANDE, DANIEL CHENET, EN-MIN SHIH, JAMES HONE, TONY HEINZ, Columbia Univ — We report a determination of the complex in-plane dielectric function of monolayer MoS₂, MoSe₂, WS₂ and WSe₂, for photon energies from 1.5 – 3 eV. The results were obtained from reflection spectra using a Kramers-Kronig constrained variational analysis. From the dielectric functions, we obtain the absolute absorbance of the monolayers. We also provide a comparison of the dielectric function for the monolayers with the corresponding bulk materials.

8:12AM F2.00002 Optical generation and detection of pure valley current in monolayer transition metal dichalcogenides1, WENYU SHAN, JIANHUI ZHOU, DI XIAO, Department of Physics, Carnegie Mellon University — Recent years have seen a surge of interest in the manipulation of the valley index of Bloch electrons, largely driven by its potential applications as valleytronics. Transition metal dichalcogenides are new types of two-dimensional materials with spin-valley coupling, and show some promise as a realization of valleytronics. In this work, we propose a practical scheme to generate a pure valley current in monolayer transition metal dichalcogenides by one-photon absorption of linearly polarized light. We show that the pure valley current can be detected by either photoluminescence measurements or the ultrafast pump-probe technique. Our method, together with the previously demonstrated generation of valley polarization, opens up the exciting possibility of ultrafast optical-only manipulation of the valley index. The tilted field effect on the valley current in experiment is also discussed.

1Acknowledgement NSF EFRI (No. 1433496), DOE (No. DE-SC0012509), and AFSOR (No. FA9550-14-1-0277)

8:24AM F2.00003 Photoluminescence and photocurrent measurement in monolayer MoTe₂, YA-QING BIE, GABRIELE GROSSO, DMITRI EFETOV, EFREN NAVARRO-MORATALLA, DIRK ENGLUND, PABLO JARILLO-HERRERO, Massachusetts Inst of Tech-MIT — 2D transition metal dichalcogenides (2D-TMD), such as MoS₂, WS₂, WSe₂, MoSe₂, have been verified with many remarkable physical properties including the indirect to direct band transition and valley dependent spin polarization. As one of the 2D-TMD family member, monolayer 2H-MoTe₂ is proved to be a direct bandgap semiconductor with strong spin orbital interaction and a significantly low bandgap ~ 1.10eV. However, the effect of the enhanced coulomb interaction arising from reduced dielectric screening in monolayer MoTe₂ has yet to be experimentally demonstrated. Here we employ the near infrared (NIR) photoluminescence and photocurrent measurement to study the quasi-particle interactions at different carrier concentration. This study sheds light on manipulating excitons in MoTe₂ and designing highly efficient NIR optoelectronic devices.
8:36 AM F2.00004 Excitons and Valley Dynamics in MoS$_2$, MoSe$_2$ and WSe$_2$ monolayers$^1$. XAVIER MARIE, Universite de Toulouse, INSA-CNRS-UPS, LPCNO — We have investigated the optical and valley properties for both neutral and charged excitons in transition metal dichalcogenide monolayers (ML): MoS$_2$, MoSe$_2$ and WSe$_2$. In WSe$_2$ MLs, we have combined linear and non-linear optical spectroscopy (one- and two-photon PLE, Second Harmonic Generation spectroscopy) to uncover the excited states of the neutral exciton. The clear identification of s and p exciton excited states combined with first principle calculations allows us to determine an exciton binding energy of the order of 600 meV. The deviation of the excited exciton spectrum from the standard Rydberg series will be discussed. Moreover we show that exciton valley coherence can be achieved following resonant one or two photon excitation [1]. The neutral and charged exciton dynamics have been measured by time-resolved photoluminescence and pump-probe Kerr rotation dynamics [2,3]. The neutral exciton valley polarization decays within about 6 ps, as a result of the intervalley coupling due the strong electron-hole Coulomb exchange interaction in bright excitons. The temperature dependence is well explained by the developed theory, taking into account the long-range exchange interaction [4]. In contrast the valley polarization decay time for the charged exciton is much longer ($\sim$ 1 ns) [5]. Finally we will compare the exciton dynamics in WSe$_2$ mono and bi-layers [6].


$^1$We acknowledge partial funding from Programme Investissements d’Avenir ANR-11- IDEX-0002-02, reference ANR-10-LABX-0037-NEXT, ERC Grant No. 306719 and ANR MoS2ValleyControl.

9:12 AM F2.00005 Imaging the grain boundaries in polycrystalline MoS$_2$ monolayer by non-invasive second harmonic generation. JINXIN CHENG, TAO JIANG, Fudan University, QINGQING JI, YANFENG ZHANG, Peking University, XINGAO GONG, WEI-TAO LIU, SHIWEI WU, Fudan University — Atomically thin transition metal dichalcogenide monolayers have showed intriguing physical properties for high performance quantum electronics. In order to utilize them in technological applications at industrial scale, mass production of this two dimensional materials via chemical vapor deposition (CVD) is demanded and urged. Despite the success of growing large-scale monolayer, limited grain size and emergence of grain boundary remain as the major hurdle being single crystalline sheets. To resolve this issue, it is necessary to image the grain and grain boundary, and further understand their formation with statistical significance. Here we used second harmonic generation (SHG) microscopy, a noninvasive coherent imaging technique, to image the grain and grain boundary in CVD grown monolayer molybdenum disulfide. The destructive interference between neighboring grains enabled us to pinpoint the location of grain boundary; the anisotropic polarization pattern permitted us to determine the type of grain boundary. Furthermore, this high-throughput characterization technique allows statistical analysis of hundreds of grain and grain boundary, unambiguously revealing that the CVD growth mechanism of monolayer MoS$_2$.

9:24 AM F2.00006 Tunable polaritons from plasmon-phonon coupling in hyperbolic media. SIYUAN DAI, Univ of California - San Diego, QIONG MA, Massachusetts Institute of Technology, SHOU-EN ZHU, Delft University of Technology, Netherlands, MENGKUN LIU, University of California, San Diego, TROND ANDERSEN, Massachusetts Institute of Technology, ZHE FEI, MICHAEL GOLDFLAM, MARTIN WAGNER, Univ of California - San Diego, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, MARK THIEMENS, Univ of California - San Diego, FRITZ KEILMANN, Ludwig-Maximilians-Universität and Center for Nanoscience, G.C.A.M. JANSSEN, Delft University of Technology, Netherlands, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology, MICHAEL FOGLER, D.N. BASOV, Univ of California - San Diego — Using infrared nano-imaging and nano-spectroscopy, we report on the tunable hyperbolic response in heterostructures comprised of a monolayer graphene deposited on hexagonal boron nitride (G-hBN). Electrostatic gating of the top graphene layer allows for modification of the wavelength and intensity of hyperbolic phonon polaritons in bulk hBN. When compared with the pristine hBN polaritons, the graphene modified ones exhibit a longer wavelength in the Type II hyperbolic region and shorter wavelength in the Type I region. Because of this modification, we achieve a 90% increase of the propagation length for graphene modified polaritons. This is a proof of principle of the tunable hyperbolic response in heterostructures comprising of G-hBN.
Intrinsic Exciton Linewidth in Monolayer Transition Metal Dichalcogenides

KAI HAO, GALAN MOODY, CHANDRIKER DASS, The University of Texas at Austin, CHANG-HSIAO CHEN, Institute of Atomic and Molecular Sciences, Academia Sinica, LAIN-JONG LI, King Abdullah University of Science & Technology (KAUST), AKSHAY SINGH, KHA TRAN, The University of Texas at Austin, GENEVIEVE CLARK, XIAODONG XU, University of Washington, GUNNAR BERGÄUSER, ERMIN MALIC, ANDREAS KNORR, Technische Universität Berlin, XIAOQIN LI, The University of Texas at Austin — Excitons in monolayer transition metal dichalcogenides (TMDCs) exhibit exceptionally large binding energy, strong optical absorption, and spin valley coupling. These characteristics make TMDCs a promising system for optoelectronics and valleytronics. An important yet unknown property of excitons in TMDCs is the intrinsic homogeneous linewidth, which reflect radiative recombination and irreversible dissipative decay. Here, we use optical coherent two-dimensional spectroscopy to reveal the exciton homogeneous linewidth in monolayer CVD grown Tungsten Diselenide (WSe2). With excitation density and temperature dependent measurements, exciton-exciton interaction and exciton-phonon interactions are quantitatively evaluated. Extrapolating to zero density and temperature, we obtain a residual homogeneous linewidth of \( \sim1.5 \text{ meV} \), which places a lower bound of 0.2 ps on the exciton radiative lifetime. This result is consistent with microscopic calculations, which suggest that fast radiative decay of delocalized excitons arises from their large oscillator strength.

We acknowledge AFOSR and NSF for funding.

Absorption spectrum and ultrafast response of monolayer and bilayer transition-metal dichalcogenides

VOLODYMYR TURKOWSKI, ALFREDO RAMIREZ-TORRES, TALAT S. RAHMAN, Department of Physics, University of Central Florida — We apply a combined time-dependent density functional theory and many-body theory approach to examine the absorption spectrum and nonequilibrium response of monolayer and bilayer MoS2, MoSe2, WS2 and WSe2 systems. A previous work we have already demonstrated [1] that the binding energies of these states in the monolayer systems are large which makes them available for room temperature applications. We analyze the possibility of ultrafast electron-hole separation in bilayer systems through inter-layer hole transfer, and show that such a possibility exists, in agreement with experimental observations. For doped systems we consider the possibility of Mahan excitonic states in monolayers and show that the binding energy of these states for the order of 10 meV. We perform a detailed analysis of the relaxation of band monolayers excited by ultrafast laser pulse by taking into account electron-phonon scattering effects, and demonstrate that ultrafast (10-100ps) processes, including luminescence, may be relevant for these materials.


Second-Harmonic Generation in a Phase-Match Free Nonlinear 2D Crystal

Mervin Zhao, Ziliang Ye, Yu Ye, Hanyu Zhu, Yuan Wang, Xiang Zhang, Univ of California - Berkeley — The second harmonic generation (SHG) produced from two-dimensional atomic crystals have been utilized to great effect in studying the grain boundaries and electronic structure of such crystals. However, the SHG in many transition metal dichalcogenides (TMDCs) only occur in odd numbered layers due to their noncentrosymmetric nature, limiting the application of their SHG. Here, we probe the SHG from the bulk noncentrosymmetric molybdenum disulfide (MoS2). Whereas the commonly studied 2H crystal phase’s antiparallel dipoles in adjacent layers give an oscillatory SH response, the parallel dipoles of each atomic layer in the 3R phase constructively interfere to amplify the second harmonic intensity. Due to this interference, we observed the phase-match free condition yielding a quadratic dependence between the intensity and layer number. Additionally, we probed the layer evolution of the A and B excitonic transitions in 3R-MoS2 using SHG spectroscopy. We find exciton splittings distinct from 2H-MoS2, resulting from the different interlayer interactions of the two polytypes.

Light matter interactions in 2D transitional metal dichalcogenides: excitonic emission and valley splitting

Ting Yu, Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, 637371, Singapore — Two-dimensional (2D) semiconductors, such as transitional-metal-dichalcogenide monolayers (TMD 1Ls), have aroused great interest because of the underlying fundamental physics (e.g. many body effects and wealth excitonic states) and the promising optoelectronic applications such as light-emitting diodes and solar cells. Here, we report excitonic emission and valley splitting of monolayer WS2 and MoS2 under electrical, optical and magnetic manipulation. Through electrical and optical injection of charge carriers, tunable excitonic emission has been realized due to interplay of various excitonic states, and basic binding energies of trions have been extracted. At low temperature, the Zeeman shifts of excitons and trions have been determined by polarization-dependent photoluminescence measurements under perpendicular magnetic fields, which reveal the breaking of valley degeneracy. Our studies provide the fundamental understanding on large excitonic and unique valleytronic effects in TMD 1Ls. Moreover, we also develop multiple strategies for managing the light emission, which opens up many possibilities for improving the performance and creating the multifunction of 2D TMD-based light emitting applications.

Optical Properties and Band Gap of Single- and Few-Layer MoTe2 Crystals

Ozgur Burak Aslan, Columbia Univ, Claudia Ruppert, Technische Universität Dortmund, Tony Heinz, Columbia Univ — Single- and few-layer crystals of exfoliated MoTe2 have been characterized spectroscopically by photoluminescence, Raman scattering, and optical absorption measurements. We find that MoTe2 in the monolayer limit displays strong photoluminescence. On the basis of complementary optical absorption results, we conclude that monolayer MoTe2 is a direct-gap semiconductor with an optical band gap of 1.10 eV. This new monolayer material extends the spectral range of atomically thin direct-gap materials from the visible to the near-infrared.

Supported by the NSF through Grant DMR-1124894 for sample preparation and characterization by the O’/ce of Naval Research for analysis. C.R. acknowledges support from the Alexander von Humboldt Foundation.
8:36AM F3.00002 Imaging current in quantum spin Hall insulator InAs/GaSb

ERIC SPANTON, Stanford Institute for Materials and Energy Sciences — Scanning superconducting quantum interference device (SQUID) microscopy allows us to visualize how currents flow in materials by imaging magnetic fields. I will give an overview of our technique and focus on the quantum spin Hall edge states we observed in Si-doped InAs/GaSb quantum wells. The main feature of 2D topological insulators is the topologically-protected edge modes that are a result of their special band structure. We used a SQUID to image current in the edge modes, which are present when the chemical potential lies in or near the insulating gap. The unique spin-texture of the edge states restricts how electrons can backscatter, leading to ballistic transport in small enough devices. In more resistive, longer devices, the backscattering becomes weaker, and the resistance of the edges due to backscattering is flat and does not match any of the allowed backscattering mechanisms which have been theoretically investigated.

9:12AM F3.00003 Magnetotransport in the topological insulator candidate InAs/GaSb

THOMAS IHN, ETH Zurich — InAs/GaSb quantum wells have been proposed as an electrically tunable two-dimensional topological insulator system. Transport can be tuned from the electron to the hole regime where the Fermi-energy crosses the hybridization gap, where topological edge states are predicted to exist. We have investigated this material system using dc magneto-transport measurements at cryogenic temperatures. In high-mobility large-area samples, a resistivity maximum is observed at the charge-neutrality point. It increases strongly with magnetic field. At the same time, a strong non-local resistance appears which we describe by a model of helical and dissipative quantum Hall edge channels shorted by residual bulk conductivity. In an attempt to reduce the bulk conductivity, we have grown samples with slightly impure Gallium. Large-area devices show a peak resistance at the charge neutrality point enhanced by almost three orders of magnitude compared to the high-mobility samples. A requirement for observing the topological insulator state is the fabrication of devices smaller than the inelastic scattering length. We have developed an optimized fabrication recipe by comparing samples produced with wet and dry etching. The former turns out to be favorable for obtaining smooth edge potentials and a width-independent electron density. With this fabrication technology we have produced small-area Hall bar devices with widths and contact separations in the micrometer range. Surprisingly these devices do not exhibit a resistance maximum at charge neutrality like large-area devices, but rather show a plateau-like local resistivity at negative gate voltages. At the same time the Hall density saturates in these devices at finite electronic densities instead of turning into the edge regime, and a systematic non-local resistance signal appears in all devices. We discuss these findings in view of conflicting fabrication issues or the proposed helical edge modes.

1Supported by the Swiss National Science Foundation via NCCR QSIT (Quantum Science and Technology).

9:48AM F3.00004 One-dimensional topological edge states of bismuth bilayers

ILYA DROZDOV, Princeton University — A quantum spin Hall (QSH) state of matter, also known as a two-dimensional (2D) topological insulator, is distinguished by one-dimensional (1D) chiral edge modes propagating along the perimeter of the system without backscattering. Among the first systems predicted to be a 2D topological insulator are bilayers of Bismuth (Bi) [1]. Despite being a well-known QSH candidate system which should in principle be accessible to scanning tunneling microscopy (STM) techniques, the experimental attempts carried out so far have suffered from edge imperfections and coupling of the edge states to the substrate. In this talk I will present recent STM experiments on bulk Bi crystals [2] which show that a subset of the predicted Bi-bilayers’ topological edge states are in fact decoupled from the states of the substrate which makes it possible to probe the 1D electronic channels experimentally using spectroscopic STM techniques. Spectroscopic features observed in STM are directly compared to model calculations. Furthermore, unique electronic structure of topological edge modes of Bi allows for quantum interference of edge-mode quasi-particles in confined geometries, which is visualized by STM and allows to reveal the absence of backscattering of electrons in the 1d edge channels - the key property of the QSH systems resulting in their remarkable coherent propagation. Additionally, I will present comparison to theoretical models of the edge state along with supporting experimental study of Bi(111) surface state’s electronic structure.


1The work at Princeton and the Princeton Nanoscale Microscopy Laboratory was supported by the ARO MURI program W911NF-12-1-0461, DARPA-SPWAR Meso program N6601-11-1-4110, NSF-DMR1104612, NSF CAREER DMR-095242, ONR-N00014-11-1-0635, and NSF-MRSEC NSF-DMR08

10:24AM F3.00005 Quantum spin Hall effect in InAs/GaSb bilayers subject to exciton condensation and magnetic field

DMITRY PIKULIN, Department of Physics and Astronomy and Quantum Matter Institute, University of British Columbia, Vancouver, Canada — Motivated by the recent experiments we study the phase diagram of the bilayer InAs/GaSb quantum wells in the presence of electron-electron interactions. The interactions lead to formation of thermodynamically stable exciton condensate. We show that in the presence of condensate but without external magnetic field the bilayer can be in three distinct insulating phases: trivial, topological, and spontaneously breaking time-reversal symmetry ones. In the applied magnetic field the bilayer remains gapped and undergoes a series of phase transitions changing from quantum spin Hall-like state to trivial insulator. We suggest transport and spectroscopic measurements for future experiments to substantiate our picture.

Tuesday, March 3, 2015 8:00AM - 11:00AM –
Session F4 APS: Undergraduate Research/Society of Physics Students III
Mayor Cockrell Room 004 –
- Sean Bentley, American Institute of Physics / Society of Physics Students

8:00AM F4.00001 Light: A Spectrum of Utility, the 2014-2015 Society of Physics Students Science Outreach Catalyst Kit

MARK SELLERS, Rhodes College, KEARNS LOUIS-JEAN, Xavier University of Louisiana, SOCIETY OF PHYSICS STUDENTS COLLABORATION, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY COLLABORATION — The Science Outreach Catalyst Kit (SOCK) is a set of activities and demonstrations designed to bolster the outreach programs of undergraduate Society of Physics Students (SPS) chapters, creating the framework for a lasting outreach program. Targeted for students ranging from kindergarten to high school, the SOCK allows students to actively engage in hands-on activities that teach them scientific skills and allow them to exercise their natural curiosity. The 2014-2015 SOCK united themes from the 2014 International Year of Crystallography and the 2015 International Year of Light to explore how light is used as a tool every day. This presentation will discuss the contents of the SOCK, which contains a large assortment of materials, such as diffraction glasses, polarizers, ultraviolet flashlights, etc. and describe the research and development of the activities. Each activity explores a different light phenomenon, such as diffraction, polarization, reflection, or fluorescence. These activities will promote critical thinking and analysis of data.

1This work was supported by the Society of Physics Students summer intern program and by the National Institute of Standards and Technology.

8:12AM F4.00002 ABSTRACT WITHDRAWN –
8:24AM F4.00003 Capacitively-coupled differential position detection in the development of a high-sensitivity torsion balance. CHARLES RACKSON, ALEX WATT, WOO-JOONG KIM, Seattle University, SEATTLE UNIVERSITY TEAM — We report on the development of a high-sensitivity torsion balance using a capacitively-coupled Wheatstone Bridge. The torsion balance will be employed to measure the Casimir Force, with a particular emphasis on the surface patch effects that are ubiquitous on metallic surfaces. We will show that these effects also play a significant role in another class of experiments involving quantum-point contacts between two metal wires.

8:36AM F4.00004 Mapped grid methods for Numerov propagation. CHRISTOPHER MADRID, JUAN BLANDON, Angelo State University, GREGORY PARKER, University of Oklahoma — The Computational toll of solving the Schroedinger equation for certain atomic systems is sometimes prohibitively heavy. We present a grid-mapping method which decreases the number of points needed, and at the same time maintains or increases accuracy for three-atom scattering. By developing a hyperspherical mapping method for Numerov propagation, scattering cross-sections can be found for a large range of energies. This method is useful for systems with very shallow bound states where the mapping will give a large number of data points inside the potential well while decreasing the number of points at a large hyper-radius. The change in grid sizes is controlled by a mapping function that is easily modified. Results are shown for scattering in the HeH₂ and HNe₂ systems.

8:48AM F4.00005 Simulation of Planetary Formation using Python. JAMES BUFKIN, DAVID BIXLER, Angelo State University — A program to simulate planetary formation was developed in the Python programming language. The program consists of randomly placed and massed bodies surrounding a central massive object in order to approximate a protoplanetary disk. The orbits of these bodies are time-stepped, with accelerations, velocities and new positions calculated in each step. Bodies are allowed to merge if their disks intersect. Numerous parameters (orbital distance, masses, number of particles, etc.) were varied in order to optimize the program. The program uses an iterative difference equation approach to solve the equations of motion using a kinematic model. Conservation of energy and angular momentum are not specifically forced, but conservation of momentum is forced during the merging of bodies. The initial program was created in Visual Python (VPython) but the current intention is to allow for higher particle count and faster processing by utilizing PyOpenCl and PyOpenGl. Current results and progress will be reported.

9:00AM F4.00006 Effects of Turbulence on Cosmic Ray Propagation in Protostar Systems. DONOVAN HERBERT, MARCO FATUZZO, Xavier University, FRED ADAMS, University of Michigan — The magnetic field associated with young stellar objects is expected to have an hour-glass geometry, i.e. the magnetic field lines are pinched together in the equatorial plane surrounding the forming star but are subsumed smoothly onto a background field at large distances. In such a structure, incoming cosmic rays experience both a funneling effect, which acts to magnify the flux impinging on the circumstellar disk, and a magnetic mirroring effect that acts to reduce that flux. These effects nearly cancel out for simple underlying magnetic field structures with respect to the leading order. However, the environments surrounding young stellar objects are expected to be highly turbulent and, thus, act to complicate these effects. We consider here how the presence of magnetic field fluctuations affects the process of magnetic mirroring, and thereby changes the flux of cosmic rays striking the circumstellar disks. These results may have significant consequences for the ionization fraction of the disk, which in turn dictates the efficiency with which disk material can accrete onto the central object.

9:12AM F4.00007 Transverse distortion effects on the Kasteleyn and KDP transition in spin ice. CURTISLEE THORNTON, TRINANJAN DATTA, Georgia Regents University — Geometrically frustrated pyrochlore oxides containing a rare-earth ion and a transition metal ion form a network of corner-sharing tetrahedra. Prominent examples include Dy₂Ti₂O₇ and Ho₂Ti₂O₇. Magnetic frustration in these compounds suppresses the formation of a long-range ordered ground state resulting in an exotic phase of matter called spin ice. Elucidating the role of external perturbations such as pressure and magnetic field is an important step towards understanding the novel KDP and Kasteleyn phase transitions arising in these classical spin ice materials. Utilizing an analytical approach based on the Husimi tree approximation, we investigate the effects of both transverse and uniaxial pressure distortion of the spin ice tetrahedra on both the KDP and Kasteleyn transition in the presence of an external magnetic field. Compared to the uniaxial distortion scenario, we find that including the effects of transverse distortion leads to further suppression of magnetization and heat capacity in both the Kasteleyn and KDP cases.

9:24AM F4.00008 ABSTRACT WITHDRAWN

9:36AM F4.00009 ABSTRACT WITHDRAWN

9:48AM F4.00010 Super Atomic Molecular Orbitals of Variably Protonated Symmetric Molecules. TANNER LATTA, KYLE DRAKE, G.P. ZHANG, Indiana State Univ — The molecular structure of symmetric molecules creates conducive conditions for delocalized orbitals. The π bonding delocalizes the valence electrons away from the individual molecules. These delocalized valence electrons allow the symmetric molecules to adapt the characteristics analogous to that of an individual atom, creating Super Atomic Molecular Orbitals, SAMOs. The symmetric molecule is then comparable to that of an individual atom with its regular atomic orbitals. When these symmetric molecules are protonated in any form, there are notable changes in the shapes of the Super Atomic Molecular Orbitals. We use the Density Functional Theory with a grid mesh method to compute the wavefunctions of these SAMOs. Then we examine the Rydberg States of these symmetric molecules through the calculated Eigenstates, and find an important trend in the filling of the SAMOs as well as relationships between variably protonated symmetric molecules. This is potentially very useful to understanding the photovoltaic effect in the fullerene- based solar cells.

1Support by U.S. Department of Energy No DE-FG02-06ER46304

10:00AM F4.00011 Comparative Study of Wavelet Basis Set and Finite-Difference Time-Domain Methods for the Time Propagation of Quantum and Classical Systems. EWA NOWARA, IRWIN GOLDBERG, St. Mary’s University (San Antonio, Texas), BRUCE JOHNSON, Rice University, RICHARD LOMBARDINI, St. Mary’s University (San Antonio, Texas) — An extensive comparison in error accumulation between a grid point method, in particular finite-difference time-domain (FDTD), and a basis set method using Daubechies wavelets is presented in the modeling of electromagnetic (EM) pulses (classical) in inhomogeneous media and quantum (QM) wavepackets interacting with various potentials. It is demonstrated that the density of wavelet functions needed to attain a certain level of accuracy is far less than needed for grid points (FDTD) translating to savings in computational memory and processing. Since neighboring wavelet basis functions have overlapping support, fictitious wavelet projections created by derivative matching (T.A. Driscoll and B. Fornberg) will be used to handle Dirichlet boundary conditions in both the EM and QM cases in order to prevent rapid error growth.
Anomaly.

Defects we consider break charge conservation symmetry and thereby provide insight into the anomalous nature of the 2/3 edge going beyond the U(1) chiral anomaly. In this talk we investigate the anomalous structure of the 2/3-edge state by testing its non-perturbative robustness to a particular type of defect. When charge conservation is broken, one might expect that there is something fundamentally anomalous about the ν = 2/3 state. However, we have protected gapless edge modes even if all symmetries are broken, including charge conservation. Since the edge protection for the 2/3 state exists even when charge conservation is broken, one might expect that there is something fundamentally anomalous about the ν = 2/3 edge beyond the usual U(1) chiral anomaly. This result contributes to understanding the relationship between temperature modification and the transverse modes of VCSEL.

1 With support from the Office of Undergraduate Research at Washington University.

10:24 AM F4.00013 Dissipative coherence of a superconducting qubit for microwave detection

TATCHER HSIEH, KATER MURCH, Washington University — Recent progress in coherent control and measurement of superconducting qubits has opened avenues to previously inaccessible regimes of metrology. Here we realize a detection scheme for microwave signals. Our scheme utilizes a superconducting transmon qubit coupled to a three-dimensional cavity. When subjected to a weak drive signal near resonance, the qubit equilibrates to a steady state coherence that arises from the competition between driven and dissipative dynamics. By measuring this steady state coherence with quantum state tomography, we map the quantum state to characteristics of the drive signal with shot noise-limited resolution. We report detection figures of merit and discuss applications to itinerant microwave fields.

10:36 AM F4.00014 Optimized reconstruction methods for imaging squeezed microwave states

ADITYA VENKATRAMANI, DAVID TOYLI, QNL, University of California, Berkeley, SAMUEL BOUTIN, Département de Physique, Université de Sherbrooke, ANDREW EDDINS, QNL, University of California, Berkeley, ALEXANDRE BLAIS, Département de Physique, Université de Sherbrooke, IRFAN SIDDIQI, QNL, University of California, Berkeley — Superconducting parametric amplifiers (paramps) are essential tools for quantum-limited measurement of superconducting qubits. A central feature of these devices is that they can ideally amplify information in one quadrature without adding noise while simultaneously squeezing fluctuations in the orthogonal quadrature. At microwave frequencies, moment-based reconstruction techniques are commonly utilized to image such squeezed states. Motivated by a desire to characterize and improve paramp squeezing performance, we have developed simulations to understand the application of these reconstruction techniques, with a focus on determining their performance at large signal gains where the amplifier output field becomes non-Gaussian. We make comparisons of this analysis to experimental data. We have also developed a complementary imaging method based on deconvolution techniques that is effective for high signal-to-noise ratios. This method benefits from a simple implementation and provides a best estimate for the output field Q function. We discuss experimental implementations of these techniques facilitated by the use of a broadband parametric amplifier.

1 This work is supported by ARO and ONR.

10:48 AM F4.00015 Toroidal moment contributions to the multiferroic acoustic susceptibility

ALEXANDER PRICE, TRINANJAN DATTA, Georgia Regents University — We consider the effects of toroidal moment corrections to the acoustic susceptibility tensor of a material that is simultaneously ferroelectric and a canted antiferromagnet (multiferroic). Using the Landau-Lifshitz equation of motion for the magnetization, the Landau-Khalatnikov relaxation equation for the electric polarization, and an equation of motion for the toroidal moment coupling, we find that the previously vanishing susceptibility components in the multiferroic channel are now non-zero. Additionally, the toroidal corrections give rise to non-zero, asymmetric susceptibility components in the magnetic, electric, and multiferroic channels with both real and imaginary corrections to the susceptibility.

1 GRU Small Grants Program
8:36AM F5.00004 Role of the continuum states in the thermodynamics of the \( \nu = 1/3 \) fractional quantum Hall effect, PETER RAUM, VITO SCAROLA, Virginia Tech — The high energy excitations of fractional quantum Hall states dictate thermodynamics at experimentally accessible temperatures. We construct a microscopic formalism for the thermodynamics of the \( \nu = 1/3 \) Laughlin state as generated by a hard core repulsive model. We use exact diagonalization of the hardcore repulsive model for small system sizes to gather statistics for the excitations. These results are extrapolated to the thermodynamic limit using an ansatz partition function that captures the ground state, low-energy excitations, and high energy continuum states. The continuum states are found to play an important role at low temperatures, even below the characteristic gap.

8:48AM F5.00005 Anisotropic gapped excitation modes in the SLL from Light Scattering\(^1\), ARON PINCZUK, Columbia University, URSULA WURSTBAUER, TU München, ANTONIO L. LEVY, Columbia University, JOHN WATSON, GEOFF C. GARDNER, MICHAEL J. MANFRA, Purdue University, KEN WEST, LOREN PFIEFFER, Princeton University — The fascinating interaction physics in the SLL supports the emergence of exotic quantum phases and unconventional FQHE states as e.g. anisotropic, possibly nematic, FQHE states at \( \nu = 5/2 \) [1] and \( \nu = 7/3 \) [2]. We explore the fascinating physics of these states by studying low-lying collective excitation spectrum from resonant inelastic light scattering (RILS) experiments. Here, we focus on the filling factor range \( 5/2 > \nu > 2 \). We observe clear signatures from gapped modes that weaken with increasing temperature for several filling factors that are known from transport to be incompressible FQHE states like \( \nu = 2+1/2, 2+3/8 \) and \( 2+1/3 \). These modes exhibit a clear dependence on filling factor, unambiguously uncovering incompressible quantum states. The lowest mode exhibits a remarkably strong polarization dependence that can be interpreted as fingerprint for the lack of rotational symmetry of the ground state. This interpretation of the observed RILS mode would support nematic FQHE states in the SLL.

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Spontaneous valley ordering in SnTe (001) surface states

Ming Xie, Department of Physics, The University of Texas at Austin, XIAO LI, Condensed Matter Theory Center, University of Maryland, FAN ZHANG, Department of Physics, The University of Texas at Dallas, ALLAN MACDONALD, Department of Physics, The University of Texas at Austin — In this work we study the spontaneous valley ordering in SnTe surface states. SnTe is a topological mirror insulator in which the bulk mirror symmetry allows robust surface states to appear on certain surfaces like (001), (111) and (110). These surface states provide a new platform to study multi-flavor Landau level physics in the quantum Hall regime. Attention has been drawn to the (001) surface by a recent experimental observation of a four-fold degenerate Landau level formed at zero energy [Science 341, 1496 (2013)]. This degeneracy arises because the single-particle bandstructure at low energies consists of four surface Dirac cones. In the presence of electron-electron interactions, however, this four-fold degeneracy is expected to be lifted. In this work we construct a theory to show that at all integer filling factors between -2 and +2 the ground state is a gapped quantum Hall state. We further demonstrate that these ground states are valley nematic phases, and discuss some experimental consequences.

Transmission Measurements in a Low Density Two-Dimensional Electron Gas in an Array of Antidots

Chi Zhang, Jian Mi, Peking University, Loren Pfieffer, Ken West, Princeton University — Under high magnetic fields, the microwave conductivity of a two-dimensional electron system containing an antidot array with fractional Landau filling was discovered [1]. On the other hand, at low temperature T=0.3 K, we have measured the transmission in the low density (n=0.6x10^11 cm^-2) ultraclean GaAs/AlGaAs sample with an array of antidots. In our measurements, we observed an interesting feature around the ν=1, 2, which may be related to the charged edge mode in the integer quantum Hall regime. [1] P. D. Ye, L. W. Engel, D. C. Tsui, J. A. Simmons, J. R. Wendt, G. A. Vawter, and J. L. Reno, Phys. Rev. B, 65, 121305 (2002).

Critical exponent in a projected lattice model for integer quantum Hall plateau transitions

Qiong Zhu, Xin Wan, Zhejiang University, R.N. Bhatt, Princeton University — Motivated by the recent numerical studies on the Chalker-Coddington network model with a larger-than-expected localization length critical exponent, we revisited the exponent calculation in the disordered Hofstadter model. We project the Hamiltonian into the lowest subband, which is the lattice analog of the lowest Landau level, and calculate the Chern number for individual eigenstates to analyze their localization properties. We compare the finite-size scaling of the total number of the conducting states, the width of the distribution of the conducting states, and the Hall conductance. We confirm that earlier calculations on the lattice model have also underestimated the localization length critical exponent and discuss the manifestation of the leading irrelevant scaling field.

Quantum Hall plateau transitions in the bulk entanglement spectrum

Xin Wan, Qiong Zhu, Zhejiang University, Guang-Ming Zhang, Tsinghua University — We discuss an alternative route to access the quantum Hall transitions via studying the so-called bulk entanglement spectrum. By partitioning the pure integer quantum Hall ground state in a checkerboard fashion we show the emergence of a quantum network with bulk gapless excitations at the Brillouin zone center without fine-tuning. The emergent critical theories have a one-to-one correspondence to the Chern number characterization of the original ground states [arXiv:1409.4916]. For example, the resulting critical theory for the ν=1 state is the (2+1)-dimensional relativistic quantum field theory characterized by a single Dirac cone spectrum and a pair of fractionalized zero-energy states. For the ν=2 state the critical theory exhibits a quadratic band crossing. The effect of disorder on the transitions will be presented.

Microwave Absorption of Edge States in Quantum Hall Droplets

Jie Zhang, Lingjie Du, Ruiyuan Liu, Ruirui Du, Department of Physics and Astronomy, Rice University, Houston, Texas, Loren Pfieffer, Ken West, Department of Electrical Engineering, Princeton University — Microwave absorption spectroscopy has been proposed as a unique tool in studies of edge physics of quantum Hall droplets (Cano et al., Phys. Rev. B 88, 165305 (2013)). In our ongoing experiment we pattern co-planar waveguide (CPW) and micrometer-size discs on the same chip of a high-mobility GaAs/AlGaAs two-dimensional electron gas. The CPW is placed inside a broadband sample holder, which is fitted with millimeter wave coax cables. The whole setup is top-loaded into a 300 mK helium3 cryostat equipped with a superconducting solenoid. In this talk the construction of the spectrometer, preliminary data, and discussions will be presented.

Thermal Hall Effect and Geometry with Torsion

Alexander Abanov, Andrey Gromov, Stony Brook University — We formulate a geometric framework that allows to study momentum and energy transport in non-relativistic systems. We show how momentum and energy current can be computed as responses to variations in geometry. It turns out that in the absence of Lorentz invariance the appropriate geometry is not Riemannian, but the Newton-Cartan geometry with temporal torsion. Our approach generalizes the classic Luttinger’s formulation of thermal transport. In particular, we clarify the geometric meaning of the fields conjugate to energy and energy current. These fields describe the geometric background with non-vanishing temporal torsion. We use the developed formalism to construct the equilibrium partition function of a non-relativistic system coupled to the NC geometry in 2+1 dimensions and to derive various thermodynamic relations. As a by-product we argue that the bulk thermal Hall conductance is not topologically protected.

Achromatic metasurface optical components by dispersive phase compensation

Federico Capasso, Harvard University — The replacement of bulk refractive elements with flat ones enables the miniaturization of optical components required for integrated optical systems. This process comes with the limitation that planar optics suffers from large chromatic aberrations due to the dispersion of the phase accumulated by light during propagation. We show that this limitation can be overcome by compensating the dispersion of the propagation phase with the wavelength-dependent phase shift imparted by a metasurface. We demonstrate dispersion-free multi-wavelength dielectric metasurface deflectors in the near-infrared and design an achromatic flat lens in the same spectral region. Our design is based on low-loss coupled dielectric resonators, which introduce a dense spectrum of modes to enable dispersive phase compensation. Achromatic metasurfaces will find applications as multi-band-pass filters, lightweight collimators, and chromatically-corrected imaging lenses.
8:36AM F6.00002 Scattering properties of semiconductor-based metamaterials with subwavelength cavities in the infrared region, ANDREY SEMICHAEVSKY, Lincoln University, PA, STEPHANIE LAW, University of Delaware — All-semiconductor (III-V) metamaterials for the IR have recently been proposed for applications in superlensing and sensing [1]. These 1-D structures have been shown to have negative effective refractive index at wavelengths around 8 µm. Some other metamaterial structures for the visible range [2] employed SiC spherical inclusions in a plasmonic (MgB2) host medium. In this paper we develop and model IR metamaterials that utilize both low-loss highly doped GaAs/InAs semiconductor thin films and 3-D structures, such as subwavelength resonant cavities. We predict the light scattering by these structures using experimentally measured dispersion relations for the doped semiconductor films. The frequency dispersions of permittivity are well fitted by the Drude model. Our future work will include the fabrication of the metamaterial structures and their optical characterization.


8:48AM F6.00003 Emission Testing Results of Thermally Stable, Metamaterial, Selective-Emitters for Thermophotovoltaics, KATHERINE LEVINSON, NORIHIKO NAKA, NICOLE PFIESTER, ABIGAIL LICHT, TOM VANDERELDE, Tufts — In thermophotovoltaics, the energy from a heated emitter is converted to electricity by a photovoltaic diode. A selective emitter can be used to emit a narrow band of wavelengths tailored to the bandgap of the photovoltaic diode. This spectral shaping improves the conversion efficiency of the diode and reduces undesirable diode heating. In our research, we study selective emitters based on metamaterials composed of repeating nanoscale structures. The emission characteristics of these materials vary based on the compositional structure, allowing the emitted spectrum to be tunable. Simulations were performed with CST Microwave Studio to design emitters with peak wavelengths ranging from 1-10 microns. The structures were then fabricated using physical vapor deposition and electron beam lithography on a sapphire substrate. Emitter materials studied include gold, platinum, and iridium. Here we report on the emission spectra of the selective emitters and the post-heating structural integrity.

9:00AM F6.00004 ABSTRACT WITHDRAWN —

9:12AM F6.00005 Enhancing harmonic generation using nonlinear Metamaterials, SINHARA SILVA, University of South Florida, Tampa, KIM SONJU, California State University, San Bernadino, JIANGFENG ZHOU, University of South Florida, Tampa — In this work, we demonstrate the double-resonator meta-atom design in a nonlinear metamaterial can significantly enhance harmonics in microwave frequency regime. Nonlinearity in the structure is introduced by adding a varactor diode in the common slit of the double split ring resonator (DSRR) design. By engineering the structure such that inner ring resonance frequency of the DSRR is twice as the outer ring resonance frequency, we have demonstrated that the second harmonic of the outer ring can be enhanced by factor of 70 compared to a conventional SRR structure. Furthermore, the second harmonic of the periodic arrays can be further improved by carefully positioning the unit cells. In addition, with the enhancement of the second harmonic, other higher order harmonics can be enhanced.

9:24AM F6.00006 Controlling the Polarization State of Light with a Dispersion-Free Metas-structure, SHANGCHI JIANG, Nanjing University — By combining the advantages of both a metallic metamaterial and a dielectric interlayer, we demonstrate the general mechanism to construct the dispersion-free metasstructure, in which the intrinsic dispersion of the metallic structures is perfectly cancelled out by the thickness-dependent dispersion of the dielectric spacing layer. As examples to apply this concept, a broadband quarter-wave plate and a half-wave plate are demonstrated. By selecting the structural parameters, the polarization state of light can be freely tuned across a broad frequency range, and all of the polarization states on the Poincare sphere can be realized dispersion free.


10:12AM F6.00008 Photon-Spin Drag on a Plasmonic Metasurface, XINGJIE NI, JUN XIAO, SUI YANG, YUAN WANG, University of California, Berkeley, XIANG ZHANG, University of California, Berkeley; Materials Sciences Division, Lawrence Berkeley National Laboratory — Classical polarized light carries spin and reveals spin-orbit coupling when propagating along a curved trajectory, however this interaction typically is very weak. Utilizing a metasurface can greatly enhance this interaction because it can bend light abruptly within an extremely small thickness due to the large induced momentum. This strong photonic spin-orbit coupling on a metasurface could drive the electrons collectively and lead to direct electric currents flowing transversely to the light-bending direction, even at normal incidence and without external magnetic fields. Such a photon-spin drag effect has never until now been demonstrated. Here we report the first direct observation of this effect on a metallic metasurface consisting of complementary nanoantennas. By inputting opposite photonic spins, we directly detect the changes inversion of the transverse current direction. This effect enables an electrical detection of photon spin-orbit interactions and provides a viable route to directly integrate modern electronic chips with the additional spin degree of freedom of light for future information processing and communication applications.

10:24AM F6.00009 Creation of optical near-field orbital angular momentum in a gold metasur-face, CHEN-BIN HUANG, CHING-FU CHEN. CHEN-TA KU, Natl Tsing Hua Univ, MING-YANG PAN, PEI-KUEN WEI, Academia Sinica — Nanocavities in a gold thin film is optimized and arranged to form a metasurface. We demonstrate both numerically and experimentally that surface plasmon vortex carrying optical orbital angular momentum can be generated using linearly-polarized optical excitation.

10:36AM F6.00010 Anisotropic Fabry Perot resonances in Metal-Dielectric Meta-Nano-Layer, DAVID KEENE, MATTHEW LEPAIN, MAXIM DURACH, Georgia Southern University — We theoretically propose a new type of mode which exists in a metal-dielectric metamaterial layer of nanoscopic width. These modes exhibit anisotropic dispersion and can be used for strongly directional emission as well as ultra-compact 90 degree polarization rotation. The anisotropic Fabry-Perot (FP) modes appear from regular FP resonances when metal strips are introduced into a dielectric layer forming a metalayer. Each regular FP resonance splits into two anisotropic FP resonances in this situation. In the metalayer structures considered in the paper a fraction of about 0.2 the lower-energy mode of a higher FP mode becomes degenerate with the higher-energy mode of a lower FR resonance and their interference produces transmission of TE polarized waves upon TM incidence from another side, promising 90 degree polarization rotators with dimensions on the order of 100 nm, an order of magnitude smaller than recently proposed by other authors. Although the described behavior is due to the metamaterial-like response of the metal-dielectric strip array the non-local effects in the structures will be discussed.

10:48AM F6.00011 Meta-Optics with Nanowire Grid Arrays: Hyperbolic Fabry-Perot Modes and Hyperbolic Tamm Plasmons, MAXIM DURACH, DAVID KEENE, MATTHEW LEPAIN, Georgia Southern Univ — In this talk we introduce a new class of structures — cavities formed by metal-dielectric metasurfaces. These cavities support a zoo of various resonances, including hyperbolic Tamm plasmons and hyperbolic Fabry-Perot modes, which feature anisotropic clover-leaf dispersion parallel to the metasurface and strong coupling between TM and TE polarizations in the modes. The properties and spectrum of the modes are highly tunable by the dimensional and material parameters of the structure and can be used for directional emission, modification of radiation produced by electric dipole emitters into magnetic dipole radiation as well as 90 degree polarization rotators and polarization rotation mirrors.
Quantum criticality of topological phase transitions in 3D interacting electronic systems

Adiabatic Pumping of Chern-Simons Axion Coupling

Anyon and Loop Braiding Statistics in Field Theories with a Topological $\Theta$-term

Interplay between geometry and topology in topological crystalline phases

Microscopic Realization of 2-Dimensional Bosonic Topological Insulators

Ab Initio Studies of the Tunability of Topological Phases of Complex Materials
9:36AM F7.00007 Fermionic Symmetry Protected Topological Phase Induced by Interaction . SHANQIANG NING, Institute for Advanced Study, Tsinghua Univ, HONGCHEN JIANG, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, ZHENGXIN LIU, Institute for Advanced Study, Tsinghua Univ — It is known that interaction can reduce the classification of topological phases in free fermion systems, for instance, the Z classes of 1D Kitaev Majorana chains with time reversal symmetry reduce to Z2 under interaction. However, strong interactions can give rise to new SPT phases which have no counterparts in free fermion systems. In this talk, I illustrate this result through an concrete example. The symmetry group we consider is U(1)xZ2. There are no topological phases for non-interacting fermions with this symmetry. When interactions are turned on, a nontrivial topological phase appears owning to the existence of nontrivial projective representation. We illustrate this result by studying a three-legged ladder of spinless fermions with strong interactions. We show that there are two gapped SPT phases, the trivial one is adiabatically connected to the band insulator, while the states in the nontrivial phase cannot be adiabatically evolved into the trivial phase without breaking symmetry.

9:48AM F7.00008 Generic Symmetry Breaking Instability of Topological Insulators due to a Novel van Hove Singularity1 , XUGANG HE, Brookhaven National Lab and Stony Brook University, XIAOXIANG XI, Photon Sciences, Brookhaven National Lab, WEI KU, Brookhaven National Lab and Stony Brook University — We point out that in the deep band-inverted state, topological insulators are generically vulnerable against symmetry breaking instability, due to a divergently large density of states of 1D-like exponent near the chemical potential. This feature at the band edge is associated with a novel van Hove singularity resulting from the development of a Mexican-hat band dispersion. We demonstrate this generic behavior via prototypical 2D and 3D models. This realization not only explains the existing experimental observations of additional phases, but also suggests a route to activate additional functionalities to topological insulators via ordering, particularly for the long-sought topological superconductivities.

10:00AM F7.00009 Symmetry Protected Topological States of Interacting Fermions and Bosons , YI-ZHUANG YOU, CENKE XU, University of California, Santa Barbara — We study the classification for a large class of interacting fermionic and bosonic symmetry protected topological (SPT) states. We define a SPT state as whether or not it is separated from the trivial state through a bulk phase transition, which is a general definition applicable to SPT states with or without spatial symmetries. We show that in all dimensions short range interactions can reduce the classification of free fermion SPT states, and we demonstrate these results by making connection between fermionic and bosonic SPT states. We first demonstrate that our formalism gives the correct classification for several known SPT states, with or without interaction, then we will generalize our method to SPT states that involve the spatial inversion symmetry.

10:12AM F7.00010 Symmetry, Defects, and Gauging of Topological Phases , PARS A BONDERS O N, MAISSAM BARKESHLI, MENG CHENG, ZHENGHAN WANG, Station Q, Microsoft Research — We examine the interplay of symmetry and topological order in 2+1D topological phases of matter. We define the topological symmetry group, characterizing symmetry of the emergent topological quantum numbers, and describe its relation with the microscopic symmetry of the physical system. We derive a general framework to classify symmetry fractionalization in topological phases, including phases that are non-Abelian and symmetries that permute the quasiparticle types and/or are anti-unitary. We develop a theory of extrinsic defects (fluxes) associated with elements of the symmetry group G, which provides a general classification of symmetry-enriched topological phases derived from a topological phase of matter with symmetry. The algebraic theory of the defects (G-crossed braided tensor category), allows one to compute many properties, such as the topologically distinct types of defects, their fusion rules, quantum dimensions, zero modes, braiding transformations, a generalized Verlinde formula, and modular transformations of the G-crossed extensions of topological phases. We also examine the promotion of the global symmetry to a local gauge invariance, wherein the extrinsic defects are turned into deconfined quasiparticle excitations, which results in a different topological phase.

10:24AM F7.00011 Kondo Breakdown in Topological Kondo Insulators1 , ONUR ERTEN, Rutgers Univ, VICTOR ALEXANDROV, PIERS COLEMAN, Rutgers University — Motivated by the observation of light surface states of SmB6, we examine the effects of surface Kondo stackings (SF) on the electronic band structure of the topological Dirac fermions protected by the time-reversal symmetry. The presence of the Kondo effect at the surface disturbs the compensation between light and heavy electrons and dopes the Dirac cone. Dispersion of these uncompensated surface states are dominated by inter-site hopping, which leads to a much lighter quasiparticles. These surface states are also highly durable against effects of magnetism and decreasing the thickness of the sample.

1Work supported by Department of Energy grant DE-FG02- 99ER45790

10:36AM F7.00012 Dirac Fermions without bulk backscattering in rhombohedral topological insulators1 , CARLOS MERA ACOSTA, MATHEUS LIMA, LEANDRO SEIXAS, ANTONIO DA SILVA, ADALBERTO FAZZIO, Instituto de Fisica, Universidade de Sao Paulo, CP 66318, 05315-970, Sao Paulo, SP, Brazil — The realization of a spintronic device using topological insulators is not trivial, because there are inherent difficulties in achieving the surface transport regime. The majority of 3D topological insulators materials (3DTI) despite of support helical metallic surface states on an insulating bulk, forming topological Dirac fermions protected by the time-reversal symmetry, exhibit electronic scattering channels due to the presence of residual continuous bulk states near the Dirac-point. From ab initio calculations, we studied the microscopic origin of the continuous bulk states in rhombohedral topological insulators materials with the space group D3h(R3m), showing that it is possible to understand the emergence of residual continuous bulk states near the Dirac-point into a six bands effective model, where the breaking of the R3 symmetry beyond the 1 point has an important role in the hybridization of the ps, py and pz atomic orbitals. Within these model, the mechanisms known to eliminate the bulk scattering, for instance: the stacking faults (SF), electric field and alloy, generated the similar effect in the electronic states of the 3DTI. Finally, we show how the surface electronic transport is modified by perturbations of bulk with SF.

1We would like to thank the financial support by Fundação de Amaparo À Pesquisa do Estado de São Paulo (FAPESP).

10:48AM F7.00013 Berry curvature induced nonlinear Hall effect in time-reversal invariant materials1 , INTI SODEMANN, LIANG FU, Massachusetts Institute of Technology — It is well-known that a non-vanishing Hall conductivity requires time-reversal symmetry breaking. However, in this work, we demonstrate that a Hall-like transverse current can occur in second-order response to an external electric field in a wide class of time-reversal invariant and inversion breaking materials. This nonlinear Hall effect arises from the dipole moment of the Berry curvature in momentum space, which generates a net anomalous velocity when the system is in a current-carrying state. We show that the nonlinear Hall coefficient is a rank-two pseudo-tensor, whose form is determined by point group symmetry. We will describe the optimal conditions and candidate materials to observe this effect.

1IS is supported by the Pappalardo Fellowship in Physics. LF is supported by DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under award DE-SC0010526.
8:00AM F8.00001 Re-visiting the O/Cu(111) system - When metastable surface oxides could become an issue!, ALOYSIUS SOON, NORINA A. RICHERT, CHANG-EUN KIM, Department of Materials Science and Engineering, Yonsei University, CATHERINE STAMPFL, School of Physics, University of Sydney. — Surface oxidation processes are crucial for the functionality of Cu-based catalytic systems used for many industrially important chemical reactions. Based on recent findings in XPS and LEED experiments, we assess the stability and population of the experimentally proposed “8”-structure, a new surface oxide phase, on the Cu(111) surface. Using density-functional theory calculations in combination with ab initio atomistic thermodynamics and Boltzmann statistical mechanics, we find that the proposed oxide superstructure is indeed metastable and that the population of the “8”-structure is competitive with the known “29” and “44” oxide film structures on Cu(111). We show that the configuration of O and Cu atoms in the first and second layers of the “8”-structure closely resembles the arrangement of atoms in the first two layers of CuO(111), where the atoms in the “8”-structure are more constricted. CuO(111) has been suggested in the literature as the most active low index facet for reactions such as water splitting under light illumination. If the “8”-structure were to form during a catalytic process, it is therefore likely to be one of the reactive phases.

8:12AM F8.00002 Oxygen disorder, a way to accommodate large tensile strains in oxide thin films, Y.Y. ZHANG, R. MISHRA, Vanderbilt University, Oak Ridge National Laboratory, T.J. PENNYCOOK, University of Oxford, A.Y. BORISEVICH, Oak Ridge National Laboratory, S.J. PENNYCOOK, University of Tennessee, S.T. PANTELIDES, Vanderbilt University, Oak Ridge National Laboratory. — Strain induced by lattice mismatch of epitaxial layers is typically accommodated by misfit dislocations. In transition-metal oxides, other strain-relaxation modes have been observed (oxygen vacancy, octahedral tilts, etc.). Here we use density functional calculations to compare the total energies of different structures and to check for negative-frequency phonon modes, which is an good indicator of instability, and explore the stability of several oxide thin films. We find that when a ZrO2 thin film is sandwiched between SrTiO3 layers (7% biaxial tensile strain), disorder in the oxygen sublattice lowers the energy by 1.4 eV/ZrO2 formula unit and, in contrast, we find that if a (LaFeO3)/(SrFeO3) superlattice is grown on a substrate that imposes an overall biaxial tensile strain, there is a competition between O sublattice disorder, formation and ordering of O vacancies, and octahedral tilts. The mechanism for strain compensation varies with the extent of the strain. We conclude that oxygen-sublattice disorder is one of many ways that tensile strain can be accommodated in transition-metal oxide films.

8:24AM F8.00003 Thermodynamic stability and band alignment at SrTiO3/GaAs(001) interface1, JOELSON COTT, RAVI DROOPAD, BYOUNGHAK LEE, Texas State University, TX 78666, USA. — The successful epitaxial growth of SrTiO3 on Si showed that it is possible to integrate the functional oxides with semiconductors incorporating unique multifunctional properties of oxides into various existing semiconductor technologies. While SrTiO3 has been also deposited on GaAs without amorphous interfacial layers, the exact interface structure has been controversial. On one hand, scanning Transmission Electron Microscopy (STEM) shows As atoms at the interface. X-ray photoelectron spectroscopy (XPS) measurements, on the other hand, do not show peaks associated with As-O bonding, indicating that the GaAs/SrTiO3 interface does not involve an As/Oxide layer, contradicting to STEM observations. Using ab initio calculations, we determine the interface structure of a SrTiO3 film on a GaAs substrate to help clarify the apparent discrepancy between the XPS and the STEM measurements. The calculations reveal that, under the condition that allows atomically abrupt interfaces, the energetically most stable interface is As/Sr/TiO2 structure, in accordance with both XPS and STEM measurements. We discuss the band offsets and the possibility of in-gap states of various interface structures.

1This work was supported by the Air Force Office of Scientific Research, Contract FA9550-10-1-0133.

8:36AM F8.00004 Study of electronic structure and magnetism at the relaxed SrTiO3/LaMO3 interface, SOHAM GHOSH, EFSTRATIOS MANOUSAKIS, Florida State Univ. — We present a density functional theory study of the nature of bands in z-terminated metal oxides. It is shown that the bandstructure of pure SrTiO3 near the fermi surface is modified by the presence of surfaces, besides being sensitive to ionic relaxations and thickness of the material. We also study the cases where layers of LaMO3 (with M = Ti, Al) have been added to create an interface. We examine doping of the SrTiO3 surface bands by the added layers as a possible reason for the presence and localization of the induced electron gas and we study the character of these bands.

8:48AM F8.00005 Lattice-mismatch Strain Effects in Electron-Doped Calcium Manganese Oxide Thin Films1, CACIE HART, GRACE YONG, ZOEY WARECKI, ADEEL CHAUDHRY, PRAKASH SHARMA, ANTHONY JOHNSON, DAVID SCHAEFER, RAJESWARI KOLAGANI, Towson University. — Electron-doped Calcium Manganese Oxide (CaMnO3−δ) thin films are of interest for use as photocatalysts and fuel cell electrodes in renewable energy applications. Oxygen stoichiometry of the films is a key parameter for the functionality in these applications. Currently, we are investigating the properties of (CaMnO3−δ) films grown by pulsed laser deposition. The thin films are epitaxially grown on LaAlO3 and SrTiO3 substrates. Both of these substrates have larger in-plane lattice parameters than CaMnO3−δ, which leads to bi-axial tensile strain in the thin films. We have characterized the thickness dependence of structural, electrical, and morphological properties of these films using high resolution x-ray diffraction, temperature dependent electrical conductivity measurements, and atomic force microscopy. The thickness dependence is characteristically different from what has been previously observed in thin films of hole-doped manganites. Our results suggest that coupling between tensile strain and oxygen deficiency affect the electrical and structural properties of the material.

1NSF Grant ECCS1128586

9:00AM F8.00006 Epitaxial growth of in-plane-dimerized, single phase NbO2 thin films for metal-insulator transition applications, AGHAM POSADAS, TOBIAS HADAMEK, ANDY O’HARA, ALEXANDER DEMKOV, University of Texas at Austin. — NbO2 is a exhibits a metal-insulator transition that may have potential applications in electronic devices. The strong conductivity change in NbO2 occurs along the dimerization direction and for devices utilizing NbO2 as a channel material (in-plane transport) such as transistors, one would like the dimerization direction to be in the plane of the film. The electrical properties of Nb oxides are strongly dependent on the oxidation state of Nb. It is therefore critical to be able to control the oxidation state of Nb during growth. Here, we describe the epitaxial growth of in-plane-dimerized NbO2 using molecular beam epitaxy on a variety of substrates (STO, LSAT, MgO, BTO and GdN), growth temperatures, and oxygen-to-niobium flux ratios. We show that the particular substrate used significantly affects the bulk and surface crystallinity, as well as the degree of oxidation. We also show the evolution of the valence and core level photoemission spectra of Nb oxides as a function of oxygen-to-niobium flux ratio and point out the optimum growth conditions to achieve phase-pure, epitaxial NbO2 films.
9:12 AM F8.00007 Band-gap engineering at a semiconductor - crystalline oxide interface. KAMYAR AHMADI-MAJLAN, MOHAMMADREZA JAHANGIR-MOGHADAM, Univ of Texas, Arlington. XUAN SHEN, Brookhaven National Laboratory, TIMOTHY DROUBAY, MARK BOWDEN, Pacific Northwest National Laboratory, MATTHEW CRYSLER, Univ of Texas, Arlington, DONG SU, Brookhaven National Laboratory, SCOTT A. CHAMBERS, Pacific Northwest National Laboratory. JOSEPH H. NGAI, Univ of Texas, Arlington — Abstract: The epitaxial growth of crystalline oxides on semiconductors provides a pathway to introduce new functionalities to semiconductor devices. Key to electrically coupling crystalline oxides with semiconductors to realize functional behavior is controlling the manner in which their bands align at interfaces. Here we apply principles of band gap engineering traditionally used at heterojunctions between conventional semiconductors to control the band offset between a single crystalline oxide and a semiconductor. Reactive molecular beam epitaxy is used to realize atomically abrupt and structurally coherent interfaces between SrZrxTi1−xO3 and Ge, in which the band-gap of the former is enhanced with Zr content x. We present structural and electrical characterization of SrZrxTi1−xO3-Ge heterojunctions for x = 0.2 to 0.75 and demonstrate the band offset can be tuned from type-II to type-I, with the latter being verified using photoemission measurements. The type-I band offset provides a platform to integrate the dielectric, ferroelectric and ferromagnetic functionalities of oxides with semiconducting devices.

9:24 AM F8.00008 Effect of post-deposition annealing on the structure and physical properties of strained epitaxial Ni1−xTi1−yO3 thin films1. TAMAS VARGA, TIMOTHY DROUBAY, LIBOR KOVARIK, SCOTT CHAMBERS, Pacific Northwest National Laboratory — Ferroelectrically induced weak ferromagnetism had been predicted in compounds MTIO3 (M=Fe,Mn,Ni) with the LINbO3-type structure. In order to stabilize this metastable structure by oxide heteroepitaxy, we attempted to grow epitaxial NiTiO3 films on Al2O3 and Fe2O3/Al2O3 substrates by pulsed laser deposition. Given the structural imperfections of the as-deposited films arising from the large lattice mismatch, which resulted in weak ferroic ordering, we investigated the effect of post-synthesis annealing on the films’ properties. Our structural data from x-ray diffraction and electron microscopy suggest that the crystalline quality of the Ni1−xTi1−yO3 films was greatly improved by annealing the films at 1000 °C for 8 hours. Our physical property characterization indicates increased ferromagnetism in the films. The specific changes in film structure and magnetic as well as polar properties will be discussed. These results suggest that the ferromagnetic properties of the films can be favorably altered by post-synthesis heat treatment.

9:36 AM F8.00009 Epitaxial Growth of CaIrO3 Single-Crystal Thin-Films. MARYAM SOURI, JOHN H. GRUENEWALD, JASMINKA TERZIC, GANG CAO, JOSEPH W. BRILL, SUNG S. AMBROSE SEO, Univ of Kentucky — Complex oxides containing 5d transition metals including iridates have attracted substantial attention due to their potential to create novel electronic and magnetic states that originate from strong spin–orbit coupling and the electron-correlation of 5d electrons. However, the progress of experimental research on the 5d transition-metal oxides is hindered by the limited number of available materials. To further understand the layered iridates (A2IrO3, A: alkaline-earth elements) featuring the J=1/2 Mott state, we have synthesized epitaxial thin-films of Ca2IrO3. The single crystal Ruddlesden-Popper (R-P) phase of Ca3n+1Ir2O3n+1 (n=1) is thermodynamically unstable; hence, we have used epitaxial-stabilization strategies to grow metastable thin-films of Ca2IrO3. The R-P phase of Ca3Ir4O7 is synthesized on yttrium aluminum oxide and lanthanum aluminum oxide substrates by pulsed laser deposition. We have studied the electronic structure of these films by transport and optical spectroscopic measurements. The dc-resistivity shows that these Ca2IrO3 thin-films are insulating with activation energy of about 100 meV. The optical spectroscopy shows that the optical gap energy is about 0.5 eV. We will discuss the electronic structure of Ca2IrO3 by comparing with Sr2IrO4 and Ba2IrO4.

9:48 AM F8.00010 Structure-Property relationship for H covered Fe3O4(001)1. FANGYANG LIU, Louisanna State Univ - Baton Rouge, ORHAN KIZILKAYA, Center for Advanced Microstructures and Devices, Louisiana State University, PHILLIP SPRUNGER, RICHARD KURTZ, RONGYING JIN, JIANDI ZHANG, WARD PLUMMER, Louisiana State Univ - Baton Rouge — Magnetite (Fe3O4), the oldest permanent magnetic material in a variety of applications.

1This work was supported in the Environmental Molecular Sciences Laboratory, a national scientific user facility sponsored by the Department of Energy’s Office of Biological and Environmental Research and located at Pacific Northwest National Laboratory.

10:00 AM F8.00011 Thin-film growth of the quasi-one-dimensional metal Li109Mo6O17. ALEXANDRA COTE, SAEED MOSHEFHEGYEGANEE, JOSUA L. COHN, University of Miami, JOHN J. NEUMEIER, Montana State University — Attempts to grow epitaxial thin films of Li109Mo6O17 by pulsed-laser deposition will be discussed. Single crystals of this quasi-one-dimensional (q1D) metal exhibit highly anisotropic Seebeck coefficients with ΔS ≈ S⊥ − S∥ ≈ 200 μV/K near 450 K (the b axis corresponds to the most conducting, q1D chain direction). Suitably oriented thin films could enable possible applications in energy detection using the transverse Seebeck effect. X-ray diffraction results will be presented for films grown from a polycrystalline target on several substrates under a narrow range of temperature and pressure conditions.

1This material is based upon work supported by the U.S. Department of Energy Office of Basic Energy Sciences grant DE-FG02-12ER46888 (Univ. Miami) and the National Science Foundation under grant DMR-0907036 (Mont. St. Univ.)


10:12 AM F8.00012 Superconducting single-crystalline YBa2Cu3O7−δ on SrTiO3 buffered Si (100). MOHAMMADREZA JAHANGIR-MOGHADAM, KAMYAR AHMADI-MAJLAN, Univ of Texas, Arlington. HAO ZHANG, Univ of Toronto, XUAN SHEN, National Laboratory of Solid State Microstructures, Nanjing University, MATTHEW CRYSLER, PATRICK CONLIN, RICKY HENSLEY, Univ of Texas, Arlington, DONG SU, Center for Functional Nanomaterials, Brookhaven National Laboratory, JOHN WEI, Univ of Toronto, JOSEPH NGAI, Univ of Texas, Arlington — The growth of crystalline oxides on semiconductors enables new functionalities to be integrated with semiconducting technologies. Here, thin films of optimally-doped (001)-oriented YBa2Cu3O7−δ are epitaxially integrated on silicon (001) through growth on a SrTiO3 buffer. The former is grown using pulsed-laser deposition and the latter is grown on Si using oxide molecular beam epitaxy. The single crystal nature of the SrTiO3 buffer enables very high transition temperatures to be achieved. For a 30 nm thick SrTiO3 buffer, YBa2Cu3O7-δ films exhibiting a transition temperature of ~ 95 K, and a narrow transition width (< 5 K) are achieved. The integration of single crystalline YBa2Cu3O7−δ on Si (001) paves the way for the potential exploration of cuprate materials in a variety of applications.
10:24AM F8.00013 Optical and magnetic properties of Ca$_3$CoMnO$_6$ thin films\textsuperscript{1}. JITENDRA SAHA, GYANESHWAR SHARMA, Graduate Student, SATYABRATA PATNAIK, Associate Professor, S PATNAIK TEAM — Ca$_3$CoMnO$_6$ is one of the initial one-dimensional Ising chain compounds that has shown large magnetoelectric coupling below its antiferromagnetic temperature (15 K). We report on the growth and characterization of Ca$_3$CoMnO$_6$ thin films deposited by pulse laser deposition. The films of thickness 220 nm are grown on 0001-oriented sapphire substrates at 750 °C. The band gap (∼ 1.73 eV) derived from UV visible absorption spectroscopy and temperature dependent resistivity is consistent with one another. It is seen that the films can be grown at various oxygen pressures but the optimal deposition pressure is found to be 5×10$^{-2}$ mbar. The effect of oxygen pressure on the texture of the film and band gap indicates that the oxygen vacancies play a major role in the optical and electrical properties of the films. AFM measurements show a homogeneous growth of the films. Magnetization measurement shows that the transition temperature increased to 39 K, much above the bulk Neel temperature. The increase in magnetic transition is supposed to be due to stronger inter-chain interaction caused by tensile strain effected by lattice mismatch.

\textsuperscript{1}CSIR and UGC Govt. of India are acknowledged for financial support.

10:48AM F8.00015 Effects of ferroelectric polarization on surface phase diagram: an evolutionary algorithm study of the BaTiO$_3$(001) surface\textsuperscript{1}. PENCHENG CHEN, YONG XU, NA WANG, Tsinghua University, ARTEM R. OGANOV, Stony Brook University, WENHUI DUAN, Tsinghua University — We have constructed the surface phase diagram of the BaTiO$_3$(001) surface by employing an evolutionary algorithm for surface structure prediction, where the ferroelectric polarization is included as a degree of freedom. Among over 1000 candidate structures explored, a surface reconstruction of $(2\times1)$-TiO is discovered to be thermodynamically stable and have the $p2mm$ plane group symmetry as observed experimentally. We find that the influence of ferroelectric polarization on the surface free energy can be either negligibly small or sizably large (over 1 eV per $(2\times1)$ supercell), depending strongly on the surface structure and resulting in a significant distinction of surface phase diagram with varying ferroelectric polarization. It is therefore feasible to control the surface stability by applying an external electric field. Our results may have important implications in understanding the surface reconstruction of ferroelectric materials and tuning surface properties.

\textsuperscript{1}We acknowledge the support of the Ministry of Science and Technology of China (Grant Nos. 2011CB921901 and 2011CB606405), and the National Natural Science Foundation of China.

Tuesday, March 3, 2015 8:00AM - 11:00AM
Session F9 DMP: Focus Session: van der Waals Bonding in Advanced Materials: Advances in Theory 006D - Adrienn Ruzsinszky-Perdew, Temple University

8:00AM F9.00001 Short-range Cut-Off of the Summed-Up van der Waals Series\textsuperscript{1}. ABHIRUP PATRA, JOHN P. PERDEW, Temple University — van der Waals interactions are important in typical van der Waals-bound systems such as noble-gas, hydrocarbon, alkali and alkaline-earth dimers. The summed-up van der Waals series \cite{1,2} works well and gives an accurate result at large separation between two atoms. But it has a strong singularity at short non-zero separation, where the two atoms touch. In this work we remove that singularity with a reasonable and physical choice of the cut-off distance. Only one fitting parameter has been introduced for the short-range cut off. The parameter in our model has been optimized for each system, and a system-averaged value has been used to get the final binding energy curves. When this correction is added to the binding energy curve from the semilocal density functional meta-GGA-M2S, we get vdW- corrected binding energy curve. These curves are compared with the results of other vdW-corrected methods such as PBE-D2 and vdW-DF2. Binding energy curves are in reasonable agreement with those from experiment. These curves also predict reasonably good equilibrium bond length. \cite{1,2}.

\textsuperscript{1}Supported by NSF (DMR)

8:12AM F9.00002 A van der Waals density functional built upon the electron-gas foundation\textsuperscript{1}. PER HYLDGAARD, Chalmers Univ. of Technology, Dept. of Microtechnology and Nanoscience –MC2, KRISTIAN BERLAND, Univ. of Oslo, Dept. of Physics, SMN, ELSEBETH SCHRÖDER, Chalmers Univ. of Technology, Dept. of Microtechnology and Nanoscience –MC2 — The vdW-DF method is designed to be a systematic extension of the constraint-based generalized-gradient approximation (GGA) and can therefore serve as general purpose density functional \cite{PRB 90,075148 (2014)}. Yet the early versions can have issues both with bulk systems and with weak chemisorption. We present a recent nonempirical version, vdW-DF-cx \cite{J. Chem. Phys. 140,18A539 (2014), PRB 89, 035412 (2014)}, that resolves these issues. The version is designed to have a consistent combination of exchange and correlation. We show that it performs well for inter-molecular binding and that it can even be better than PBE for describing cohesion and structure of molecules and solids.

\textsuperscript{1}The work was supported by the Swedish Research Council (VR), by the Chalmers Areas of Advance: Materials, and by the Swedish National Infrastructure for Computing.

8:24AM F9.00003 A Local Representation Of The Dielectric Response Function\textsuperscript{1}. DEYU LU, XI-AOCHUAN GE, Brookhaven National Laboratory — The screened dielectric response function ($\chi$) is a fundamental physical quantity that captures the many-electron correlation effects, key to the accurate description of van der Waals dispersion interaction in the ground state and a range of excited state properties. Although $\chi$ is non-local by definition, a real space partition of $\chi$ onto local structural motifs can help us gain further physical insight into, e.g., effective local screening properties. Because the construction of bare response function, $\chi_{0}$, is associated with the product of electron - hole orbitals, standard localization procedures for electron wave functions can not be directly applied. In this work, we propose a new method to decompose $\chi_{0}$ into contributions from local response functions. Exemplary results of finite and bulk systems are discussed.

\textsuperscript{1}Research carried out at the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.
8:36AM F9.00004 An Efficient Coupled Dipole Method: TCDM1, HYE-YOUNG KIM, Southeastern Louisiana Univ — An overview of a memory-efficient and cost-effective method, called Trace-Coupled Dipole Method (TCDM), which can accurately predict the van der Waals (vdW) forces between dielectric materials will be presented. CDM is an intrinsically atomistic method which includes all the many-body interaction terms self-consistently. TCDM, an alternative way to execute CDM, is to obtain VDW interaction energy by calculating the trace of a 3NX3 matrix, rather than its eigenvalues. It will be demonstrated that the power series expansion in TCDM is equivalent to that of the perturbation theory. The advantage of adopting TCDM over the conventional perturbation theory or CDM will also be discussed. The use of TCDM will make it practical for any interested future users to calculate the accurate VDW interaction in large systems like those found in computer simulation studies without serious increase in computational burden.

1This research is supported by the Louisiana Board of Regents-RCS grant (LEQSF(2012-15)-RD-A-19).

8:48AM F9.00005 Electronic Properties of Polarizable Systems with Self-Consistent Interatomic van der Waals Density Functional, NICOLA FERRI, Fritz Haber Institute der MPG, ROBERT A. DISTASIO JR., Princeton University, ALBERTO AMBROSETTI, Fritz Haber Institute der MPG, ROBERTO CAR, Princeton University, MATTHIAS SCHEFFLER, ALEXANDRE TKATCHENKO, Fritz Haber Institute der MPG — Ubiquitous long-range van der Waals (vdW) interactions play a fundamental role in the structure and stability of a wide range of systems. Within the DFT framework, the vdW energy represents a crucial, but tiny part of the total energy, hence its influence on the electronic density, n(r), and electronic properties is typically assumed to be rather small. Here, we address this question via a fully self-consistent (SC) implementation of the interatomic Tkatchenko-Scheffler vdW functional [1] and its extension to surfaces [2]. Self-consistency leads to large changes in the binding energies and electrostatic moments of highly polarizable alkali metal dimers. For some metal surfaces, vdW interactions increase dipole moments and induce non-trivial charge rearrangements, leading to visible changes in the metal workfunctions. Similar behavior is observed for molecules adsorbed on metals. Our study reveals a non-trivial connection between electrostatics and long-range electron correlation effects. [1] A. Tkatchenko and M. Scheffler PRL (2009). [2] V. G. Ruiz, W. Liu, E. Zojer, M. Scheffer, and A. Tkatchenko PRL (2012).

9:00AM F9.00006 Many-body dispersion meets non-local density functionals: A unified approach for van der Waals correlations, JAN HERMANN, MATTHIAS SCHEFFLER, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der Max-Planck-Gesellschaft — It is an ongoing challenge to develop an efficient method for van der Waals (vdW) non-local correlation within DFT which would be both accurate and broadly applicable. Current approaches can be loosely divided into the fragment-based ones, two-point density functionals and methods based on the density-density response function. The fragment-based models utilize parameters not derivable from the electron density. Two-point approaches are explicit density functionals, but difficult to generalize to include many-body correlations. Here, we show that these seemingly contrasting approaches can be unified within a single framework based on the adiabatic-connection formalism in the random-phase approximation. We use a local response-function model from the VV09 functional[1] together with the many-body dispersion approach to create an atom-based model with no external parameters. We introduce a consistent correlation-functional-based coupling of the short- and long-range correlation energy. We show that this unification provides new insights into the different approaches, naturally deals with the partitioning of ionic and delocalized states and paves path towards self-consistent description of many-body vdW correlations.

1O. A. Vydrov, T. Van Voorhis, Phys. Rev. Lett. 103, 063004

9:12AM F9.00007 Repulsive van der Waals forces and other delights from the Lifshitz approach, ADRIAN PARSEGIAN, Univ. Massachusetts, Amherst — No abstract available.

9:48AM F9.00008 Farsightedness of the Correlation Energy in Polarizable Non-Metallic Nanostructures, ALBERTO AMBROSETTI, Università degli Studi di Padova, NICOLA FERRI, Fritz-Haber Institut der Max Planck Gesellschaft, Berlin, ROBERT D. DAMSTASIO, Princeton University, Princeton, ALEXANDRE TKATCHENKO, Fritz Haber Institut der Max Planck Gesellschaft, Berlin — The success of semi-local approaches to the electron correlation energy is commonly attributed to the relative nearsightedness of the electronic matter—a powerful concept introduced by M. Kohn. However, recent theoretical and experimental evidence indicates that electron correlation can be characterized by strong “action at a distance”, especially in low-dimensional polarizable nanomaterials. Here we systematically analyze the influence of relevant properties, namely dimensionality, topology and polarizability, on the convergence and power laws governing the correlation energy. Using an accurate model system of coupled quantum harmonic oscillators we find that many-body effects can induce collective and strongly delocalized charge-fluctuation modes. These modes are ultimately responsible for a marked non-locality of the response, and an unconventional power-law decay of the dispersion interaction, which significantly deviates from the asymptotic predictions of finite-order perturbative theories. Notably, the degree of farsightedness of the correlation energy could possibly be tuned, opening the way to an appropriate control of the interaction in complex polarizable nanostructures.

10:00AM F9.00009 Van der Waals Interactions Between Subsystems with Overlapping Electron Density1, MICHELE PAVANELLO, Rutgers Univ - Newark — The subsystem formulation of DFT known as Frozen Density Embedding (FDE) provides a divide-and-conquer approach to Kohn–Sham DFT for weakly bound systems. We claim that a subsystem formulation of DFT can simplify both the theoretical framework and the computational effort for calculating the electronic structure of condensed phase systems. In addition, the naturally subsystem-like form of molecular aggregates makes subsystem DFT a better descriptor of the underlying physics than regular DFT of the supersystem. As an example, we present a novel van der Waals theory based on subsystem DFT which can treat seamlessly non-overlapping as well as overlapping subsystem electron densities. The theory is amenable to sensible approximations, such as RPA, and offers natural algorithms to fold in post-RPA corrections. Application of the theory to the computation of binding energies of dimers in the S22 set, as well as computation of selected potential energy surfaces is presented.

1M.P. acknowledges funding by NSF IIA-1404739 and CBET-1438493

10:12AM F9.00010 Adiabatic-connection fluctuation-dissipation DFT for the structural properties of solids - the renormalized ALDA and other electron gas kernels1, CHRISTOPHER PATRICK, KRISTIAN THYGESEN, Department of Physics, Technical University of Denmark — The adiabatic-connection fluctuation-dissipation formula of density-functional theory (ACFD-DFT) provides a natural pathway for the calculation of electron correlation energies going beyond the random-phase approximation (RPA). The key ingredient of ACFD-DFT is the exchange-correlation kernel $\text{xc}$. Recent theoretical and experimental evidence indicates that the exchange-correlation kernel is the key to accurately model the van der Waals (vdW) forces between dielectric materials will be presented. CDM is an intrinsically atomistic method which includes all the many-body interaction terms self-consistently. TCDM, an alternative way to execute CDM, is to obtain VDW interaction energy by calculating the trace of a $3N\times3N$ matrix, rather than its eigenvalues. It will be demonstrated that the power series expansion in TCDM is equivalent to that of the perturbation theory. The advantage of adopting TCDM over the conventional perturbation theory or CDM will also be discussed. The use of TCDM will make it practical for any interested future users to calculate the accurate VDW interaction in large systems like those found in computer simulation studies without serious increase in computational burden.

1Research supported by the Danish Council for Independent Research’s Sapere Aude Program, Grant No. 11-1051390
10:24AM F9.00011 The role of delocalization error in non-covalent interactions from dispersion-corrected density-functional theory, ALBERTO OTERO DE LA ROZA, National Institute for Nanotechnology-NRC — Extensive benchmarking of dispersion-corrected density functional theory (dDFT) methods has shown that it is nowadays feasible to calculate, with great accuracy, binding energies of small dimers and lattice energies of molecular crystals. However, there are many outstanding questions that can only be answered by a proper understanding of the interplay between base functional and dispersion correction. In this talk, I explore how delocalization error from the exchange-correlation functional impacts the calculation of non-covalent donor-acceptor interactions. Delocalization error arises from the failure of most functionals to model the long-range behavior of the exchange-correlation hole. Its primary consequence for non-covalent interactions is that the stability of donor-acceptor interactions is overestimated. Errors caused by delocalization error are particularly harmful in systems with strong and extensive hydrogen-bonded networks (water clusters and ice) or strong donor-acceptor interactions (halogen bonding), and cannot be corrected using a pairwise dispersion correction. In addition, I present how delocalization error affects real-life applications of dDFT, such as molecular adsorption on iron-oxide nanoparticles and surfaces.

10:36AM F9.00012 Ultra-long-ranged dispersion interaction between degenerate molecules, JOHN DOBSON, Griffith Univ, ANDREAS SAVIN, CNRS, UPMC Sorbonne Universities — It is known (see e.g. [1]) that extended nano-systems with zero electronic gaps can exhibit dispersion interactions that fall off with unexpected powers of distance \( D \). We seek to find a similar phenomenon between finite molecules that have a strictly degenerate many-electron groundstate (zero gap). As a toy model we take \( H_2 \) with the atoms constrained to lie on an equilateral triangle of side \( a \), using a minimal (s) basis set, and with spin-orbit coupling omitted. Rotational symmetry at fixed spins guarantees a degenerate time-reversed pair of three-electron states. For sufficiently small atomic spacing \( a \) where inter-atomic hopping kinetic energy dominates the electron-electron repulsion, these degenerate time-reversed pairs of states are many-electron groundstates. We confirm this groundstate degeneracy via limited-basis CI calculations. We show that the resulting dispersion energy between two such constrained \( H_2 \) molecules falls off as \( D^{3.5} \) instead of the usual \( D^6 \). Within the classification scheme proposed in ref [2], this effect can be interpreted as a “type C non-additivity” of the dispersion interaction. This model may be relevant to metal atom clusters.

1 JFD acknowledges Australian Research Council Grant DP1096240. We benefited from discussions with Prof. Janos Anany and Dr. Ru-Fen Liu.

10:48AM F9.00013 Optimization of a van der Waals Density Functional for water, MICHELLE FRITZ, Universidad Autonoma de Madrid, MARIVI FERNANDEZ-SERRA, Stony Brook University, JOSE M. SOLER, Universidad Autonoma de Madrid — In particular, delicate systems, like liquid water, ab initio exchange and correlation functionals are simply not accurate enough for many practical applications. In these cases, fitting the functional to reference data is a sensible alternative to empirical interatomic potentials. However, a global optimization requires functional forms that depend on many parameters and the usual trial and error strategy becomes cumbersome and suboptimal. We present a general and powerful optimization scheme called data projection onto parameter space (DPPS). In an arbitrarily large parameter space, DPPS expands the vector of unknown parameters in vectors of known data. Poorly sampled subspaces are determined by the physically-motivated functional shape of ab initio functionals, using Bayes’ theory to combine this prior information with reference energies and electron densities of monomers, clusters, and condensed phases of water.

We acknowledge support from FIS2012-37549 (MF and JMS) and DOE Early Career Award No. DE-SC0003871 (M.-V.F.-S.)

Tuesday, March 3, 2015 8:00AM - 11:00AM —
Session F10 DCMP: Magnetism and Topological Insulators 007A - Jim Eckstein, University of Illinois-Urbana

8:00AM F10.00001 Room Temperature Ferromagnetism on the Topological Insulators Surface by Proximity Effect, FERHAT KATMIS, MIT, VALERIA LAUTER, Oak Ridge National Lab., VAHID SAZGARI, ISMET I. KAYA, Sabanci University, DONALD HEIMAN, Northeastern University, JAGADEESH MOODERA, MIT — Generating exchange-induced ferromagnetism on the surface of a topological insulator (TI) with a ferromagnetic layer (FM) provides a cleaner approach for realizing a ferromagnetic TI that may lead to exhibiting other quantum functionality. Here we demonstrate further that room temperature magnetic state may be reached in the TI and FM heterostructures through magnetic proximity-induced time reversal symmetry breaking on the TI surface. Using different magnetic characterization methods we provide evidence of this enhanced proximity-induced magnetism in TI. We show that such effects persist up to room temperature, far above the Curie temperature of the FM, signifying a significantly different behavior in TI. The project supported by grants NSF (DMR-1207469), MIT MRSEC through the MRSEC Program of the NSF (DMR-0817962) and NSF (ECCS-1402738). 1. “Exchange-Coupling-Induced Symmetry Breaking in Topological Insulators”, Peng Wei, et al, PRL. 110, 186807 (2013).

8:12AM F10.00002 A first-principles study of magnetic phase transitions in Fe-doped Bi2Se3, JOEONGWOO KIM, SEUNG-HOON JHI, Pohang Univ of Sci & Tech — Magnetic impurities perturb helical surface states of topological insulators because they act as the spin-flipping scattering centers. Counter-intuitively, the energy gap of the surface states, presumably opened by such scattering, decreases with Fe concentration in Fe-doped topological insulating Bi2Te3 [1]. In addition, the ground magnetic phase of the compound is changed as Fe concentration is increased, which is atypical in dilute magnetic semiconductors. We study the magnetic phase transition and the behavior of surface states in Fe-doped Bi2Se3 using first-principles calculations. We find that the localized spin states of Fe atoms are aligned via hybridization with conduction electrons at dilute doping regimes (<1.7 %) but, at dense impurity levels (>1.7%), are ordered mainly via the super-exchange interaction. We show that topological surface states are sensitive to the type of magnetic ordering of adjacent Fe impurities and that the ground magnetic phase barely perturbs the linear band dispersion and the helical nature of the surface states. This finding explains the observation of the band gap of the surface-states in the presence of magnetic impurities.


8:36AM F10.00004 Signatures of Dirac fermion-mediated magnetic order 1, PAOLO SESSI, FELIX REIS, THOMAS BATHON, Institute of Physics, University of Wuerzburg, Germany, KONSTANTIN KOKH, OLEG TERESHCHENKO, Novosibirsk State University, Novosibirsk, Russia, MATTHIAS BODE, Institute of Physics, University of Wuerzburg, Germany — The spin-momentum locking of topological states offers an ideal platform to explore novel magneto-electric effects. These intimately depend on the ability to manipulate the spin texture in a controlled way. Here, we combine low-temperature scanning tunneling microscopy with single-atom deposition technique to directly map the evolution of the electronic properties of topological states under the influence of different magnetic perturbations. By analyzing energy-resolved quasi-particle interference maps, we reveal signatures of Dirac fermion-mediated surface magnetic order for extremely dilute adatom concentrations. By using different magnetic elements and coverages, we find that this striking observation crucially depends on two parameters: single adatoms magnetic anisotropy direction and energy-level alignment.

8:48AM F10.00005 Magnetization Dynamics of a Ferromagnet Attached to the Surface State of a Topological Insulator: A Time Dependent Keldysh Green Function Approach 1, FARZAD MAHFOUZI, NICHOLAS KIOUSIS, Department of Physics and Astronomy, California State University, Northridge — Motivated by the recent experiments on the Spin Orbit Torque (SOT) generated by the Topological Insulators (TI) we investigate the conditions under which the SOT due to the in-plane current flowing through the surface state can switch the magnetic orientation of a ferromagnet attached to the TI. Using the Keldysh Green function approach, we developed the theoretical formalism for a classical system coupled to an electronic system out of equilibrium due to both bias voltage and the adiabatic variation of the classical degree of freedom. In this approach the quantities of interest that are calculated have the form of the generalized Fisher-Lee formula describing the electronic current and spin accumulation in terms of the Green functions in a unified approach. We show that due to the Edlestein effect the direction of the easy axis changes with the applied voltage which makes it difficult to separate the SOT into field like and anti-damping like components.

9:00AM F10.00006 Magnetization switching of a nanomagnet by spin polarized surface states of a topological insulator 1, URMIMALA ROY, RIK DEY, TANMOY PRAMANIK, BAHINAM GHOSH, LEONARD F. REGISTER, SANJAY K. BANERJEE, Microelectronics Research Center, The University of Texas at Austin — Due to the spin-momentum helical locking, a charge current supported by the topological insulator (TI) surface states leads to a spin accumulation at the TI surface. In this theoretical study, we consider a thermally-stable, conducting nanomagnet subject to spin-polarized current injection from TI surface states, in order to evaluate possible non-volatile memory applications such as in spin-transfer-torque random access memory. We simulate parallel transport in the TI and the ferromagnetic metal, and evaluate the efficiency of magnetization switching for varying ease of transport between the TI and the ferromagnetic metal. With the assumed parameters, transport in the TI beneath the ferromagnetic metal is diffusive in nature at room temperature and is modeled by drift-diffusion simulation, which we believe to be sufficient for this purpose, and allows for rapid interpretation. We use self-consistent transport and magnetization dynamics calculation to predict switching time and energy spent per write operation. Based on our simulation, we believe that a large in-plane resistivity of the ferromagnetic layer—perhaps not a simple ferromagnetic metal layer—along with an interface with the TI that is transparent to charge transport, will lead to minimum switching time and write energy.

9:12AM F10.00007 The influence of proximity induced ferromagnetism, superconductivity and Fermi-velocity on evolution of Berry phase in Bi$_2$Se$_3$ topological insulator 1, PARIJAT SENGUPTA, University of Wisconsin-Madison — Bi$_2$Se$_3$ is a well-known 3D-topological insulators (TI) with a non-trivial Berry phase of $\pi$ attributed to the topology of the band structure. The Berry phase shows non-topological deviations from $\pi$ in presence of a perturbation that destroys time reversal symmetry and gives rise to a quantum system with massive Dirac fermions and finite band gap. Such a band gap opening is achieved on account of the exchange field of a ferromagnet or the intrinsic energy gap of a superconductor that influences the topological insulator surface states by virtue of the proximity effect. The Berry phase of such gapped systems with massive Dirac fermions is considered. Additionally, it is shown that the Berry phase for such a system also depends on the Fermi-velocity of the surface states which can be tuned as a function of the TI film thickness. The role of higher order warping terms in the surface state Hamiltonian which influences deviations to the Berry phase is evaluated. Finally, a connection between Berry phase and circular dichroism is examined through explicit calculation of the optical matrix elements.

9:24AM F10.00008 Quantum Anomalous Hall Effect in Magnetic Insulator Heterostructure 1, GANG XU, JING WANG, Stanford University, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, XIAOLIANG QI, SHOUCHENG ZHANG, Stanford University, STANFORD UNIVERSITY COLLABORATION, INSTITUTE OF PHYSICS, CAS, CHINA COLLABORATION, MAX PLANCK INSTITUTE FOR CHEMICAL PHYSICS OF SOLIDS, DRESDEN, GERMANY COLLABORATION — Based on ab initio calculations, we predict that a monolayer of Cr-doped (Bi$_2$Sb)$_3$Te$_3$ and Gd$_2$ heterostructure is a quantum anomalous Hall insulator with a non-trivial band gap up to 38 meV. The principle behind our prediction is that the band inversion between two topologically trivial fermionic insulators can result in a non-zero Chern number, which offers a better route toward novel topological materials.

9:36AM F10.00009 Persistent ferromagnetism and topological phase transition at the interface of a superconductor and a topological insulator 1, WEI QIN, ZHENYU ZHANG, University of Science and Technology of China — At the interface of an $s$-wave superconductor and a three-dimensional topological insulator, Majorana zero modes and Majorana helical states have been predicted to exist respectively around magnetic vortices and geometrical edges. Here we first show that randomly distributed magnetic impurities at such an interface will induce bound states that broaden into impurity bands inside (but near the edges of) the superconducting gap, which remains open unless the impurity concentration is too high. Next we find that an increase in the superconducting gap suppresses both the oscillation magnitude and period of the RKKY interaction between two magnetic impurities. Within a mean field approximation, the ferromagnetic Curie temperature is found to be essentially independent of the superconducting gap, an intriguing phenomenon due to a compensation effect between the short-range ferromagnetic and long-range anti-ferromagnetic interactions. The existence of robust superconductivity and persistent ferromagnetism at the interface allows realization of a novel topological phase transition from a non-chiral to a chiral superconducting state at sufficiently low temperatures, providing a new platform for topological quantum computation.

1Supported by NSF of China.
9:48AM F10.00010 Revealing dissipationless chiral edge channel in magnetic topological insulator via non-local transport measurement. WEI-LI LEE, Institute of Physics, Academia Sinica, Taipei, XUFENG KOU, Department of Electrical Engineering, University of California, Los Angeles, SHIH-TING GUO, Institute of Physics, Academia Sinica, Taipei, YABIN FAN, LEI PAN, MURONG LANG, Department of Electrical Engineering, University of California, Los Angeles, YING JIANG, Department of Materials Science and Engineering, Zhejiang University, Hangzhou, QIMING SHAO, ANDUN ZHONG, Kimia University of Technology, Tehran, AROOP DAS, University of Maryland at College Park, PENG WEI, MIT, BISWARUP SATPATHI, Saha Institute of Nuclear Physics, JAGADEESH M. MODDAR, MIT, DON HEIMAN, Northeastern University — The observation of dissipationless edge states, which are the hallmark of a topological state, is a key step toward understanding the quantum Hall effect (QHE) in topological insulators. In this work, we present the first observation of dissipationless chiral edge states in a thin film of magnetic topological insulator Cr$_x$(Bi$_9$Sb$_9$)$_2$Se$_3$ grown by MBE technique. The measurement of the dissipationless edge state was performed using a novel nonlocal transport technique, which allows us to access and manipulate the edge states in a controlled manner. The results demonstrate the potential of magnetic topological insulators for future spintronics applications.

10:00AM F10.00011 Inducing magnetism onto the surface of a topological crystalline insulator. BADDIH A. ASSAF, Northeastern University, FERNAT KATMIS, PENG WEI, MIT, BISWARUP SATPATHI, Saha Institute of Nuclear Physics, JAGADEESH M. MODDAR, MIT, DON HEIMAN, Northeastern University — Magnetically-doped topological crystalline insulators (TCI) have been predicted to host a quantum anomalous Hall effect characterized by a Chern number, as large as a C=4 [1]. An alternative way to achieve this quantum state is by inducing magnetism onto the surface via magnetic proximity with a ferromagnetic insulator such as EuS. Similar to the proximity effect achieved in EuS/Bi2Se3 bilayers [2], we have induced magnetism onto the TCI SnTe in an MBE-grown SnTe/EuS/SnTe trilayer. Transport measurements at T=2K exhibit an anomalous Hall effect that is induced at the SnTe surfaces by the insulating ferromagnet EuS. The in-plane magnetoresistance (MR) exhibits a pronounced hysteresis that is isotropic with the direction of the EuS magnetization. Unlike the case of ferromagnetic semiconductors and metals, where the in-plane MR is highly anisotropic as a result of spin-scattering, the present MR is evidence of additional conduction inside the domain-walls at the EuS-SnTe interfaces. Further MR measurements in the minor loop regime confirm this effect. This work is a significant step toward realizing quantum states in TCI thin films. [1] C. Fang, et al. Phys. Rev. Lett. 112, 046801 (2014). [2] P. Wei et al. Phys. Rev. Lett. 18, 186807 (2013).

10:12AM F10.00012 Electrically Tunable Magnetism in Magnetic Topological Insulators. SHOUCHENG ZHANG, JING WANG, BIAO LIAN, Stanford Univ — The external controllability of the magnetic properties in topological insulators would be important both for fundamental and practical interests. Here we predict the electric-field control of ferromagnetism in a thin film of insulating magnetic topological insulators. The decrease of band inversion by the application of electric fields results in a reduction of magnetic susceptibility, and hence in the modification of magnetism. Remarkably, the electric control of magnetic order could even induce the magnetic quantum phase transition from ferromagnetism to paramagnetism. We further propose a topological transistor device in which the dissipationless charge transport of chiral edge states is controlled by an electric field. The simultaneous electric control of magnetic order and chiral edge channel in such a device may lead to electronic and spintronic applications for topological insulators.


10:36AM F10.00014 Imaging Dirac-Mass Disorder from Magnetic Dopant-Atoms in the Ferromagnetic Topological Insulator Cr$_x$(Bi$_9$Sb$_9$)$_2$Se$_3$ – Part II. CHUNG KOO KIM, INHEE LEE, BNL, JINHO LEE, Brooklyn National Laboratory, JINHO LEE, Seoul National University, SIMON BILLINGE, Columbia University, RUIJIAN ZHONG, JOHN SCHNEELOCH, TIANGSHENG LIU, JOHN TRANQUADA, GENDA GU, Brookhaven National Laboratory, J. C. SEAMUS DAVIS, Cornell University — We present Part II of the spectroscopic imaging - scanning tunneling microscopy (SI-STM) study of ferromagnetic Cr$_x$(Bi$_9$Sb$_9$)$_2$Se$_3$ single crystals measured at 4.5 K. As Part II we show how both spectroscopic analysis in real and momentum space demonstrate the coincident Dirac mass gap identified. Distribution of gap width, gap center, and gap anisotropy will be discussed. The anticipated relationship $\Delta(r) \propto n(r)$ is confirmed throughout, and exhibits an electron-dopant interaction energy $J^* = 145$ meV$^{-1}$. These observations reveal how magnetic dopant atoms actually generate the TI mass gap and that, to achieve the novel physics expected of time-reversal-symmetry breaking TI materials, control of the resulting Dirac-mass gap disorder will be essential.

10:48AM F10.00015 Spin-based Mach-Zehnder interferometry in topological insulator p-n junctions. RONI ILAN, University of California, Berkeley, FERNANDO DE JUAN, JOEL MOORE, University of California, Berkeley and Lawrence Berkeley National Laboratory, Berkeley — A p-n junction, an interface between two regions of a material populated with carriers of opposite charge, is a basic building block of solid state electronic devices. From the fundamental physics perspective, it often serves as a tool to reveal the unconventional transport behavior of novel materials. We show that a p-n junction made from a three dimensional topological insulator in a magnetic field realizes an electronic Mach-Zehnder interferometer with virtually perfect visibility. This is owed to the confinement of the topological Dirac fermion state to a closed two-dimensional surface, which offers the unprecedented possibility of utilizing external fields to design networks of chiral modes wrapping around the bulk in closed trajectories, without the need of complex constrictions or etching. Remarkably, this junction also acts as a spin filter, where the path of the particle is tied to the direction of spin propagation. It therefore constitutes a novel and highly tunable spintronic device where spin polarized input and output currents are naturally formed and could be accessed and manipulated separately.

Tuesday, March 3, 2015 8:00AM - 11:00AM – Session F11 DCMP: Odd-Parity Superconductivity 007B - Daoxin Yao, Sun Yat-sen University
8:00AM F11.00001 Influence of Fermi Surface Geometry and Geometric Phases on Spin-Triplet correlations in Superconductor-Ferromagnet Hybrid Structures1, MATTHIAS ESCHRIG, Royal Holloway, University of London — During the past 15 years a new field has emerged, which combines superconductivity and spintronics, with the goal to pave a way for new types of devices for applications combining the virtues of both, namely quantum coherence and interference on one side, and spin-selectivity and spin magnetism on the other. The building block of this new “spin-supertronics” are spin-triplet Cooper pairs, which are generated at the interface between a conventional superconducting and a ferromagnetic material. Non-collinear magnetic inhomogeneity mixes triplet pairs among each other, thus creating long-ranged equal-spin Cooper pairs in the ferromagnet, and non-collinear inhomogeneity introduces geometric phases giving rise to unusual current phase relations. Considerable Fermi surface mismatch is unavoidable for hybrid structures involving strongly spin-polarized ferromagnets. We perform calculations showing that Fermi surface geometry has important implications for the sign and magnitude of induced triplet correlations in the superconductor, as well as for the generation of spin currents. We discuss under which conditions spin currents are generated, and how the triplet correlations can be maximized for applications.

1This work is supported by the Engineering and Physical Science Research Council (EPSRC Grant No. EP/J010618/1).

8:12AM F11.00002 Proximity-induced triplet superconductivity in Rashba materials1, CHRISTOPHER REEG, SAURABH MAITI, DMITRII MASLOV, Univ of Florida - Gainesville — We study a proximity junction between a conventional $s$-wave superconductor and a conductor with Rashba spin-orbit coupling. Our specific focus is on the spin structure of the induced pairing in the Rashba conductor, where the mixing of spin-up and spin-down states converts the purely spin-singlet Cooper pairs of the superconductor into a mixture of spin-singlet and spin-triplet pairs. Because the induced triplet component of the pairing is generated entirely by a singlet order parameter and a single-particle spin-orbit term that preserves time-reversal symmetry, the triplet component is expected to persist even in the presence of disorder. We also propose an experimental setup to verify the triplet nature of the induced pairing.

1This work was supported by the National Science Foundation via grant NSF DMR-1308972.

8:24AM F11.00003 Possible correlation-driven odd-parity superconductivity in LaNi$_7$/8Co$_1$/8O$_3$ (111) bilayers, BING YE, ANDREJ MESAROS, YING RAN, Boston College — Using the functional renormalization group technique we demonstrate a route for potentially high temperature odd-parity superconductivity in ferromagnetic materials caused by repulsive electron interactions, where the superconducting pairing is driven by charge-density wave fluctuations. Our model is directly applicable to a lightly cobalt-doped LaNiO$_3$ bilayer grown in the (111) direction. As the on-site repulsive interaction grows, a charge-density wave state with a charge pattern that respects all point-group symmetries of the bilayer is replaced by a superconducting state with an $f$-wave pairing.

8:36AM F11.00004 Spin-Triplet Superconductivity in Sr$_2$RuO$_4$ due to Orbital and Spin Fluctuations: 2D fRG Analysis, MASHAISHI TSUCHIZU, YOUCHI YAMAKAWA, Department of Physics, Nagoya University, SEICHIKO ONARI, Department of Physics, Okayama University, HIROSHI KONTANI, Department of Physics, Nagoya University — We study the mechanism of the triplet superconductivity in Sr$_2$RuO$_4$, by applying the functional renormalization group (fRG) method to the multi-orbital Hubbard model [1]. Thanks to the vertex correction, we observe the strong spin and orbital fluctuations at $Q \approx (2\pi/3, 2\pi/3)$ in the quasi-one-dimensional Fermi surfaces (which are composed of $d_{xz}$ and $d_{yz}$ orbitals). Moreover, due to the cooperation of spin and orbital fluctuations, the triplet superconductivity emerges where the superconducting gap is given by the linear combination of $\Delta_k(k) \approx \sin(3k_x \pi, \sin(3k_y \pi)$ [2]. These results can also be confirmed by a diagrammatic calculation of the vertex correction.


8:48AM F11.00005 ABSTRACT WITHDRAWN —

9:00AM F11.00006 Search for half-flux-quantum Little-Parks oscillations in mesoscopic rings of Sr$_2$RuO$_4$. XINXIN CAI, BRIAN ZAKRZEWSKI, YIQUN YING, Pennysylvania State Univ, DAVID FOBES, TIJIANG LIU, ZHIQIANG MAO, Tulane University, YING LIU, Pennsylvania State Univ — Recent cantilever magnetometry measurements on micron-sized, doubly-connected crystals of Sr$_2$RuO$_4$ have indicated that a half-flux-quantum state may be present in this material. To provide independent evidence for the presence of this new topological object by electrical transport measurements and examine its stability, we carried out Little-Parks (L-P) oscillation measurements, which trace out the phase boundary indicated that a half-flux-quantum state may be present in this material. To provide independent evidence for the presence of this new topological object by electrical transport measurements and examine its stability, we carried out Little-Parks (L-P) oscillation measurements, which trace out the phase boundary of a system, on mesoscopic rings of Sr$_2$RuO$_4$. Sr$_2$RuO$_4$ rings were fabricated using a combination of mechanical exfoliation of Sr$_2$RuO$_4$ single crystals, photolithography, and focused ion beam techniques. Without an in-plane magnetic field, large-amplitude resistance oscillations of a full-flux quantum were found in the upper critical field data of Kittaka et al. [2009 Phys. Rev. B 80, 174514] are obtained.

This work is supported by DOE under grant DE-FG02-04ER46159.

9:12AM F11.00007 Large Chern Number and Edge Currents in Sr$_2$RuO$_4$. THOMAS SCAFFIDI, STEVEN SIMON, University of Oxford — Using the results of a previously reported microscopic calculation, we show that the most favored chiral superconducting order parameter in Sr$_2$RuO$_4$ has Chern number $|C| = 7$ in the weak coupling limit. This order parameter has a momentum dependence of the type $\sin(k_x) \cos(k_y) + i \sin(k_y) \cos(k_x)$ and lies in the same irreducible representation $E_u$ of the tetragonal point group as the usually assumed gap function $\sin(k_y) + i \sin(k_x)$. While the latter gap function leads to $C = 1$, the former leads to $C = -7$, which is only allowed for an $E_u$ gap function since the tetragonal symmetry only fixes $C$ modulo 4. Since it was shown that the edge currents of a $|C| > 1$ superconductor vanish exactly in the continuum limit, and can be strongly reduced on the lattice, this form of order parameter could help resolve the experimental observation of time-reversal symmetry breaking and yet the absence of observed edge currents in Sr$_2$RuO$_4$.

9:24AM F11.00008 Is the anisotropy of the upper critical field of Sr$_2$RuO$_4$ consistent with a helical $p$-wave state?, RICHARD KLEMM, Univ of Central Florida, JINGCHUAN ZHANG, QIANG GU, University of Science and Technology Beijing, CHRISTOPHER LOESCHER, Univ of Central Florida — We calculate the angular and temperature $T$ dependencies of the upper critical field $H_{c2}(\theta, \phi, T)$ for the $C_4v$ point group helical $p$-wave states, assuming a single uniaxial ellipsoidal Fermi surface, Pauli limiting, and strong spin-orbit coupling that locks the spin-triplet d-vectors onto the layers. Good fits to the Sr$_2$RuO$_4$ $H_{c2,0}(\theta, T)$ data of Kittaka et al. [2009 Phys. Rev. B 80, 174514] are obtained. Helical states with $\hat{d}(k) = k_x \hat{x} - k_y \hat{y}$ and $k_x \hat{x} + k_y \hat{y}$ or $k_x \hat{x} + k_y \hat{y}$ and $k_x \hat{x} - k_y \hat{y}$ produce $H_{c2}(90^\circ, \phi, T)$ that greatly exceed (or do not exhibit) the four-fold azimuthal anisotropy magnitudes observed in Sr$_2$RuO$_4$ by Kittaka et al. and by Mao et al. [2000 Phys. Rev. Lett. 84, 991], respectively.
9:36AM F11.00009 Possible f-wave pairing in the low-doping regime of monolayer MoS$_2$. CARSTEN HONERKAMP, JIE YUAN, RWTH Aachen University — We investigate the possible superconducting pairing state in a theoretical model for monolayer-MoS$_2$ by using the temperature-flow functional renormalization group (fRG). In the low doping regime, the dominant instability lies in the odd-parity pairing channel. It has a f-wave pairing structure within the D$_{3h}$ point-group symmetry. We also compute the fRG phase diagram below the van-Hove filling. In the superconducting regime, the critical temperature grows with increasing doping, comparable to the experiments. We demonstrate that the pairing is driven by ferromagnetic fluctuations. When the band filling is close to the van-Hove filling, the system favors a ferromagnetic state.

9:48AM F11.00010 Possible restoration of superconductivity in the quasi-one-dimensional conductor Li$_{1-y}$Mo$_y$O$_{17}$ in pulsed high magnetic field $H \approx 100 \, T$. OTAR SEPPER, ANDREI LEBED, University of Arizona — We present a theoretical study of restoration of superconductivity in the form of the triplet reentrant superconducting phase in the quasi-one-dimensional (Q1D) conductor. Substitution of known band and superconducting parameters of the presumably triplet Q1D superconductor Li$_{1-y}$Mo$_y$O$_{17}$ into our theoretical equations shows that such restoration can happen in non-destructive pulsed magnetic fields of the order of $H \approx 100 \, T$. We investigate in detail how small inclinations of a direction of magnetic field from its optimal experimental geometry decrease the superconducting transition temperature of the reentrant phase, which is important for its experimental discovery. If confirmed experimentally, the reentrant superconducting phase in Li$_{1-y}$Mo$_y$O$_{17}$ would be the first example of the survival of superconductivity in ultra high magnetic fields and would, in addition, unequivocally confirm the spin-triplet pairing nature in this compound.

This work was supported by the NSF under Grant No. DMR-1104512

10:00AM F11.00011 Fluctuation effects in a two-component p-wave superconductor. MARK H. FISCHER, EREZ BERG, Weizmann Institute of Science — For a tetragonal material, order parameters of $p_x$ and $p_y$ symmetry are related by rotation and hence have the same $T_c$. This degeneracy can be lifted by a symmetry-breaking field, like (uniaxial) in-plane strain, such that at $T_c$, the order parameter is only of $p_x$ or $p_y$. Only at a lower temperature also the respective other order parameter condenses. We analyze consequences of (thermal) fluctuations on these transition temperatures within a Ginzburg-Landau approach to obtain a comprehensive strain-temperature phase diagram. We find that the fluctuations can both enhance or suppress the effect of the symmetry breaking field, and even drive the system into a preemptive chiral phase. Possible consequences for the spin-triplet superconductor Sr$_2$RuO$_4$ will be discussed.

10:12AM F11.00012 Long range p-wave proximity effect into a disordered metal!. AYDIN CEM KESEK, CMTC, Univ. of MD, VALENTIN STANEV, CMTC, Univ.of MD, VICTOR GALITSKI, CMTC and JQI, Univ. of MD & School of Physics, Monash. — We use quasiclassical methods of superconductivity to study the superconducting proximity effect from a topological p-wave superconductor into a disordered one-dimensional metallic wire. We demonstrate that the corresponding Eliashberg equations with disorder reduce to a closed non-linear equation for the superconducting component of the matrix Green’s function. Remarkably, this equation is formally equivalent to a classical mechanical system (i.e., Newton’s equations), with the Green function corresponding to a coordinate of a fictitious particle and the coordinate along the wire corresponding to time. This mapping allows to obtain exact solutions in the disordered nanowire in terms of elliptic functions. A surprising result that comes out of this solution is that the p-wave superconductivity proximity-induced into the disordered metal remains long-range, decaying as slowly as the conventional s-wave superconductivity. It is also shown that impurity scattering leads to the appearance of a zero-energy peak.

This research was supported by DOE-BES DESC0001911 (VG & VS), NSF-CAREER DMR- 0847224 (ACK), and Simons Foundation.

10:24AM F11.00013 Colossal proximity effect in a superconducting triplet spin valve based on the half-metallic ferromagnet CrO$_2$. AMRITA SINGH, STEFANO VOLTAN, KAVEH LAHABI, JAN AARTS, Kamerlingh Onnes Laboratory — Combining superconductors (S) and ferromagnets (F) offers the opportunity to create a new class of superconducting spintron devices. In particular, the S/F interface can be specifically engineered to convert singlet Cooper pairs to spin-polarized triplet Cooper pairs. The efficiency of this process can be studied using a so-called triplet spin valve (TSV), which is composed of two F-layers and an S-layer. When the magnetization in the two F-layers are not collinear, singlet states can be drained from the S-layer, and injected as triplet generation is therefore signalled by a decrease of the critical temperature $T_c$. Here, we build highly efficient TSVs using a 100% spin-polarized half-metallic ferromagnet, CrO$_2$. The application of large out of plane magnetic fields results in an extremely strong suppression of $T_c$, by almost a Kelvin. The observed effect is nearly an order of magnitude larger than previous studies on TSVs with standard ferromagnets. Furthermore, we clearly demonstrate that this triplet proximity effect is strongly dependent on the transparency and spin activity of the interface. Our results are particularly important in view of the growing interest in generating long range triplet supercurrents for dissipationless spintronics.

10:36AM F11.00014 Quantum Limit in a Magnetic Field for Triplet Superconductivity in a Quasi-One-Dimensional Conductor1, ANDREI LEBED, OTAR SEPPER, Department of Physics, University of Arizona — We theoretically consider the upper critical magnetic field, perpendicular to a conducting axis in a triplet quasi-one-dimensional superconductor [1]. In particular, we demonstrate that, at high magnetic fields, the orbital effects against superconductivity in a magnetic field are reversible and, therefore, superconductivity can restore. It is important that the above mentioned quantum limit can be achieved in presumably triplet quasi-one-dimensional superconductor Li$_{1-y}$Mo$_y$O$_{17}$ [J.-F. Mercure et al., Phys. Rev. Lett. 108, 187003 (2012)] at laboratory available pulsed magnetic fields of the order of $H \approx 500 - 700 \, T$. [1] A.G. Lebed and O. Sepper, Phys. Rev. B 90, 024510 (2014).

This work was supported by the NSF under Grant No DMR-1104512

10:48AM F11.00015 Universal spin-triplet superconducting correlation of Majorana Fermions, XIU LIU, JAY DEEP SAU, Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland, College Park, Maryland 20742-4111, USA. — In this work, we show that Majorana fermions (MFs) on the boundary of topological superconductors (TSCs) only have spin-triplet superconducting correlation no matter what the bulk superconducting gap is singlet or triplet. This is universal for all TSCs as long as they have, on the boundary, odd number of MFs for BDI or D class and odd number pairs of MFs for DIII class. As a result, the Andreev reflection induced by the Majorana fermions always introduces spin-triplet Cooper pairs in the leads. This spin-triplet condensate results in the the spin-orbit coupling (SOC) controlled oscillatory correlation critical current without $0 - \pi$ transition in the TSC/SOC-semiconductor/TSC Josephson junction. The observation of this unique current-phase relation can serve as a signal of Majorana fermions. Moreover our study open a new way to manipulate Majorana fermions based on their spin-triplet superconducting correlation.

Tuesday, March 3, 2015 8:00AM - 11:00AM –
Session F12 DMP GERA FIAP DCOMP: Focus Session: Thermoelectric Materials and Applications 007C - Lilia Woods, University of South Florida
Thermoelectric energy harvester based on quantum well superlattices

YUNJIN CHOI, ANDREW JORDAN, University of Rochester — We propose a nanoscale heat engine based on quantum well superlattices for harvesting thermal energy. A hot cavity is connected via superlattices to electronic reservoirs, and the electron transport through the superlattice by gaining energy from the hot cavity converts heat into electrical power. The energy gain is determined by the composite superlattices system. Therefore, the electric and heat current of electrons for simplified miniband transport of the superlattices give tunable conditions for the maximal generated power or efficiency. In addition, we analyze the phonon transport of the superlattices and show the reduction of the phonon thermal conductivity at high temperature which is beneficial for the highly efficient thermoelectric devices [1]. Combination of the electron and phonon transport shows an optimal configuration for the best performance of energy harvester. We discuss and compare our result with the energy harvester based on resonant quantum wells [2].


Self-propagating high temperature synthesis for compound thermoelectrics and new criterion for applicability of combustion processing

XINFENG TANG, XIANLI SU, Wuhan University of Technology, CITIRAD UHER, University of Michigan, TANG’S GROUP TEAM, UHER’S GROUP TEAM — Here we report compound thermoelectric materials (Bi$_2$Te$_3$, Bi$_2$Se$_3$, Cu$_2$Se, Cu$_5$SnSe$_3$, half-Heusler alloys, lead chalcogenides, skutterudites, and magnesium silicides) with thermoelectric properties comparable with materials prepared by the traditional routes of synthesis can be synthesized at a minimal cost and on the time scale of seconds using the self-propagating high temperature synthesis method. Moreover, we found that the criterion often quoted in the literature as the necessary preconditions for combustion synthesis, $T_{ad} \geq 1800$ K, is not universal and certainly not applicable to thermoelectric compound semiconductors. Instead, we offer new empirically-based criterion, $T_{ad}/T_{in} \geq 1$, i.e., the adiabatic temperature must be high enough to melt the lower melting point component, which covers all materials synthesized by self-propagating high temperature synthesis, including the high temperature refractory compounds for which the $T_{ad} \geq 1800$ K criterion was originally developed. Our work opens a new avenue for ultra-fast, low cost, mass production fabrication of efficient thermoelectric materials and the new criterion greatly broadens the scope of materials that can be successfully synthesized by self-propagating high temperature synthesis. 3

1We wish to acknowledge support from the National Basic Research Program of China (973 program) under project 2013CB632502.

NbFeSb based p-type half-Heusler for power generation applications

GRI JOH, GMZ Energy Inc. RAN HE, University of Houston, MICHAEL ENGBER, GMZ Energy Inc. GEORGE SAMSONIDZE, Robert Bosch LLC, TEJ PANTA, EKRAJ DAHAL, GMZ Energy Inc. KESHAB DAHAL, University of Houston, JIAN YANG, GMZ Energy Inc. YUCHENG LAN, University of Houston, BORIS KOZINSKY, Robert Bosch LLC. ZHIFENG REN, University of Houston — We report peak dimensionless figure-of-merit (ZT) of 1.2 at 700 K, is not universal and certainly not applicable to thermoelectric compound semiconductors. Instead, we offer new empirically-based criterion, $T_{ad}/T_{in} \geq 1$, i.e., the adiabatic temperature must be high enough to melt the lower melting point component, which covers all materials synthesized by self-propagating high temperature synthesis, including the high temperature refractory compounds for which the $T_{ad} \geq 1800$ K criterion was originally developed. Our work opens a new avenue for ultra-fast, low cost, mass production fabrication of efficient thermoelectric materials and the new criterion greatly broadens the scope of materials that can be successfully synthesized by self-propagating high temperature synthesis.

3Supported by US DOE

Automotive Thermoelectric Waste Heat Recovery

GREGORY P. MEISNER, General Motors Research and Development — Considerable fuel energy, as much as 70%, is not converted to useful work by internal combustion engines but is instead rejected as waste heat, and more than half of the waste heat, nearly 40% of fuel energy, is contained in vehicle exhaust gas. This provides an opportunity to recover some of the wasted fuel energy and convert it from heat into useful work, subject to the laws of thermodynamics, and thereby improve vehicle energy efficiency. Thermoelectric (TE) materials have been extensively researched and TE devices are now being developed for operation at high temperatures corresponding to automotive exhaust gases for direct solid-state conversion of heat into electricity. This has stimulated substantial progress in the development of practical TE generator (TEG) systems for large-scale commercialization. A significant enabler of this progress has been the US Department of Energy’s Vehicle Technologies Program through funding for low cost solutions for automotive TE waste heat recovery to improve fuel economy. Our current project at General Motors has culminated in the identification of the potential supply chain for all components and assembly of an automotive TEG. A significant focus has been to develop integrated and iterative modeling tools for a fully optimized TEG design that includes all components and subsystems (TE modules, heat exchangers, thermal interfaces, electrical interconnects, power conditioning, and vehicle integration for maximal use of TEG power). We have built and tested a new, low-cost Initial TEG prototype based on state-of-the-art production-scale skutterudite TE modules, novel heat exchanger designs, and practical solutions to the many technical challenges for optimum TEG performance. We will use the results for our Initial TEG prototype to refine our modeling and design tools for a Final automotive TEG system prototype. Our recent results will be presented. Thanks to: J.R. Salvador, E.R. Gundlach, D. Thompson, N.K. Bucknor, M.G. Reynolds, K. Rober, F.R. Stabler; Marlau, JPL, Dana, Delphi E&S, Eberspacher, Molycorp, University of Washington, Purdue University, Michigan State University, ORNL, BNL.

1Supported by US DOE

Anharmonic phonons in type I clathrates

KATSU MIYAKI, JIAZHENG WU, HIDEKAZU SHIMOTANI, Tohoku University — A systematic study on the anharmonicity of phonons is made for thermoelectric single crystal type-I clathrates based on their heat capacity $C_P$ at low temperatures (T) down to 360 mK. The low-T linear terms $\kappa_0 + \gamma T$ of $C_P$, including the tunneling-term of the atoms accommodated in the host cages ($\gamma T T > \alpha T$), and the Sommerfeld itinerant-electron term $(\gamma T)$ are successfully separated through careful measurements of single crystals with various carrier concentrations. The values of the density of anharmonic potentials are deduced. The effective mass $(m^*)$ enhancement is also determined from $\gamma T$ values and the electron-phonon interaction strength $(\lambda)$ can be evaluated from these values. It is shown that both the thermal conductivities $(\kappa)$ and the electron-phonon interaction strength $(\lambda)$ are quantitatively in good agreement with the $\alpha$ parameters deduced from the present experiments. The boson peaks observed at low energy excitations are discussed in relation to the $\alpha$ values.
9:24AM F12.00006 Large local distortions around the Ba site in Ba$_8$Ga$_2$$_x$X$_{38}$, X=Si, Sn$^1$. TREVOR KEIBER, Univ of California-Santa Cruz, FRANK BRIDGES, PATRICK NAST, UC Santa Cruz, SCOTT MEDLING, Australian National University, TOSHIRO TAKABATAKE, Hiroshima University — We report an Extended X-ray Absorption Fine Structure (EXAFS) analysis of thermoelectric type-I clathrates, Ba$_8$Ga$_{16}$X$_{38}$, X=Si,Sn. These clathrates have a cage-like crystal structure filled with “rattler” atoms (Ba) located near the center of the cages (Ga-X). In contrast to the results for Ba$_8$Ga$_{16}$Ge$_{38}$, our results show that for X=Si,Sn the average pair distances within the cages (Ga-Sn, Ga-Ga, Ga-Si, Sn-Sn) are significantly different than the average distances found from diffraction. Direct measurements of the Ba K edge suggests that the environment about Ba is very highly disordered for X=Sn,Si compared to X=Ge, with surprisingly short Ba-X/Ga distances; likely the Ba2 site is significantly off center. For Si, the Ba K first neighbor peak is substantially reduced in size and shifted to lower r due to interference effects from many different Ba neighbor distances. For X=Sn the Ba-Ga/Sn distances are even shorter, and there is a split peak with very low amplitude suggesting a very disordered environment. The mixed distances of the cage atoms, the very short Ba-Ga/X distances, as well as the disorder about the Ba site, suggest that the cage structure is buckled. This disorder will lead to increased scattering for both phonons and electrons.

$^1$This work supported under NSF grant DMR1005568.

9:36AM F12.00007 Effect of Alkaline Metal Filling on the Structural Properties of Type-II Clathrate A$_x$M$_{136}$(A = Na,K,Rb,Cs; M = Group IV Atom; 0$<x$$\leq$24). CHARLES MYLES, DONG XUE, Texas Tech University — Early investigations of the properties of the Type II clathrate Na$_x$Si$_{136}$ (0$<x$$\leq$24) $^1$[1] have found that, as the composition x increases, the Si$_{136}$ lattice exhibits framework contraction upon filling (0$<x$$<8$), followed by an expansion of the unit cell volume (9$<x$$<24$). Stimulated by this discovery of a non-monotonic structural response to cage filling by the guests, we have performed a systematic, first-principles study of the composition-framework interaction in the large and small cages in the Type II clathrates Si$_{136}$, Ge$_{136}$, and Sn$_{136}$. Our calculations are based on the VASP code and we have considered Na, K, Rb, and Cs guests for 0$<x$$\leq$24. An emphasis in our study is on how the guest atom size affects the dynamical behavior of the host material. We focus on the host lattice structural expansion or compression as x increases. We also present and discuss calculations of the effective potential energy curves for the guest-host interactions in these materials. Our results are correlated with the damping (or anharmonic) oscillations of the guests. These results are useful as an indication of the expected behavior of the guest “rattling” phonon modes in these materials. Among other results, we find that some guests are weakly bonded in the host cages and others are unstable around the cage centers.

$^1$Beekman, Nenghabi, Biswas, Myles, Yaittinger, Grin, Nolas, Inorganic Chemistry 49, 5338 (2010).

9:48AM F12.00008 First Principles Study of the Vibrational and Thermal Properties of the Type-II Clathrates A$_x$Ga$_8$Sn$_{136}$-x (x = 8,16,24; A = Rb,Cs). DONG XUE, CHARLES MYLES, Texas Tech University — We have performed first-principles calculations of the vibrational and thermal properties of the semiconductor clathrates Rb$_x$Ga$_8$Sn$_{136}$-x and Cs$_x$Ga$_8$Sn$_{136}$-x for x = 8, 16, and 24. Our calculations used the VASP code to obtain the equilibrium geometries and the PHONOPY code to obtain the harmonic phonon modes. For x = 24, the phonon dispersion relations predict an upshift of the low-lying optical modes (~30cm$^{-1}$) in the presence of the light guest (“rattler”) Rb. We also find large isotropic atomic displacement parameters ($u_{iso}$) when the Rb occupies the large cages (Sn$_{28}$). The modes associated with these guests should contribute strongly to lowering the lattice thermal constant (kL). This is reinforced by our evaluation of the guest-associated effective potential energy curves E(x). Our calculated effective harmonic spring constants K for these guests show that a simple harmonic oscillator model is in good agreement with the first principles lattice dynamical calculations. The similarity between $\omega_{oa} = (K/M)^{1/2}$ and our computed guest phonon frequencies implies that anharmonic contributions to the guest vibrational modes are not significant. Our calculations of the vibrational contribution to the specific heat and our estimation of $k_L$ are also presented and discussed.

10:00AM F12.00009 Study on Transport and Mechanical Properties of La and Ce Double Filled p-type Skutterudites$^1$. TULASHI DAHAL, Department of Physics and TCSUH, University of Houston, TX 77204, SONIKA GAHALWAT, Department of Mechanical Engineering, University of Houston, TX 77204, QING JIE, HEE SEOK KIM, KESHAB DAHAL, WEISHUI LIU, Department of Physics and TCSUH, University of Houston, TX 77204, YUCHENG LAN, Department of Physics, Morgan State University, MD 21251, KENNETH WHITE, Department of Mechanical Engineering, University of Houston, TX 77204, ZHIFENG REN, Department of Physics and TCSUH, University of Houston, TX 77204, REN’S GROUP TEAM — Optimizing the thermoelectric performance of p-type skutterudites is extremely challenging due to several factors such as low Seebeck voltage and bipolar contribution in electrical and thermal conductivity at elevated temperature, leading to small ZT value. In this work, we report improved thermoelectric performance of La and Ce double filled p-type skutterudites by melting-quenching-annealing-ball milling-hot pressing. The observed high power factor (~35 μW cm$^{-1}$ K$^{-2}$ at 500 °C) and low thermal conductivity (~2.5 W m$^{-1}$ K$^{-1}$ at 500 °C) leads to a peak ZT about 1.1 in the optimized composition, With a ΔT of 475 °C between heat source and sink, the estimated output power density in the best sample is ~8 W cm$^{-2}$. The nano-indentation experiment reveals that the hardness and Young’s modulus of elasticity of the sample is much better than Bi$_2$Te$_3$ and PbTe-based samples, indicating skutterudites are suitable for practical applications where mechanical strength is also important.

$^1$US Department of Energy

10:12AM F12.00010 Local structure in ball-milled and Ni substituted Nd$_x$Fe$_{4-x}$Ni$_2$Sb$_{12}$.$^1$. FRANK BRIDGES, FELIPE RIVAS, MARKUS SHORT, TREVOR KEIBER, Physics Dept. UC Santa Cruz, Santa Cruz CA 95064, PETER ROGL, Institute of Physical Chemistry, University of Vienna, Austria — We report EXAFS measurements at the Nd L$_{III}$, Fe, and Sb K edges in Nd$_x$Fe$_{4-x}$Ni$_2$Sb$_{12}$. Recent measurements show thatball-milled Nd$_4$Fe$_{12}$Sb$_{12}$, with ~150 nm size particles, significantly improved the figure of merit (ZT) by 22 %, compared to material with 10 μm sized particles. Since ball milling can produce significant disorder and even amorphization, which would lower the thermal conductivity, we compared the local structure for ball-milled and hand ground samples. We find that the average local structure is essentially unchanged by ball milling; the reduced particle size reduces the phonon mean free path, thereby reducing the thermal conductivity. When Ni is substituted on the Fe site, together with a decreased concentration of Nd, we find the largest changes in disorder are about the Nd atoms; there is little disorder of the first few neighbors about the Fe site. Further the local distortions are not uniform; the lattice constant decreases with Ni concentration, but the Nd-Sb bond length slightly expands while the Sb-Sb contracts more than expected. Some consequences are discussed.

$^1$Support: NSF DMR1005568
10:24 AM F12.00011 Thermoelectric properties of GeTe-CuInTe₂ alloys, SI HUI, Department of Mechanical Engineering, University of Michigan, Ann Arbor, JAMES SALVADOR, Chemical and Materials Systems Laboratory, GM R&D Center, Warren, HUI SUN, Department of Physics, University of Michigan, Ann Arbor, KEVIN PIPE, Department of Mechanical Engineering, Department of Electrical Engineering, University of Michigan, Ann Arbor, CTIRAD UHER, Department of Physics, University of Michigan, Ann Arbor — GeTe-AgSbTe₂ and PbTe-AgSbTe₂ alloys, known as TAGS and LAST respectively, are excellent thermoelectric materials. By alloying the matrix with other ternary compounds, the thermal conductivity is significantly reduced due to the enhancement of phonon scattering by formation of nano-sized secondary phases and disturbance to the lattice. Meanwhile, since the ternary compound AgSbTe₂ also exhibits good thermoelectric properties and Ag¹⁺ and Sb²⁺ tend to replace two Ge atoms at the same time, the mobility, and thus the power factor, will not be influenced much by this alloying. In this work, we replaced the ternary compound AgSbTe₂ by CuInTe₂ which does not contain the expensive element Ag and also exhibits good thermoelectric properties. We measured the Seebeck coefficient, electrical conductivity, thermal conductivity and Hall coefficient, and observed that CuInTe₂ almost has no influence on the power factor but does reduce the thermal conductivity. ZT was observed to improve to 1.2 at 800K for (Ge₃Te₇)₀.₉₇(CuInTe₂)₀.₀₃. We believe that ZT will be further enhanced at larger CuInTe₂ fractions due to further reduced thermal conductivity.

10:36 AM F12.00012 Thermoelectric and Lattice Dynamical Properties of Ge₃Sb₂Te₅, SAIKAT MUKHOPADHYAY, JIFENG SUN, Oak Ridge National Laboratory, Oak Ridge, TN, ALASKA SUBEDI, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany, DAVID SINGH, Oak Ridge National Laboratory, Oak Ridge, TN — Ge₃Sb₂Te₅ (GST) has been widely used as phase-change materials in optical data storage media and nonvolatile RAM devices. At elevated temperature, GST is known to undergo subsequent structural transitions from a non-conducting amorphous to (metastable) disordered cubic phase and then to a conducting hexagonal phase above 300°C. Given that hexagonal-GST has already been reported to have promising thermoelectric properties and transport properties critically depend on the bonding information, a direct correlation between its structural- and transport properties needs to be established. In this talk, we will present the evolution of thermoelectric and lattice dynamical properties of GST in different phases via first principles calculations based on density functional theory. A better understanding of the origin of low-thermal conductivity in hexagonal-GST may provide critical information for further improvement of its thermoelectric figure of merit (ZT).

10:48 AM F12.00013 Calculation of Phonon Conductivity and Seebeck Coefficient in Cu-Ni Alloy, YUSUKE KONISHI, YOSHIHIRO ASAI, NRI-AIST — In recent years, thermoelectric materials have been attracting a lot of attention because they are expected to be applied for utilization of waste heat. Many kinds of materials are studied for this purpose; semiconductors, alloys, organic materials, etc. In 2010, a giant Peltier effect was observed in a Cu-Ni/Au junction [1]. It is considered that this giant Peltier effect is caused by nano-scale phase separation formed in the sputtering process. Although this material is a great candidate for a thermoelectric material, we need to find the condition for a large thermoelectric properties of Cu-Ni alloy by using nonequilibrium molecular dynamics simulation and calculated Seebeck coefficients via ab-initio methods. [1] A. Sugihara et al., Appl. Phys. Exp. 3, 065204 (2010).

Tuesday, March 3, 2015 8:00 AM - 11:00 AM — Session F13 DCMP: Quantum Dots, Wires And Wells: Electronic Phenomena 007D - Paul Simmonds, Boise State University

8:00 AM F13.00001 Using Dissipation to Stabilize a Quantum Critical Point in Two Quantum Dots, GU ZHANG, Duke Univ, EDUARDO NOVAIS, UFABC, Brazil, HAROLD BARANGER, Duke Univ — We show how dissipation could be used to stabilize the two-impurity Kondo critical point in a double dot system. In the absence of dissipation, this intermediate coupling fixed point cannot be reached because charge transfer from the source to drain lead, always present in a realistic system, is a relevant perturbation. By using dissipative leads, as recently introduced in single dot experiments, this charge transfer can be suppressed, thus allowing the intermediate-coupling non-Fermi-liquid quantum critical point to be reached. We expect that when dissipation exceeds a critical value, zero conductance will be observed except at this critical point, which then is its experimental signature. We also studied the effect of dissipation on the two critical points at which the interdot exchange flows either to zero or infinity.

1 Work supported in part by the U.S. DOE Division of Materials Sciences and Engineering (DE-SC0005237).

8:12 AM F13.00002 Stabilizing lateral strained-Si/SiGe material quantum dots, SERGEI STUDENIKIN, G. POULIN-LAMARRE, A. SACHRAJDA, National Research Council of Canada, T. LU, N. BISHOP, T. PLUYM, P. KOTULA, M. LILLY, M. CARROLL, Sandia National Laboratories — In enhancement-mode SiGe quantum dot structures [2], 2DEG electrons are generated via the application of a positive global gate. The carrier mobility in such structures is limited by disorder potential at the oxide/silicon interface. Recently it was shown that the deteriorating effect of charge fluctuations can be substantially mitigated by incorporating a shielding electron layer at the surface — a thin Si quantum well cap layer [1,2]. This cap layer can, however, cause instabilities, drifts and hysteretic behaviour. In this work we study the stability of a tunable quantum dot defined by lateral gates in a Si/SiGe structure with a thin silicon cap layer and Si3N4 dielectric layer between the global gate and the structure [2]. Different "stabilization" procedures are explored to stabilise the device using both dc transport and charge sensing measurements at 300 mK.


8:24 AM F13.00003 Beyond hydrostatic strain in empirical pseudopotentials for the electronic structure of InGaAs quantum dots, CEYHUN BULUTAY, ASLI CAKAN, Bilkent University — Self-assembled quantum dots (SAQDs) are among the prime candidates for realizing semiconductor quantum wire systems. Even though much progress has been achieved toward understanding their electronic structure, more efforts are needed to reach the desired quantitative level for a precise control of the carrier and nuclear spin degrees of freedom. In this respect, the empirical pseudopotential method has been highly successful for structures involving more than hundred thousand atoms. However, due to lack of self-consistency, their use in strained environments, as in SAQDs, requires vital improvement. The main contribution of this work is to develop empirical pseudopotentials valid for inhomogeneous strain environments caused by cation alloying in InGaAs SAQDs. In our presentation, we first validate our approach with the ab initio density functional theory results based on Projector Augmented-Wave technique. This is followed by a comparison of the electronic structure results with and without strain-dependent pseudopotentials for InGaAs SAQDs having an alloy composition of 20-30% indium, which is typically the case in the current samples.

1Supported by TUBITAK with the Project No. 112T178.
9:00AM F13.00006 Spin-orbit coupling in semiconductor nanowires: Physical limits for Majorana states. 


9:36AM F13.00009 Electrical and thermal transport in inhomogeneous quantum wires.

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

\[1\] J. F. and M. G. acknowledge support from DFG SFB 689.


Characterization of NiSi nanowires as field emitters and limitations of Fowler-Nordheim model at the nanoscale

AМИНА B. BELKADI, University of Colorado - Boulder, E. GALE, Khalifa University - KUSTAR, A.F. ISAKOVIC, Khalifa University - KUSTAR, KSRС — Nanoscale field emitters are of technological interest because of the anticipated faster turn-on time, better sustainability and compactness. This report focuses on NiSi nanowires as field emitters for two reasons: (a) possible enhancement of field emission in nanoscale field emitters over bulk, and (b) achieving the same field emission properties as in bulk, but at a lower energy cost. To this end, we have grown, fabricated and characterized NiSi nanowires as field emitters. Depending on the geometry of the NiSi nanowires (aspect ratio, shape etc.), the relevant major field emission parameters, such as (1) the turn-on field, (2) the work function, and (3) the field enhancement factor, can be comparable or even superior to other recently explored nanoscale field emitters, such as CdS and ZnO. We also report on a comparative performance of various nanoscale field emitters and on the difficulties in the performance comparison in the light of relatively poor applicability of the standard Fowler-Nordheim model for field emission analysis for the case of the nanoscale field emitters. Proposed modifications are discussed.

Ultra-low noise atomically patterned nanostructures in Si

SAQUIB SHAMIM, Department of Physics, Indian Institute of Science, Bangalore 560012, India, BENT WEBER, MICHELLE Y. SIMMONS, Centre of Excellence for Quantum Computation and Communication Technology, University of New South Wales, Sydney 2052, Australia, ARINDAM GHOSH, Department of Physics, Indian Institute of Science, Bangalore 560012, India — Advancement in scanning tunnelling microscopy (STM) based lithography has made it possible to achieve low resistivity atomic scale wires and single donor quantum dot devices in silicon. Due to extreme sensitivity of these devices to any disorder or charge traps, it is of paramount importance to explore the noise magnitude in these systems. Here we investigate low frequency noise measurements in two STM patterned atomic scale wires of phosphorous dopants in Si of diameters 4.5 nm and 1.5 nm. The variation of noise with gate voltage indicates that the noise arises due to trapping-detrapping of electrons between the wire and charged traps. The Hooge parameter for these wires is 10⁻¹² to 10⁻¹³ (for different gate voltages), which is one of the lowest reported for any one-dimensional system. The reason for such low noise magnitude can be two-fold. First, a complete monolithic fabrication procedure avoids any direct metallic contact to the one-dimensional system and hence prevents any Schottky barrier. Second possibility is that the Coulomb repulsion between the charges on traps doesn’t allow many traps to be activated simultaneously. Aimed at being the backbone of silicon quantum computation scheme, a reduced noise in these devices is technologically crucial.

Understanding electronic band-edge properties of GaSbAs/GaAs nanostructures through k.p theory simulations

CHRISTINA JONES, EMMANOUIL KIOUPAKIS, University of Michigan - Ann Arbor — Gallium antimonide (GaSb) nanostructures embedded in gallium arsenide (GaAs) have been predicted by theory and have been found experimentally to demonstrate both type-I and type-II band alignment. The ability of GaSb nanostructures to exhibit two band alignment types makes them versatile in applications such as LEDs, photodetectors, and charge-based memory elements. We present a systematic study of the mechanisms behind the band alignment type in order to understand the underlying physics behind the alignment transition and allow for prediction and optimization of electronic properties. We employ the eight-band k.p method through a commercially available software package (nextnano) to calculate the band structure by self-consistently solving the Schroedinger and Poisson equations including strain and polarization charges. Results obtained for GaSbAs/GaAs quantum wells show both type-I and type-II band alignment depending on strain and composition. Calculated band-edges are compared to published experimental results.

Resonant Subband Landau Level Coupling in GaAs/AlGaAs/GaAs Coupled Quantum Wells

LI-CHUN TUNG, University of North Dakota, DMITRY SMIRNOV, National High Magnetic Field Laboratory — Subband energies and intersubband couplings of symmetric GaAs/AlGaAs/GaAs coupled quantum wells have been investigated by magneto-infrared spectroscopy at 4K up to 35T. Most of the proposed quantum well infrared photodetectors consist of coupled quantum wells, and the detection of infrared photons is accomplished via exciting bound electrons of lower subbands to a continuous state via intersubband transitions. With the presence of a small in-plane magnetic field, subbands due to the mixing of wave functions of individual quantum wells are studied by the anti-level crossing resonance of the Landau levels belonging to different subbands. The observed coupling between the first subband of the coupled quantum wells (Symmetric mixing of the lowest subbands of the individual quantum wells) to the third subband is observed, while the others are forbidden. The symmetry selection rule for the intersubband transitions of symmetric coupled quantum wells will be discussed in the presentation.

Mott transition in the coupled quantum wells with the external periodic potential

OLEG BERMAN, ROMAN KEZERASHVILI, New York City College of Technology of CUNY, Brooklyn NY, USA, YURII LOZOVIK, Institute of Spectroscopy, Troitsk, Russia, KLAUS ZIEGLER, University of Augsburg, Augsburg, Germany — We study a system of spatially separated electrons and holes in two coupled quantum wells within a temperature-dependent mean-field approach. A periodic potential is applied to the quantum wells which allows us to modify the spectral properties of the electrons and the holes. This system exhibits a rich phase diagram, consisting of a BCS phase with electron-hole pairs, an electron-hole plasma and a bosonic Mott phase of tightly bound electron-hole pairs. The latter have no phase coherence in contrast to the pairs in the BCS phase. We discuss the transitions between the different phases in terms of temperature, density and interaction strength.

Terahertz spectroscopy of two-dimensional electron-hole pairs: probing Mott physics of magneto-excitons

QI ZHANG, WEILU GAO, Rice University, JOHN WATSON, MICHAEL MANFRA, Purdue University, JUNICHIRO KONO, Rice University — Density-dependent Coulomb interactions can drive electron-hole (e−h) pairs in semiconductors through an excitonic Mott transition from an excitonic gas into an e−h plasma. Theoretical studies suggest that these interactions can be strongly modified by an external magnetic field, including the absence of inter-exciton interactions in the high magnetic field limit in two dimensions, due to an e−h charge symmetry, which results in ultrastable magneto-excitons. Here, we present a systematic experimental study of e−h pairs in photo-excited undoped GaAs quantum wells in magnetic fields with ultrafast terahertz spectroscopy. We simultaneously monitored the dynamics of the intraexcitonic 1s→2p transition (which splits into 1s→2pυ and 1s→2pl transitions in a magnetic field) and the cyclotron resonance of unbound electrons and holes up to 10 Tesla. We found that the 1s→2pυ absorption feature is robust at high magnetic fields even under high excitation fluences, indicating magnetically enhanced stability of excitons. We will discuss the Mott physics of magneto-excitons as a function of temperature, e−h pair density, optical pump delay time, as well as magnetic field, and also compare two-dimensional excitons in GaAs quantum wells with three-dimensional excitons in bulk GaAs.
8:00AM F14.00001 Carbon defects as sources of the green and yellow luminescence bands in undoped GaN\(^1\), Denis Demchenko, Michael Reshchikov, Virginia Commonwealth University — In high-purity GaN grown by hydride vapor-phase epitaxy (HVPE), the commonly observed yellow luminescence (YL) band gives way to a green luminescence (GL) band at high excitation intensity. Based on hybrid functional calculations and experimental photoluminescence measurements, we propose that the GL band with a maximum at 2.4 eV is caused by transitions of electrons from the conduction band to the 0/+ level of the isolated C\(_N\) defect. The YL band with a maximum at 2.1 eV, related to the transitions via the /-0 level of the same defect can be observed only for some high-purity HVPE samples. However, in less pure GaN samples (HVPE samples with larger O and C concentrations, as well as all MOVCD grown samples), no GL band is observed and another YL band with a maximum at 2.2 eV dominates the PL spectrum. The latter is attributed to the C\(_N\)O\(_3\) complex.

\(^1\)This work was supported by the National Science Foundation (DMR-1410125) and the Thomas F. and Kate Miller Jeffress Memorial Trust.

8:12AM F14.00002 Density Functional Theory Calculations of Activation Energies for Carrier Capture by Defects in Semiconductors, Normand Modine, Alan Wright, Stephen Lee, Sandia National Laboratories — Carrier recombination due to defects can have a major impact on device performance. The rate of defect-induced recombination is determined by both defect levels and carrier capture cross-sections. Density functional theory (DFT) has been widely and successfully used to predict defect levels, but only recently has work begun to focus on using DFT to determine carrier capture cross-sections. Lang and Henry worked out the fundamental theory of carrier-capture by multiphonon emission in the 1970s and showed that, above the Debye temperature, carrier-capture cross-sections differ between defects primarily due to differences in their carrier capture activation energies. We present an approach to using DFT to calculate carrier capture activation energies that does not depend on an assumed configuration coordinate and that fully accounts for anharmonic effects, which can substantially modify carrier activation energies. We demonstrate our approach for the -3/-2 level of the Ga vacancy in wurtzite GaN. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

8:24AM F14.00003 Defect identification in semiconductors with positron annihilation: experiment and theory, Filip Tuomisto, Aalto University — Positron annihilation spectroscopy is a very powerful technique for the detection, identification and quantification of vacancy-type defects in semiconductors. In the past decades, it has been used to reveal the relationship between optoelectronic properties and specific defects in a wide variety of materials - examples include parasitic yellow luminescence in GaN, dominant acceptor defects in ZnO and broad-band absorption causing brown coloration in natural diamond. In typical binary compound semiconductors, the selective sensitivity of the technique is rather strongly limited to cation vacancies that possess significant open volume and suitable charge (negative of neutral). On the other hand, oxygen vacancies in oxide semiconductors are a widely debated topic. The properties attributed to oxygen vacancies include the inherent n-type conduction, poor p-type dopability, coloration (absorption), deep level luminescence and non-radiative recombination, while the only direct experimental evidence of their existence has been obtained on the crystal surface. We will present recent advances in combining state-of-the-art positron annihilation experiments and ab initio computational approaches. The latter can be used to model both the positron lifetime and the electron-positron momentum distribution - quantities that can be non-directly correlated in the experiments. We will present results from these methods to study vacancy-type defects in III-nitride semiconductors (GaN, AlN, InN) and oxides such as ZnO, SnO\(_2\), In\(_2\)O\(_3\) and Gd\(_2\)O\(_3\). We will show that cation-vacancy-related defects are important compensating centers in all these materials when they are n-type. In addition, we will show that anion (N, O) vacancies can be detected when they appear as complexes with cation vacancies.

9:00AM F14.00004 The role of surface kinetics on defect generation and propagation during epitaxy of WBG semiconductors, Angel Yanguang-Gil, Argonne Natl Lab — One of the greatest challenges in the application of WBG semiconductors to power electronics and optoelectronic applications is how to mitigate the impact of electrically active defects on device performance. While this is an issue that traditionally has been tackled through process development, from a fundamental point of view we still have a limited knowledge on the interplay between epitaxial growth and defect generation. This interaction goes both ways, with surface kinetics promoting the formation of surface defects that get incorporated into the bulk, and the surface defects and surface morphology driving the kinetics of the growth process. In this work we explore the interplay between surface kinetics and 0D and 1D defects during epitaxy. By combining molecular dynamics and kinetic Monte Carlo simulations we have focused on understanding how surface kinetics promotes the formation of defects, and identified the surface configurations that are more likely to lead to point defects incorporated in the bulk. Conversely, we have also studied the impact of existing defects, in particular the interaction of surface species and surface steps with threading dislocations. Our target materials are GaN, AlN, and SiC.

9:12AM F14.00005 Dilute-P GaNP Semiconductor Alloy for Visible Light Emitter, Chee-Keong Tan, Nelson Tansu, Center for Photonics and Nanoelectronics, Department of Electrical and Computer Engineering, Lehigh University — Group III-Nitride semiconductor alloy in particular InGaN alloy is widely employed as the active media for the solid state lighting applications. In addition to the InGaN alloy, dilute-As GaNAs alloy has recently been suggested as the potential material for high efficiency solid state lighting devices. In conjunction with dilute-As GaNAs alloy, dilute-P GaNP alloy has the potential for its use in light emitting applications. The literature on dilute-P GaNP alloy is severely limited, thus the understanding of electronic properties of dilute-P GaNP alloys is important. In this work we present the analysis of the electronic properties of dilute-P GaNP alloys through First-Principle Density Functional Theory (DFT). Our analysis shows that the replacement of N atoms with Phosphorus (P) atoms in the GaN alloy leads to significant changes in the band structure including the band gap and effective mass. In addition, our finding indicates minimal interband Auger recombination in the dilute-P GaNP alloys as compared to InGaN alloy, suggesting the potential of GaNP alloys as high efficiency visible light emitter. The electronic properties of the dilute-P GaNP alloys will be discussed in detail.

9:24AM F14.00006 The donor-acceptor relationship in HVPE GaN:Fe Substrates\(^3\), Ustun Sunay, University of Alabama at Birmingham — GaN is a wide bandgap semiconductor plagued by a high concentration of residual donors, typically from unintentionally incorporated Si or O. The effect of these donors can be masked by doping with deep acceptors, such as Fe, which compensates the donors creating a semi-insulating material that can be used for RF applications. Compensation is thought to occur when the Fe\(^{3+}\) acceptor captures a donor electron, creating Fe\(^{2+}\) and a partially compensated donor. A recent photo-EPR spectroscopy study of lightly Fe-doped (1x10\(^{17}\) cm\(^{-3}\)) bulk GaN showed the existence of neutral donors and Fe\(^{3+}\) simultaneously. The presence of both calls into question the current understanding of compensation. To further understand donor-acceptor compensation, bulk GaN grown via hydride vapor epitaxy was intentionally codoped with Si donors and Fe acceptors in ratios ranging from 0.01 to 1.55. Both species were present in 3.5 K EPR spectra, but the Fe\(^{3+}\) acceptor signal decreased, and the neutral donor signal increased monotonically as the Si:Fe ratio increased. While this shows that Fe\(^{3+}\) partially compensates the neutral donor, interpretation of photo-EPR experiments suggests that some donors and acceptors are not interacting and that there is a multi-step mechanism for compensation. Cathodoluminescence (CL) results showed striated regions of luminescence intensity which indicate defect concentration non-uniformity. The leading explanation for the EPR and CL results is a physical separation between the donors and acceptors, leading to local variations in the Si:Fe ratio.

\(^3\)This work is funded by the National Science Foundation DMR-1308446.
9:36AM F14.00007 The Role of Oxygen on the Nature and Stability of Eu Centers in Eu doped Gallium Nitride, BRANDON MITCHELL, Department of Physics and Astronomy, University of Mt. Union, 1972 Clark Ave, Alliance, OH, 44601, USA, DOLF TIMMERMAN, ZHU WAXING, JUNICHI TAKATSU, MASAKI MATSUDA, Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, Suita, Osaka 565-0871, Japan, KATHARINA LORENZ, EDUARDO ALVES, Instituto Superior Técnico, Campus Tecnológico e Nuclear, Estrada Nacional 10, P-2695-066 Bobadela LRS, Portugal, ATSUŠI KOIZUMI, YASUFUMI FUJIWARA, Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, Suita, Osaka 565-0871, Japan, VOLKMAR DIEROLF, Department of Physics and Astronomy, Leibniz Universität Hannover, Department of Physics and Astronomy, Leibniz Universität Hannover, 30167 Hannover, Germany, and Department of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University, Suita, Osaka 565-0871, Japan. — Growth of high quality, free-standing GaN substrates is essential for further improvement of nitride device performance. Unfortunately, many bulk growth methods introduce unacceptable amounts of O donors. Samples studied in this work were grown by the high-pressure nitrogen solution method on (0001) sapphire with Mg-doped GaN substrates characterized by 4 K electron paramagnetic resonance (EPR) spectroscopy. No EPR signal is detected in the undoped samples. However, a nearly isotropic spectrum with g-value of 1.984 and a line-width of 120 G is observed in the doped sample after illumination with 2.8 eV light. Concentration of the center was estimated to be 10^{17} cm^{-3} while secondary ion mass spectroscopy revealed Mg and O levels of 10^{16} cm^{-3}, Si, C, and Be levels of 10^{17} cm^{-3}. Time-dependent photo-EPR data were well fit by a single defect-to-band transition model with a defect level of 0.67 eV above the valence band. This value is close to that predicted for the Be acceptor. Together with the similar concentrations of the EPR center and Be, the data suggest that the signal may be due to the accidental Be; however, a review of the literature suggests additional possibilities, such as a vacancy-related defect.

9:48AM F14.00008 Computational nano-material design of exotic luminescent materials based upon europium doped gallium nitrides, AKIRA MASAGO, TETSUYA FUKUSHIMA, Graduate School of Engineering Science, Osaka University, KAZUNORI SATO, Graduate School of Engineering, Osaka University, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University — Eu-doped GaN has attracted much attention, because the red light luminescence ability provides us with expectations to realize monolithic full-color LEDs, which work on seamless conditions such as substrates, electrodes, and operating bias voltages. Toward implementation of multifunctional activity into the luminescent materials using the spinoidal nano-structures, we investigate atomic configurations and magnetic structures of the GaN crystal codoped with Eu, Mg, Si, O, and/or the vacancies using the density functional method (DFT) calculations. Our calculations show that the impurity clustered distributions are energetically favorable more than the homogeneous distribution. Moreover, analyses of the formation energy and binding energy suggest that the clustered distributions are spontaneously formed by the nano-spinoidal decomposition. Though the host matrix has no magnetic moments, the cluster has finite magnetic moments, where Zener’s p–f exchange interaction works between the Eu f-state and the nearby np-states.

10:00AM F14.00009 Stabilization of free-standing GaN foils by threading edge dislocations, ROMAN GRÖGER, Institute of Physics of Materials and CEITEC IPM, Academy of Sciences of the Czech Republic, LUCIEN LECONTE, Université Lille 1, France — Computational studies of core structures of 1/3(1120) threading edge dislocations in bulk GaN predict the existence of a 5/7-atom ring configuration when viewed along the [001] direction. While this agrees with recent high-resolution electron microscopy observations, previous studies also reveal the existence of an 8-atom ring configuration. We employ molecular statics calculations to show that the core stability of the threading edge dislocation in free-standing GaN foils depends on the foil thickness and the terminations of their surfaces. For the foil thickness above 6 nm, the edge dislocation is predicted to possess the 5/7-atom ring core structure. However, with decreasing thickness and depending on surface terminations the minimum energy core structure may change to both 8-atom ring and 4-atom ring configurations. By quantifying the interaction energy of the dislocation with the surface of the foil, we show that there exist conditions for which the threading edge dislocation in the foil is more stable than in the bulk.

10:12AM F14.00010 Atomic and electronic structures of (GaN)_{1-x}(ZnO)_{x} alloys: the role of short-range order, JIAN LIU, PHILIP ALLEN, State Univ of NY- Stony Brook — (GaN)_{1-x}(ZnO)_{x} solid solution is a promising photocatalyst for efficient water splitting under visible illumination. For theoretical modeling, the special quasirandom structure (SQS) method which assumes random site occupancy is widely used. We have previously shown, with density-functional theory (DFT) total energy calculations, cluster expansion, and Monte Carlo simulations, that short-range order (SRO) is significant due to the non-isovalency. Thus it is desirable to include SRO in the construction of supercells. Inspired by the SQS method, we construct the “special quasi-ordered structure” (SQoS) supercells. Subsequent DFT calculations show that the atomic and electronic structures of SQS and SQoS alloys differ significantly. The SRO and (x,T) dependence of the valence band maximum stem mainly from the anti-bonding hybrids of N2p and Zn3d states. This suggests the possibility of engineering the band gap by tuning SRO. We also explore bond length distribution and bond angle variation over the composition-temperature (x,T) phase space using bond valence method (BVM). The validity of our BVM model is tested by DFT total energy calculations.

1 Supported by DOE grant No. DE-FG02-08ER46550.

10:24AM F14.00011 EPR detected defect center in bulk GaN substrates grown by high pressure nitrogen solution method, J. DASHDORJ, M.E. ZVANUT, Univ of Alabama - Birmingham, M.M. BOCKOWSKI, Institute of High Pressure Physics, Poland — Growth of high quality, free-standing GaN substrates is essential for further improvement of nitride device performance. Unfortunately, many bulk growth methods introduce unacceptable amounts of O donors. Samples studied in this work were grown by the high-pressure nitrogen solution method on (0001) sapphire with Mg-doped GaN substrates characterized by 4 K electron paramagnetic resonance (EPR) spectroscopy. No EPR signal is detected in the undoped samples. However, a nearly isotropic spectrum with g-value of 1.984 and a line-width of 120 G is observed in the doped sample after illumination with 2.8 eV light. Concentration of the center was estimated to be 10^{17} cm^{-3} while secondary ion mass spectroscopy revealed Mg and O levels of 10^{16} cm^{-3}, Si, C, and Be levels of 10^{17} cm^{-3}. Time-dependent photo-EPR data were well fit by a single defect-to-band transition model with a defect level of 0.67 eV above the valence band. This value is close to that predicted for the Be acceptor. Together with the similar concentrations of the EPR center and Be, the data suggest that the signal may be due to the accidental Be; however, a review of the literature suggests additional possibilities, such as a vacancy-related defect.

1 This work is supported by NSF.

Tuesday, March 3, 2015 8:00AM - 10:48AM — Session F15 DMP: Focus Session: Exciton and Electron Transport in Nanostructures 008B - Richard Haglund, Vanderbilt University

8:00AM F15.00001 Exciton Transport in Nanostructured Solids, VLADIMIR BULOVIC, M.I.T. — Transport of nanoscale energy in the form of excitons is at the core of operation of nanostructured optoelectronic devices such as solar cells, light-emitting diodes and excitonic transistors. Of particular importance is the relationship between exciton transport and bandcage disorder, the defining characteristic of molecular and nanostructured materials. The talk will present recent advancements in directly visualizing exciton transport, with spatial, temporal and spectral evolution recorded for molecular crystals, disordered thin films, and colloidal quantum dot solids. Our measurements demonstrate that the mechanism of exciton transport depends strongly on the nanostructure morphology and the design of nanoscale building blocks. In addition, the talk will show that the excitonic energy landscape can be directly manipulated in solid-state thin films using dipole–dipole interactions, which can be increased under mechanical pressure, or molecular doping with polar molecules, leading to dramatic shifts in the exciton energy structure.
8:36AM F15.00002 Spectral Road Map of Strain-Split Bulk GaAs Excitons: Evidence of Excitation-Induced Dephasing. DANIEL WEBBER, KIMBERLEY HALL, Dalhousie University, BRIAN WILMER, ALAN BRISTOW, West Virginia University, XINYU LIU, MARGARET DOBRWOLSKA, JACEK FURDYNA, University of Notre Dame — Thin films of bulk GaAs studied with two-dimensional coherent spectroscopy reveal strain-split heavy- (HH) and light-hole (LH) excitons with quantum interference. Excitation overlapping the HH continuum show strong excitation-induced dephasing (EID) and emission at the HH exciton for collinear polarization. The results are consistent with excitations beyond the perturbative $\chi^{(3)}$ regime. Cross-linear polarization suppresses the HH emission and enhances the LH exciton as well as HH bie exciton emission. Two-quantum spectra at low excitation concentrations are also consistent with HH and LH exciton interference and EID. Results are compared to four-wave mixing transients that require modelling for interpretation.

8:48AM F15.00003 Nonlinear, driven-dissipative hydrodynamics and effective chiral description of an exciton-polariton superfluid. MANAS KULKARNI, GERMAN KOLMAKOV, New York City College of Technology, City University of New York — Given recent remarkable experimental success on capturing hydrodynamic features of exciton-polariton condensates in optical microcavities and their potential implications for quantum and optical computing and information technologies, we present an effective chiral description for such systems. This description captures the fingerprints of hydrodynamics, namely, nonlinearity, dispersion and dissipation in the exciton-polariton system. The resulting chiral equation for the condensate perturbation wave dynamics is found to be of Burgers-type thereby providing a more transparent understanding of the complicated underlying coupled exciton-photon dynamics. By using analytical calculations and numerical simulations, we describe the phenomenon of polariton shock waves, solitons and defects in such systems. Our mapping is expected to have broad implications for other polariton and photon systems including dipolar exciton and magnon condensates. This mapping can further help one in engineering a delicate balance between the pump and damping to produce stable optical signals propagating in polariton circuits.

9:00AM F15.00004 Recipe for Topological Polaritons1, TORSTEN KARZIG, CHARLES-EDOUARD BARDYN, Caltech, NETANEEL LINDNER, Technion, GIL REFAEL, Caltech — The interaction between light and matter can give rise to novel topological states. This principle was recently exemplified in Floquet topological insulators, where classical light was used to induce a topological electronic band structure. Here, in contrast, we show that mixing single photons with excitons can result in new topological polaritonic states — or “topolaritons”. Taken separately, the underlying photons and excitons are topologically trivial. Combined appropriately, however, they give rise to non-trivial polaritonic bands with chiral edge modes allowing for unidirectional polariton propagation. The main ingredient in our construction is an exciton-photon coupling with a phase that winds in momentum space. We demonstrate how this winding emerges from spin-orbit coupling in the electronic system and an applied Zeeman field. We discuss the requirements for obtaining a sizable topological gap in the polariton spectrum.

1funded by the Institute for Quantum Information and Matter, the Bi-National Science Foundation and I-Core: the Israeli Excellence Center “Circle of Light”, and Darpa under funding for FENA, and the Swiss National Science Foundation.

9:12AM F15.00005 Topological Polaritons and Excitons in Garden Variety Systems1, CHARLES-EDOUARD BARDYN, TORSTEN KARZIG, GIL REFAEL, Caltech, TIM LIEW, Nanyang Technological University — Topological polaritons (aka topolaritons) present a new frontier for topological behavior in solid-state systems. They combine light and matter, which allows to probe and manipulate them in a variety of ways. They can also be made strongly interacting due to their excitonic component. Here we present a scheme which allows to realize topolaritons in garden variety zinc-blende quantum wells. Our proposal requires a moderate magnetic field and a potential landscape which can be implemented, e.g., via surface acoustic waves or patterning. We identify indirect excitons in double quantum wells as a particularly appealing alternative for topological states in exciton-based systems. Indirect excitons are robust and long lived (with lifetimes up to milliseconds), and, therefore, provide a flexible platform for the realization, probing, and utilization of topological coupled light-matter states.

1Funded by: Institute for Quantum Information and Matter, Swiss National Science Foundation, Packard Foundation, NSF.

9:24AM F15.00006 Excitonic condensation in spatially separated 1D systems1, DAVID ABERGEL, NORDITA — We introduce the concept of excitonic condensation between spatially separated ground state populations of 1D electrons and holes mediated by their attractive direct Coulomb interaction. Candidate systems for observing this phenomenon include semiconductor quantum wires, core-shell nanowires, stacked graphene nanoribbons, and carbon nanotubes. We focus on the core-shell nanowire system and present calculations of the excitonic gap (which characterizes the stability of the condensate) and the critical temperature of the condensate. We also discuss additional effects such as the dependence on the material parameters, the presence of multiple bands, and spin or valley degeneracy. We show that 1D systems may have substantial improvement in the critical temperature of the condensate over comparable 2D systems because the screening of the inter-layer Coulomb interaction is weaker.

1This work was supported by ERC DM-321031 and by Nordita.

9:36AM F15.00007 Kondo Physics in 4f metals: Gadolinium nanocontacts. BERNAT OLIVERA, CARLOS UNTIEDT, University of Alicante (Spain), ELKE SCHEER, University of Konstanz (Germany) — The study of electron transport in conducting materials at the nanoscale can be carried out by using Scanning Tunneling Microscope (STM) and Mechanically Controllable Break Junction techniques (MCBJ). At such scales, Kondo effect vanishes the magnetic properties of the 3d transition metals Fe, Co and Ni. The 4f rare earth metals are an interesting aim of study because of their strong magnetic properties among other things. At our laboratories we have measured gadolinium with both STM and MCBJ techniques. This work is supported by the LDRD program at ORNL. Portion of this research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

9:48AM F15.00008 Theory of space charge limited currents in films and nanowires with dopants1, XIAOGUANG ZHANG, Department of Physics and Quantum Theory Project, University of Florida, SOKRATES PANTELIDES, Department of Physics and Astronomy, Vanderbilt University — We show that proper description of the space charge limited currents (SCLC) in a homogenous bulk material must account fully for the effect of the dopants and the interplay between dopants and traps [1]. The sharp rise in the current at the trap-filled-limit (TFL) is partially mitigated by the dopant energy levels and the Frenkel effect, namely the lowering of the ionization energy by the electric field, which is screened by the free carriers. In nanowires, lack of effective screening causes the trap occupation at small biases to reach a high level comparable to the TFL in bulk. This explains the high current density in SCLCs observed in nanowires. [1] X.-G. Zhang and S. T. Pantelides, Phys. Rev. Lett. 108, 266602 (2012).

1This work is supported by the LDRD program at ORNL. Portion of this research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.
10:00AM F15.00009 Long Minority Carrier Diffusion Lengths in Bridged Silicon Nanowires¹. DONG YU, MARK TRIPPLETT, YIMING YANG, UC Davis, FRANCOIS LEONARD, ALEC TALIN, Sandia National Lab, SAIF ISLAM, UC Davis — Nanowires have large surface areas which create new challenges for their optoelectronic applications. Lithographic processes involved in device fabrication and substrate interfaces can lead to surface defects and substantially reduce charge carrier lifetimes and diffusion lengths. Here, we show that using a bridging method to suspend pristine nanowires allows for circumventing detrimental fabrication steps and interfacial effects associated with planar device architectures. We report electron diffusion lengths up to 2.7 µm in bridged silicon nanowire devices, much longer than previously reported values for silicon nanowires with a diameter of 100 nm. Strikingly, electron diffusion lengths are reduced to only 45 nm in planar devices incorporating nanowires grown under the same conditions. The highly scalable and low-cost silicon nano-bridge devices with the demonstrated long diffusion lengths may find exciting applications in photovoltaics, image sensing and photodetectors.

1DMD-1310678, CMMI-1235592, DEAC01-94-AL85000

10:12AM F15.00010 Analytical Perturbative Treatment of Multiterminal Nonequilibrium Anderson Impurity Models¹. NOBUHIKO TANIGUCHI, University of Tsukuba — We investigate analytically the nonequilibrium Anderson impurity model connecting with multiterminal leads. Within the validity of the second-order perturbation regarding the interaction strength, the full dependence on frequency and bias voltage of the nonequilibrium self-energy and spectral function is determined for a generic multiterminal setting where the current preservation has been an issue. Our analytical perturbative treatment respects the current conservation as well as the spectral sum rule, and it encompasses Fermi-liquid and non-Fermi-liquid behaviors, showing that increasing finite-bias voltage leads to a crossover from the Kondo resonance to the Coulomb blockade phenomena. Analysis on two-terminal and multiterminal settings shows that finite-bias voltage does not split the Kondo resonance in this order; no specific structure due to multiple leads emerges in the spectral function. Overall bias dependence is quite similar to finite-temperature effect, which could be understood by help of the Ward identity and the limit of $N \gg 1$ terminals.

¹Grant-in-Aid for Scientific Research (No.26060032, MEXT, Japan).

10:24AM F15.00011 Kondo effects and interference in transport through single molecules, JENS PAASKE, KIM GEORG LIND PEDERSEN, PER HEDEGAARD, The Niels Bohr Institute, University of Copenhagen — Quantum transport through single molecules or quantum dot arrays with spin-degenerate ground states can be dominated by Kondo effects at low temperatures. In contrast to the single impurity case, quantum interference plays a significant role in such ‘multi-orbital’ systems and may have a strong influence on the possible Kondo physics: deciding between single- or multi-channel screening and even ferromagnetic Kondo effect. We investigate a range of smaller molecules with source, and drain electrodes attached in different specific contacting geometries. The interacting pi-electron system is treated by means of exact diagonalization, and combining with a perturbative treatment of molecule-lead tunnel couplings, we calculate the zero-bias cotunneling conductance as a function of a gate-voltage shifting the Fermi level across a time dependent impurity in a linear chain are studied theoretically using the Floquet formalism. We obtain the exact reflection coefficient for a wide range of parameters. Our results compare well with known approximations in the high frequency regime. Furthermore, at lower frequencies we observe new features and a significant departure from the approximated predictions. Below a well defined frequency the impurity couples waves of differing $k$-values. As a result, the impurity not only splits the incident wave into a transmitting and a reflecting part of the same wave number $k$, but also waves of differing $k$ emerge from the perturbed site. The amplitude of these waves is also obtained.

10:36AM F15.00012 Quantum transport in linear chains under periodic perturbations, DANIEL THUBERG, SEBASTIAN REYES, Facultad de Física, Pontificia Universidad Católica de Chile, Avda.Vicuña Mackenna 4860, Macul, Santiago, Chile, SEBASTIAN EGGERT, Department of Physics, Univ. Kaiserslautern, Erwin Schrodinger Str., D-67663 Kaiserslautern, Germany — Quantum transport properties across a time dependent impurity in a linear chain are studied theoretically using the Floquet formalism. We obtain the exact reflection coefficient for a wide range of parameters. Our results compare well with known approximations in the high frequency regime. Furthermore, at lower frequencies we observe new features and a significant departure from the approximated predictions. Below a well defined frequency the impurity couples waves of differing $k$-values. As a result, the impurity not only splits the incident wave into a transmitting and a reflecting part of the same wave number $k$, but also waves of differing $k$ emerge from the perturbed site. The amplitude of these waves is also obtained.

Tuesday, March 3, 2015 8:00AM - 10:48AM — Session F16 DMP DCOMP: Focus Session: Search for New Fe-based Superconductors I 101AB
- Qiang Li, Brookhaven National Laboratory

8:00AM F16.00001 Why are the Tc,s so high in rare-earth doped CaFe2As2 single crystals and ultrathin FeSe epi-films?¹. C.W. CHU, TCSUH and Department of Physics, University of Houston — Recent reports of non-bulk superconductivity with unexpectedly high onset-Tc,s up to 49 K in the Pr-doped CaFe2As2 [(Ca,Pr)122] single crystals [1] and up to 100 K in one-unit-cell (1UC) FeSe epi-films [2], respectively, offer an unusual opportunity to seek an answer to the question posed in the title. Through systematic compositional, structural, resistive, and magnetic investigations on (Ca,R)122 single crystals with R = La, Ce, Pr, and Nd, we have observed a doping-level-independent Tc, a large magnetic anisotropy, and the existence of mesoscopic-2D structures in these crystals, thus providing evidence consistent with the proposed interface-enhanced Tc in these naturally assembled Fe-based superconductors. Similar resistive and magnetic measurements were also made on the 1-4UC FeSe ultra thin epi-films. We have detected a Meissner state below 1 Oe with extensive weak-links up to ∼ 100 K, unconnected small superconducting patches up to ∼ 40 K, and an unusual dispersion of diamagnetic moment with frequency up to 80 K. The unusual frequency dependences of the diamagnetic moment observed in the films at different temperature ranges suggest that collective excitations of electron and/or spin nature may exist in the FeSe films below 20 K and 40-80 K. The experimental results will be presented and the implications discussed.


¹Collaborators: Liangzi Deng, Bing Lv, Fengyan Wei, and Yu-Yi Xue, University of Houston; Li-Li Wang, Xu-Cun Ma, and Qi-Kun Xue, Tsinghua University, Beijing.
K-doping takes place at the spacing layer while FeAs layers remain intact. In contrast, Co substitution in BaFe$_2$As$_2$ hole asymmetry in the phase diagram of iron-based superconductors is well illustrated in doped BaFe$_{1+y}$As$_2$. The electron-to-conduction electron ratio in these systems is close to 1, which plays a crucial role in the electron-hole asymmetry. In this talk, I will present the magnetic and structural transitions of La$_{0.2}$Ba$_{1.8}$Fe$_2$As$_2$, La$_{0.5-x}$Na$_{0.5+x}$Fe$_2$As$_2$, or even compounds with other rare earth and alkali ions in the spacing layer, provides a new material platform for the study of iron-based superconductors. The material could be tuned from electron-doped to hole-doped by varying the ratio between the alkali metal and rare earth ions.

9:00AM F16.00004 The structural and magnetic phase transitions in a “parent” Fe pnictide compound. NI NI, Department of Physics and Astronomy, University of California, Los Angeles, JARED ALLRED, Materials Science Division, Argonne National Laboratory, HUJBIO CAO, WEI TIAN, Quantum Condensed Matter Division, Oak Ridge National Laboratory, LIAN LIU, Department of Physics, Columbia University, KYUIL CHOI, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, MATTHEW KROGSTAD, Materials Science Division, Argonne National Laboratory, JIE MA, Quantum Condensed Matter Division, Oak Ridge National Laboratory, KEITH TADDEI, Materials Science Division, Argonne National Laboratory, MAKARIY TANATAR, RUSLAN PROZOROV, Ames laboratory and Department of Physics and Astronomy, Iowa State University, MASAAKI MATSUDA, Quantum Condensed Matter Division, Oak Ridge National Laboratory, STEPHAN ROSENKRANZ, Materials Science Division, Argonne National Laboratory, YASUTOMO UEMURA, Department of Physics, Columbia University, SHAN JIANG, Department of Physics and Astronomy, University of California, Los Angeles — We will present transport, thermodynamic, synchrotron X-ray, neutron diffraction, SR, ARPES and polarized optical image measurements on the “parent” compound of the 112 high Tc superconducting Fe pnictide family. Structural and magnetic phase transitions are revealed. Detailed magnetic structure was solved by single crystal neutron diffraction. We will discuss the similarity and difference of these transitions comparing to the parent compounds of other Fe pnictide superconductors.

9:12AM F16.00005 Study on the non-bulk superconductivity in CaFe$_{2-x}$As$_2$ single crystals under different annealing conditions. K. ZHAO, B. LV, I. Z. DENG, Y. Y. XUE, Texas Center for Superconductivity and Department of Physics, University of Houston, C. W. CHU, Texas Center for Superconductivity and Department of Physics, University of Houston, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley — The interplay between SDW and tetragonal/collapsed tetragonal (Tc/T) structural transition in CaFe$_{2-x}$As$_2$ single crystals under different annealing conditions has been thoroughly investigated, while the occurrence of filamentary superconductivity with Tc ~ 10K remains mysterious. In this talk, I will present our studies on the interplay of magnetism, structural transition, and superconductivity in the undoped CaFe$_{2-x}$As$_2$ single crystals obtained under different synthetic conditions and annealing procedures. The dihedral shift has been detected for the first time and taken as an evidence of superconducting High temperature annealing and temperature annealing driving CaFe$_{2-x}$As$_2$ into the cT ground state and the T ground state, respectively. The superconducting signal is maximized in the condition where the sample reaches the unstable region at the border of these two. The detailed results and their implications will be presented and discussed.

9:24AM F16.00006 First-principles study on the specific heat of optimally hole-doped BaFe$_2$As$_2$ compound. HYUNGJU OH, SINISA COH, MARVIN L. COHEN, UC Berkeley, Lawrence Berkeley National Laboratory — We present density functional calculation of optimally K-doped BaFe$_2$As$_2$, including a modification of the GGA potential by adding a repulsive term (GGA + A). We tune the additional repulsive term until the occupied bandwidth of the M-point pocket agrees with experimental data. The calculated Sommerfeld coefficient and electron-phonon coupling constant yield a theoretical specific heat coefficient comparable to the experimental one. In addition, overall band structure and Fermi surface topology are improved with respect to the experiment. This work was supported by NSF Grant No. DMR10-1006184 and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by the DOE at Lawrence Berkeley National Laboratory’s NERSC facility.

9:36AM F16.00007 High-temperature superconductivity from fine-tuning of Fermi-surface singularities in iron oxypnictides. ALIAKSEI CHARNUKHA, Physics Department, University of California - San Diego, La Jolla, CA 92093, USA — In the family of iron-based superconductors, 1111-type materials exhibit superconductivity with the highest transition temperature Tc=55K. Early theoretical predictions of their electronic structure revealed multiple large circular sheets of the Fermi surface. Here we use ARPES to show that two prototypical compounds of the 1111 type are at odds with this description. Their low-energy band structure is formed by the edges of several bands, which are pulled to the Fermi level from the depths of the theoretically predicted band structure by strong electronic interactions. We further demonstrate that although their low-energy electronic looks remarkably similar, the Tc differs by a factor of 2. Upon closer examination we uncover that one of the bands in the higher-Tc compound sinks to 2.3meV below the Fermi level and thus does not produce a Fermi surface. And yet we find that it hosts a superconducting energy gap 10x larger than the same band in the lower-Tc sister compound. Our results show that the Fermi-surface singularities in the iron-oxypnictides dramatically affect their low-energy electronic properties, including superconductivity, and must therefore be explicitly taken into account in any attempt to understand the pairing mechanism.

9:48AM F16.00008 Mott Kondo Insulating Behavior in Iron-Oxylachalogenides. BYRON FREELON, Physics Department, Massachusetts Institute of Technology, Cambridge, MA, YUHAO LIU, Lawrence Berkeley National Laboratory, JUNG-LENG CHEN, Department of Physics, Tamkang University, LUIS CRACO, Instituto de Fisica. Universidad Federal de Mato Grosso, Curitiba, Brazil, MUKUL LAAD, The Institute of Mathematical Sciences, CIT Campus, Chennai, India, STEFANO LEONI, School of Chemistry, Cardiff University, JIAQI CHEN, LI TAO, MINGHU FANG, Department of Physics, Zhejiang University, Hangzhou, China, RXOKAN FLAUA, ZAHRAN YAMANI, Canadian Neutron Beam Centre, Canadian Neutron Beam Centre, National Research Council, Chalk River Labs, Chalk River Ontario, Canada, YI-SHENG LIU, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, CHINGLIN CHANG, Department of Physics, Tamkang University, J.-H. GUO, ZAHID HUSSAIN, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA — The findings of unconventional high-Tc superconductivity (HTSC) in Fe arsenides and selenides have reinvigorated HTSC research. The outstanding debate over how the normal state gives way to HTSC in cuprates has emerged in discussions on possible HTSC mechanisms in Fe-based superconductors. Does Fe-based HTSC result as a pairing instability of a conventional Landau-Fermi liquid (NFL), or as one of a non-NFL, akin to the cuprates? One possible way to address this important question is to investigate Fe-based materials that exhibit a Mott insulating parent phase as in the cuprates. Here we present a study of such materials. We performed a combined experimental-theoretical investigation of the Fe-oxylachalogenides (FeOCh) series La$_2$O$_2$Fe$_2$O$_{12}$ (M =S, Se), the latest among the Fe-based materials with the potential to show unconventional high-Tc superconductivity (HTSC).
10:00AM F16.00009 Correlation effects in KFe$_2$As$_2$, RbFe$_2$As$_2$ and CsFe$_2$As$_2$. STEFFEN BACKES, HARALD O. JESCHKE, ROSER VALENTI, University Frankfurt — We perform a systematic LDA+DMFT study of the iron-pnictide series KFe$_2$As$_2$, RbFe$_2$As$_2$ and CsFe$_2$As$_2$ and compare with available experiments. We find not only strong orbital-dependent renormalizations and Fermi surface topology changes compared to the local-density approximation but also interesting features at higher binding energies. We discuss the observation of a possible orbitally-selective instability as a function of isoelectronic doping.  

$^1$Research funded within DFG SPP 1458.


$^3$Backes et al., in preparation

10:12AM F16.00010 Electronic Properties of Fe-based Ladder Compounds, FEI DU, Jilin University, KENYA OHGUSHI, Tohoku University, YUTAKA UEDA, Toyota Physical and Chemical Institute — The crystal structure of Fe-based superconductors found so far have two-dimensional conducting planes composed of a square lattice of Fe atoms coordinated tetrahedrally by pnictogens or chalcogens. Although there is no report on the discovery of superconductivity in Fe-based materials with one-dimensional structures, elucidating electronic states of such compounds is expected to give an important clue to the mechanism of superconductivity as well as a strong hint for searching new superconductors. We here report on electronic properties of a series of quasi-one-dimensional spin-ladder compounds AFe$_2$X$_2$ ($A = K$, Cs, Ba; $X = S, Se$) with a special focus on a solid-solution AFe$_2$($S_1-x$,$Se_x$)$_3$. We demonstrate that fruitful electronic states emerge as a consequence of the strong electron correlation effect and quantum fluctuations in a low dimensional crystal structure. The following is the list of papers directly related to this talk: [1] Y. Nambu, et al., Phys. Rev. B, 85 064413 (2012). [2] F. Du, et al, Phys. Rev. B 85, 214436 (2012). [3] F. Du, et al, Phys. Rev. B 90, 085143 (2014).

10:24AM F16.00011 H$_2$O(0) and the Kondo Effect in FeSe$_{0.7}$Te$_{0.9}$ Epitaxial Films, NICHOLAS CORNELL, ANVAR ZAKHIDOV, UT Dallas, MARCELO JAIME, MPA-CMMS, LANL, JUIE HUANG, HAYAN WANG, TAMU, MYRON SALAMON, UT Dallas — High-quality, [001]-oriented epitaxial films of FeSe$_{0.7}$Te$_{0.9}$ have been grown on SrTiO$_3$. They are found to have increased critical temperatures and critical fields relative to both bulk samples and thin films of the sister compound, FeSe$_{0.5}$Te$_{0.5}$. Critical field values in excess of 114 T have been reported based on WHH theory. In addition to these improved properties, some samples show resistance minima above Tc, reminiscent of the Kondo effect, presumably from excess Fe. We report results of a high field investigation of these thin films that reveals an empirical zero-temperature value of H$_c2(0)$ ≈ 46 T along [001], significantly less than the WHH estimate, but still exceeding the maximum strong coupling correction to the Pauli limit. Large negative magnetoresistance above the critical field confirms the presence of Kondo behavior in the normal state and persists without saturation up to 60 T. Why the measured critical field exceeds the paramagnetic limit remains a question. However, a Kondo temperature that exceeds the superconducting Tc can lead to overestimated WHH upper critical fields and could explain the wide variation in Tc and H$_c2$ among the “11” iron chalcogenides.

10:36AM F16.00012 High Critical Field Superconductivity in FeSe$_{0.1}$Te$_{0.9}$ Coated Carbon Nanotubes, HAIYAN WANG, post doc. NICHOLAS CORNELL, Professor, Texas A&M University, JUIE HUANG, graduate student in TAMU, MYRON SALAMON, ANVAR ZAKHIDOV, Professor of Physics, University of Texas at Dallas, ANVAR ZAKHIDOV AND HAIYAN WANG TEAM, UTD AND TAMU AFSOR TEAM — Thin films of FeSe$_{0.1}$Te$_{0.9}$, grown on SrTi03, have been shown to possess an increased critical temperature, field, and current relative to both bulk samples of FeSe$_{0.1}$Te$_{0.9}$ and thin films of the related compound FeSe$_{0.5}$Te$_{0.5}$. Empirical measurement of FeSe$_{0.1}$Te$_{0.9}$ thin films reveal a zero temperature Hc2(0) ~ 45T. Carbon nanotubes are a promising lightweight flexible material for superconducting applications and have proven a robust substrate when conformally coated by superconducting MgB2. Thin film coatings of FeSe$_{0.1}$Te$_{0.9}$ have been deposited via pulsed laser deposition on dry-drawn multiwall carbon nanotube sheets drawn from CVD grown forests. While true zero resistance isn’t achieved due to inter-connectivity issues or junction effects in multiwall CNT case, clear superconducting transitions with R reaching zero can be seen on other single wall CNT, and non-oriented carbon nanotube substrates. Properties of these superconducting FeSe$_{0.1}$Te$_{0.9}$@SWCNT thin films are discussed.

Tuesday, March 3, 2015 8:00AM - 11:00AM
Session F17 DMP: Focus Session: Two-dimensional Materials Design 102AB - Aleskey Kolmogorov, Binghamton University, SUNY

8:00AM F17.00001 New two dimensional compounds: beyond graphene, SEBASTIEN LEBEGUE, CRM2 Laboratory, Jean Barriol Institute, Nancy — In the field of nanosciences, the quest for materials with reduced dimensionality is only at its beginning. While a lot of effort has been put initially on graphene, the focus has been extended in the last past years to functionalized graphene, boron nitride, silicene, and transition metal dichalcogenides in the form of single layers. Although these two-dimensional compounds offer a larger range of properties than graphene, there is a constant need for new materials presenting equivalent or superior performances to the ones already known. Here I will present an approach that we have used to discover potential new two-dimensional materials. This approach corresponds to perform datamining in the Inorganic Crystal Structure Database using simple geometrical criteria, and allowed us to identify nearly 40 new materials that could be exfoliated into two-dimensional sheets. Then, their electronic structure (density of states and bandstructure) was obtained with density functional theory to predict whether the two-dimensional material is metallic or insulating, as well as if it undergoes magnetic ordering at low temperatures. If time allows, I will also present some of our recent results concerning the electronic structure of transition metal dichalcogenides bilayers.

8:36AM F17.00002 New-class of Semiconducting 2D materials: Tin Dichalcogenides (SnX2), CAN ATACA, Department of Materials Science and Engineering, Massachusetts Institute of Technology, KEDI WU, School for Engineering of Matter, Transport and Energy, Arizona State University, KAYAHAN SARITAS, Department of Materials Science and Engineering, Massachusetts Institute of Technology, SEFAATTIN TONGAY, School for Engineering of Matter, Transport and Energy, Arizona State University, JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology — Recent studies have focused on a new generation of atomically thin films of semiconducting transition metal dichalcogenides (MX2) have been fabricated and investigated in monolayer, bilayer and few layer form. In this work, we investigated the electronic, optical and elastic properties of single and few layer and bulk SnX2 ($X=S$, Se) both theoretically and experimentally. Using density functional theory (DFT) we carried out stability analysis through phonon and electronic, optical and elastic structure calculations. Single-layer SnX2s are mechanically exfoliated and Raman and photoluminescence (PL) measurements are taken. UV-Vis absorption spectrum together with PL measurements and DFT calculations yield an indirect gap of ~ 2.5 eV for SnS2 and SnSe structures (bulk). Tunability of the energy band gap and indirect-direct gap transitions are investigated by controlling the number of layers and applied stress. Lowering the number of layers decreases the indirect gap (0.4-0.3 eV), but indirect-direct gap transition occurs when layer-layer distance is reduced. Due to flexibility in engineering the electronic and optical properties, SnX2 compounds are promising materials for future optoelectronic nanoscale applications.
8:48AM F17.00003 Computational design of p-type contacts for MoS$_2$-based electronic devices

PRIYANK KUMAR, Massachusetts Institute of Technology, TIZIANA MUSSO, ADAM FOSTER, Aalto University, JEFFREY GROSSMAN, Massachusetts Institute of Technology — The excellent physical and semiconducting properties of transition metal dichalcogenide (TMDC) monolayers make them promising for many applications. A well-known example is MoS$_2$, which has gained significant attention as a channel material for next-generation transistors. While n-type MoS$_2$ field-effect transistors (n-FETs) can be fabricated with relative ease, fabrication of p-FETs remains a challenge as the Fermi-level of elemental metals used as contacts are pinned close to the conduction band, leading to large p-type Schottky barrier heights (SBHs). Using \textit{ab initio} computations, we model and propose efficient hole contacts utilizing high work function oxide-based hole injection materials, with the aim of advancing p-type MoS$_2$ device technology. Our calculations will highlight the possibility to tune and lower the p-type SBH at the metal/semiconductor interface by controlling the structural properties of oxide materials. Taken together, our results provide an interesting platform for experimental design of next-generation MoS$_2$-based electronic and optoelectronic devices.

9:00AM F17.00004 Computational Design of 2D materials for Energy Applications

QIANG SUN, Peking University — Since the successful synthesis of graphene, tremendous efforts have been devoted to two-dimensional monolayers such as boron nitride (BN), silicene and MoS$_2$. These 2D materials exhibit a large variety of physical and chemical properties with unprecedented applications. Here we report our recent studies of computational design of 2D materials for fuel cell applications which include hydrogen storage, CO$_2$ capture, CO conversion and O$_2$ reduction.

9:12AM F17.00005 Systematic Enumeration of sp$^3$ Nanotethroes and Computational Study of their Properties

ENSNI XU, PAUL E. LAMMERT, Department of Physics, Pennsylvania State University, VINCENT H. CRESPI, Department of Physics, Material Science and Engineering and Chemistry, Pennsylvania State University — A novel 1D allotrope of carbon arise from slow decompression of solid benzene in high-pressure (GPa) cells, wherein columns of benzene, guided by “topochemical” constraint as six-valent 1D super-atoms, rehybridize into a crystal of sp$^3$ nanotethroes. We exhaustively enumerate the allowed hexavalent bonding topologies and discovered several new low-energy allotropes not previously described. The intermediate conformational nature of these systems — stiffer than a polymer, more reconfigurable than a nanowire or nanotube — allows the translational repeat unit for interatomic connectivity (“topological unit cell”) to deviate from the crystallographic unit cell. A topological unit of 12 carbons accommodates thirty-seven distinct chemically stable nanotethroes, fourteen of which are within 80 meV/carbon of the most stable member. Careful optimization of apriori helicity reveals the most stable structures to be chiral; several are stiffer (per carbon atom) than bulk diamond. They have the large gaps of saturated hydrocarbons, but reasonable routes exist towards producing semiconducting variants. We generalize Euler’s rules for ring counting to cover these systems, and propose a naming convention that can be generalized to handle a broad range of progenitor molecules.

9:24AM F17.00006 ABSTRACT WITHDRAWN

9:36AM F17.00007 A Pentagon Based Carbon Sheet

QIAN WANG, SHUNHONG ZHANG, Center for Applied Physics and Technology, Peking University, JIAN ZHOU, Physics Department, Virginia Commonwealth University, XIAOSHUANG CHEN, Shanghai Institute of Technical Physics, Chinese Academy of Science, YOSHIIKU KAWAZOE, Institute for Material Research, Tohoku University, Japan, PURU JENA, Physics Department, Virginia Commonwealth University, A INTERNATIONAL TEAM COLLABORATION — A new two-dimensional (2D) meta-stable carbon allotrope, penta-graphene, composed entirely of carbon pentagons and resembling the Cairo pentagonal tiling, is proposed. State-of-the-art theoretical calculations confirm that the new carbon polymorph is not only dynamically and mechanically stable, but also can withstand temperatures as high as 1000 K. Due to its unique atomic configuration penta-graphene has an unusual negative Poisson’s ratio (NPR) and ultra-high ideal strength that can even outperform graphene. Furthermore, unlike graphene that needs to be functionalized for opening a band gap, penta-graphene possesses an intrinsic quasi-direct band gap as large as 3.25 eV - close to that of ZnO and GaN. Equally important, when rolled up, penta-graphene can form a pentagon-based nanotube. The resulting penta-carbon nanotubes are semiconducting regardless of their chirality. When stacked in different patterns, dynamically and thermally stable 3D twin structures of T12-carbon are generated with band gaps even larger than that of T12-carbon. The versatility of penta-graphene and its derivatives are expected to have broad applications in nanoelectronics and nanomechanics.

9:48AM F17.00008 The size and shape dependence of graphene domain on the band gap of h-BN

CHERNO B. KAH, SALLIYA KIRIGEENAHAGE, LYLE SMITH, MING YU, CHAKRAM JAYANTHI, SHIYU WU, University of Louisville — This talk will report the structure and electronic characteristics of graphene domains embedded in a hexagonal boron-nitride sheet (h-BN) with the goal of band gap tuning in mind. Different shapes (triangular, circular, rectangular, and irregular structures) and sizes of graphene domains will be studied. The structural stability of these hybrid materials will be studied using a new generation of the semi-empirical Hamiltonian (SCELDAO) developed recently [arXiv:1408.4931]. It is found that the lattice mismatch between graphene domains and the h-BN generates large strain, leading to a reduction or a symmetry breaking of the hexagonal lattice of h-BN. The extent of the strain depends on the shape and the size of the domain, as well as on the distribution of B atoms around the graphene domains. This effect also creates impurity states in the band gap of h-BN and changes the band gap. The interplay between the shape and size of graphene domains, the local strain around the domains and the nature of the impurity states on the band gap of h-BN will be discussed.

10:00AM F17.00009 Plenty of motion at the bottom: atomically thin, free-standing liquid gold

PEKKA KOSKINEN, TOPI KORHONEN, Nanoscience center, Department of Physics, University of Jyvaskyla, Finland — Recent experiments have shown that, in addition to covalent materials, also metals like iron can display an atomically thin free-standing solid phase. This phase can be created when existing hole in free-standing graphene is patched by metal atoms. Here we investigate such a metal patch by density-functional -based electronic and molecular dynamics simulations, while the patching material is gold. Simulations show that while at room temperature gold displays a solid phase, at elevated temperatures it displays an atomically thin liquid phase. This stability of free-standing gold to remain planar even upon two-dimensional diffusion is outright remarkable and has its origins in relativistic effects.

10:12AM F17.00010 Dirac Loops in Carbon Allotropes

KIERAN MULLEN, BRUNO UCHOA, Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, D. GLATZHOFER, Department of Chemistry and Biochemistry, University of Oklahoma — We propose a family of structures that have “Dirac loops”: closed lines in momentum space with Dirac-like quasiparticles, on which the density of states vanishes linearly with energy. The structures all possess the planar trigonal connectivity present in graphene, but are three dimensional. We discuss the consequences of their multiply-connected Fermi surface for transport, including the presence of three dimensional Integer Quantum Hall effect. In the presence of spin-orbit coupling, we show that those structures may have topological surface states. We discuss the feasibility of realizing the structures as an allotrope of carbon.

1Work supported by NSF grants DMR-1310407 and DMR-1352604.
10:24AM F17.00011 Effects of interlayer Sn-Sn lone pair interaction on the band gap of bulk and nanosheet SnO

1NAOTO UMEAWA, Natl Inst for Materials Sci, WEI ZHOU, Tianjin University — Effects of interlayer lone-pair interactions on the electronic structure of SnO are firstly explored by the density-functional theory. Our comprehensive study reveals that the band gap of SnO opens as increase in the interlayer Sn-Sn distance. The effect is rationalized by the character of band edges which consists of bonding and anti-bonding states from interlayer lone pair interactions. The band edges for several nanosheets and strained double-layer SnO are estimated. We conclude that the double-layer SnO is a promising material for visible-light driven photocatalyst for hydrogen evolution.

1This work is supported by the Japan Science and Technology Agency (JST) Precursory Research for Embryonic Science and Technology (PRESTO) program.

10:36AM F17.00012 Phosphorene Oxide: Stability and electronic properties of a novel 2D material

1GAOXUE WANG, RAVIDRA PANDEY, Michigan Tech Univ, SHASHI P. KARNA, US Army Research Laboratory — Phosphorene, the monolayer form of the (black) phosphorus, was recently exfoliated from its bulk counterpart. Phosphorene oxide, by analogy to graphene oxide, is expected to have novel chemical and electronic properties, and may provide an alternative route to synthesis of phosphorene. In this letter, we investigate physical and chemical properties of the phosphorene oxide including its formation by the oxygen adsorption on the bare phosphorene. Analysis of the phonon dispersion curves finds stoichiometric and non-stoichiometric oxide configurations to be stable at ambient conditions, thus suggesting that the oxygen sorption may not degrade the phosphorene. The nature of the band gap of the oxides depends on the degree of the functionalization of phosphorene; indirect gap is predicted for the non-stoichiometric configurations whereas a direct gap is predicted for the stoichiometric oxide. Application of the mechanical strain and external electric field leads to tunability of the band gap of the phosphorene oxide. In contrast to the case of the bare phosphorene, dependence of the diode-like asymmetric current-voltage response on the degree of stoichiometry is predicted for the phosphorene oxide.

8:00AM F18.00001 Observation of Antiferromagnetic Correlations in the Hubbard Model with Ultracold Atoms

1RANDALL HULET2. Rice University — Ultracold atoms on optical lattices form a versatile platform for studying many-body physics, with the potential of addressing some of the most important issues in strongly correlated matter. Progress, however, has been stymied by an inability to create sufficiently low temperatures in an optical lattice. In this talk, I will present our experimental results on the characterization of the three-dimensional Hubbard model near half-filling, realized using two spin-states of fermionic atomic lithium (6)Li). We have developed a compensated optical lattice that has enabled, for the first time, the achievement of temperatures that are below the tunneling energy, t. We use in-situ imaging to extract the central density of the gas, and to determine its local compressibility. For intermediate to strong interactions, we observe the emergence of a density plateau and a reduction of the compressibility, indicative of the formation of a Mott insulator. Comparisons to state-of-the-art numerical simulations of the Hubbard model over a wide range of interactions set an upper limit for the temperature T < t. The Hubbard model is known to exhibit antiferromagnetism at temperatures below the Neel temperature TN. We have detected antiferromagnetic correlations in this system by spin-sensitive Bragg scattering of light. We deduce the temperature of the atoms in the lattice by comparing the light scattering to determinantal quantum Monte Carlo and numerical linked-cluster expansion calculations to find that T/t = 0.51 ± 0.06, corresponding to 1.47N. Further refinement of the compensated lattice may produce even lower temperatures which, along with light scattering thermometry, have important implications for achieving other novel quantum states of matter.

1Supported by DARPA/ARO, ONR, NSF.
3P.M. Duarte et al., arXiv:1409.8348
4R.A. Hart et al., arXiv:1407.5932

8:36AM F18.00002 Spin Transport in a Unitary Fermi Gas

JOSEPH THYWIISSEN, University of Toronto — We study spin transport in a quantum degenerate Fermi gas of 40K near an s-wave interaction resonance. The starting point of our measurements is a transversely spin-polarized gas, where each atom is in a superposition of the lowest two Zeeman eigenstates. In the presence of an external gradient, a spin texture develops across the cloud, which drives diffusive spin currents. Spin transport is described with two coefficients: D∥, the transverse spin diffusivity, and γ, the Leggett-Rice parameter. Diffusion is a dissipative effect that increases the entropy of the gas, eventually creating a mixture of spin states. γ parameters the rate at which spin current precesses around the local magnetization. Using a spin-echo sequence, we measure these transport parameters for a range of interaction strengths and temperatures. At unitarity, for a normal-state gas initially at one fifth of the Fermi temperature, we find D∥ = 2.3(4) h/m and γ = 1.08(9), where m is the atomic mass. In the limit of zero temperature, γ and D∥ are scale-invariant universal parameters of the unitary Fermi gas. The value of D∥ reveals strong scattering and is near its proposed quantum limit, such that the inferred value of the transport lifetime τ∥ is comparable to h/ϵ. This raises the possibility that incoherent transport may play a role. The nonzero value of γ tells us that spin waves in unitary Fermi gas are dispersive, or in other words, that the gas has a spin stiffness in the long-wavelength limit. Time permitting, we will also discuss a time-resolved measurement of the contact, through which we observe the microscopic transformation of the gas from ideal to strongly correlated.
HENDRIK HAMANN, IBM T J Watson Research Center — In the past most information on the internet has been originated by humans or support topological quantum excitations such as Majorana and Weyl fermions. Generated synthetic gauge fields, such as artificial spin-orbit coupling or band hybridization in driven optical lattices. I will show that such FF superfluids can be generated when the spin populations are imbalanced.


This work is supported by ARO, AFOSR and NSF.

9:48AM F18.00004 Pairing phenomena in quasi-2D Fermi gases , MEERA PARISH, Univ Coll London — Quasi-two-dimensional Fermi systems are both of fundamental interest and technological importance. Recent advances in cold-atom experiments have now made it possible to investigate model quasi-2D Fermi gases in a controlled manner. In this talk, I will discuss the different regimes in the attractive Fermi gas and how these can be dramatically modified by the finite transverse width of the quasi-2D system. In particular, I find that the critical temperature for pairing and superfluidity can be enhanced by relaxing the transverse confinement and perturbing away from the 2D limit. I will also discuss the exotic phases that may be generated when the spin populations are imbalanced.

10:24AM F18.00005 Strongly Interacting Fermi Gases of Atoms and Molecules , MARTIN ZWIERLEIN, MIT-Harvard Center for Ultracold Atoms, Research Laboratory of Electronics, and Department of Physics, MIT, Cambridge, MA, USA — In recent years, ultracold gases of fermionic atoms have become a new platform for the realization of paradigmatic forms of strongly interacting matter. Feshbach scattering resonances allow to tune the interactions between atoms and to realize the crossover from Bose-Einstein condensation of molecules to Bardeen-Cooper-Schrieffer superfluidity of long-range Cooper pairs. On resonance, we encounter the unitary Fermi gas, with universal properties that closely correspond to those of dilute neutron matter in the crust of neutron stars, and to nuclear matter. I will present our recent study of solitonic excitations in this novel superfluid, the creation of planar solitons and the subsequent cascade into vortex rings and solitonic vortices. In the presence of spin imbalance, solitons are predicted stabilize, a hallmark of the Larkin-Ovchinnikov phase. To induce strong interactions one may also quench the atoms’ kinetic energy in optical lattices. Of great interest here is the realization of the Fermi-Hubbard model, believed to hold the key to understanding high-temperature superconductors. We recently realized imaging of fermionic atoms with single-site resolution in optical lattices, an important step towards the direct observation of magnetic order. Finally, strong, long-range dipolar interactions can lead to novel states of fermionic matter such as topological superfluids. We have created chemically stable, strongly dipolar fermionic molecules, opening up prospects for observing a strongly interacting degenerate Fermi gas with dominant dipolar interactions.

Tuesday, March 3, 2015 8:00AM - 11:00AM — Session F19 FIAP: Invited Session: Physical Analytics Mission Room 103B - Supratik Guha, IBM

8:00AM F19.00001 Physical Analytics: An emerging field with real-world applications and impact , HENDRIK HAMANN, IBM T J Watson Research Center — In the past most information on the internet has been originated by humans or computers. However with the emergence of cyber-physical systems, vast amount of data is now being created by sensors from devices, machines etc digitizing the physical world. While cyber-physical systems are subject to active research around the world, the vast amount of actual data generated from the physical world has attracted so far little attention from the engineering and physics community. In this presentation we use examples to highlight the opportunities in this new subject of “Physical Analytics” for highly inter-disciplinary research (including physics, engineering and computer science), which aims understanding real-world physical systems by leveraging cyber-physical technologies. More specifically, the convergence of the physical world with the digital domain allows applying physical principles to everyday problems in a much more effective and informed way than what was possible in the past. Very much like traditional applied physics and engineering has made enormous advances and changed our lives by making detailed measurements to understand the physics of an engineered device, we can now apply the same rigor and principles to understand large-scale physical systems. In the talk we first present a set of “configurable” enabling technologies for Physical Analytics including ultralow power sensing and communication technologies, physical big data management technologies, numerical modeling for physical systems, machine learning based physical model blending, and physical analytics based automation and control. Then we discuss in detail several concrete applications of Physical Analytics ranging from energy management in buildings and data centers, environmental sensing and controls, precision agriculture to renewable energy forecasting and management.


9:00AM F19.00003 Physics of Financial Markets: Can we Understand the Unpredictable Phenomenon of Flash Crashes? , H. EUGENE STANLEY, Boston University Center for Polymer Studies — Dangerous vulnerability is hiding in complex systems. Indeed, disasters ranging from abrupt financial “flash crashes” and large-scale power outages to sudden death among the elderly dramatically exemplify this fact. While we can understand the cause of most events in complex systems, sudden unexpected “black swans” whether in economics or in the “physicists world” cry out for insight. To design more resilient systems we will describe recent results seeking understanding of these black swans. In many real-world phenomena, such as brain seizures in neuroscience or sudden market crashes in finance, after an inactive period of time a significant part of the damaged network is capable of spontaneously becoming active again. The process often occurs repeatedly. To model this marked network recovery, we examine the effect of local node recoveries and stochastic contiguous spreading, and find that they can lead to the spontaneous emergence of macroscopic “phase-flipping” phenomena. The fraction of active nodes switches back and forth between the two network collective modes characterized by high network activity and low network activity. Furthermore, the system exhibits a strong hysteresis behavior analogous to phase transitions near a critical point [A. Majdanzic, B. Podobnik, S. V. Buldyrev, D. Y. Kenett, S. Havlin, and H. E. Stanley, “Spontaneous Recovery in Dynamic Networks,” Nature Physics 10 , 34 (2014)].

This work was carried out in collaboration with a number of colleagues, chief among whom are A. Majdanzic, B. Podobnik, S. V. Buldyrev, D. Y. Kenett, and S. Havlin.
I will also briefly discuss focus areas for future advances, and speculate on ultimate performance limits for coherent Raman imaging. Improvements in this field would provide an unprecedented combination of speed, sensitivity, and chemical selectivity \[1\]. Using this system we are able to obtain high quality Raman spectra in a reasonably short amount of time, sometimes less than a second. This has enabled us to conduct a variety of experiments that were previously inaccessible. Some of these experiments include investigations of the glass transition temperature in thin PS films, measures of enhanced surface mobility in glassy PS, and a simple picture of how we can use surface mobility to develop an understanding of the thin film glass transition. Finally, I will discuss the relation between the length scale of surface mobility to the long discussed yield and plastic flow, which has little impact on the flow stress. Eyring proposed that stress increases the rate of molecular rearrangements in solids and this is the source of nonlinearity in many models. Our group has developed an optical technique to measure molecular mobility and shown that mobility during deformation can increase by more than a factor of 1000. In this talk, I will highlight recent progress including understanding the role of deformation temperature and a comparison between molecular and mechanical relaxation times. Results from recent computer simulations and molecular theories will be discussed. Finally, some comments will be made on the deformation of polymer glasses in comparison to colloidal and metallic glasses.

**Tuesday, March 3, 2015 8:00AM - 11:00AM** — Session F20 DPOLY: Invited Session: Polymer Physics Prize

**8:00AM F20.00001 Polymer Prize Lecture: A perspective on the deformation of polymer glasses**, MARK EDIGER, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706 — The mechanical properties of polymer glasses, including yield and plastic flow, are important for many applications. In contrast to the flow of polymer melts, plastic flow is poorly understood at a fundamental level. One reason for this is that the deformation of polymer glasses typically occurs in a highly nonlinear regime, e.g., doubling the strain rate has little impact on the flow stress. Eyring proposed that stress increases the rate of molecular rearrangements in solids and this is the source of nonlinearity in many models. Our group has developed an optical technique to measure molecular mobility and shown that mobility during deformation can increase by more than a factor of 1000. In this talk, I will highlight recent progress including understanding the role of deformation temperature and a comparison between molecular and mechanical relaxation times. Results from recent computer simulations and molecular theories will be discussed. Finally, some comments will be made on the deformation of polymer glasses in comparison to colloidal and metallic glasses.

**8:36AM F20.00002 Nanoparticles in liquid crystals, and liquid crystals in nanoparticles**, JUAN DE PABLO, Institute for Molecular Engineering, University of Chicago — Liquid crystals are remarkably sensitive to interfacial interactions. Small perturbations at a liquid crystal interface, for example, can be propagated over relatively long length scales, thereby providing the basis for a wide range of applications that rely on amplification of molecular events into macroscopic observables. Our recent research efforts have focused on the reverse phenomenon; that is, we have sought to manipulate the interfacial assembly of nanoparticles or the organization of surface active molecules by controlling the structure of a liquid crystal. This presentation will consist of a review of the basic principles that are responsible for liquid crystal-mediated interactions, followed by demonstrations of those principles in the context of two types of systems. In the first, a liquid crystal is used to direct the assembly of nanoparticles; through a combination of molecular and continuum models, it is found that minute changes in interfacial energy and particle size lead to liquid-crystal induced attractions that can span multiple orders of magnitude. Theoretical predictions are confirmed by experimental observations, which also suggest that LC-mediated assembly provides an effective means for fabricating plasmonic devices. In the second system, the structure of a liquid crystal is controlled by confinement in submicron droplets. The morphology of the liquid crystal in a drop depends on a delicate balance between bulk and interfacial contributions to the free energy; that balance can be easily perturbed by adsorption of analytes or nanoparticles at the interface, thereby providing the basis for development of hierarchical assembly of responsive, anisotropic materials. Theoretical predictions also indicate that the three-dimensional order of a liquid crystal can be projected onto a two-dimensional interface, and give rise to novel nanostructures that are not found in simple isotropic fluids.

**9:12AM F20.00003 Broadband Coherent Raman Scattering for Rapid Spectroscopic Imaging**, MARCUS CICERONE, National Institute of Standards and Technology — Over the past ten years, coherent Raman imaging (CRI) has evolved from a curiosity to a practical tool for investigating many classes of biological and material questions. An important key to this evolution has been the ability to rapidly obtain information from many spectral peaks. Most vibrational spectroscopic information is found in the fingerprint region where spontaneous Raman can be used to achieve >3 signal to noise ratio for weak fingerprint peaks in biological systems, but typically requires acquisition times of several seconds; too slow for imaging. Coherent Raman methods have previously been unable to acquire high quality fingerprint spectra. We have overcome this limitation by developing a highly efficient signal excitation paradigm and appropriately harnessing the nonresonant background (NRB) signal that accompanies the resonant signal of interest. With these and other innovations, we have developed a CRI approach based on broadband coherent anti-Stokes Raman scattering (BCARS) that provides an unprecedented combination of speed, sensitivity, and chemical selectivity \[1\]. Using this system we are able to obtain high quality Raman spectra in the fingerprint and CH stretch regions from biological specimens at 3.5 ms, enabling rapid, label-free chemical imaging of even delicate samples. I will briefly put our approach in context with the broader CRI field, describe key technical features of the present imaging system and provide application examples in materials and biology. I will also briefly discuss focus areas for future advances, and speculate on ultimate performance limits for coherent Raman imaging.

10:24AM F20.00005 Surface Mediated Self-Assembly of Amyloid Peptides1, ZAHRA FAHKRAAI, University of Pennsylvania — Amyloid fibrils have been considered as causative agents in many neurodegenerative diseases, including Alzheimer’s disease, Parkinson’s disease, type II diabetes and amyloidosis. Amyloid fibrils form when proteins or peptides misfold into one dimensional crystals of stacked beta-sheets. In solution, amyloid fibrils form through a nucleation and growth mechanism. The rate limiting nucleation step requires a critical concentration much larger than those measured in physiological conditions. As such the exact origins of the seeds or oligomers that result in the formation of fully mature fibrils in the body remain topic intense studies. It has been suggested that surfaces and interfaces can enhance the fibrillation rate. However, studies of the mechanism and kinetics of the surface-mediated fibrillation are technologically challenging due to the small size of the oligomer and proteofibril species. Using smart sample preparation technique to dry the samples after various incubation times we are able to study the kinetics of fibril formation both in solution and in the vicinity of various surfaces using high-resolution atomic force microscopy. These studies elucidate the role of surfaces in catalyzing amyloid peptide formation through a nucleation-free process. The nucleation free self-assembly is rapid and requires much smaller concentrations of peptides or proteins. We show that this process resembles diffusion limited aggregation and is governed by the peptide adhesion rate, two -dimensional diffusion of the peptides on the surface, and preferential interactions between the peptides. These studies suggest an alternative pathway for amyloid formation may exist, which could lead to new criteria for disease prevention and alternative therapies.

1 Research was partially supported by a seed grant from the National Institute of Aging of the National Institutes of Health (NIH) under Award Number P30AG010124 (PI: John Trojanowski) and the University of Pennsylvania.

Tuesday, March 3, 2015 8:00AM - 11:00AM —
Session F21 GIMS: Focus Session: Advances in Scanned Probe Microscopy II: High Frequencies and Optical Techniques 201 - Fabian Natterer, National Institute of Standards and Technology

8:00AM F21.00001 Measurement of Radiation Pressure in an Ambient Environment, DAKANG MA, JOSEPH GARRETT, JEREMY MUNDAY, University of Maryland - College Park — Light has momentum and thus exerts “radiation pressure” when it is reflected or absorbed due to the conservation of momentum. Micromechanical transducers and oscillators are suitable for measurement and utilization of radiation pressure due to their high sensitivities. However, other light-induced mechanical deformations such as photothermal effects often obscure accurate measurements of radiation pressure in these systems. In this work, we investigate the radiation pressure and photothermal force on an uncoated silicon nitride microcantilever under illumination by a 660 nm laser in an ambient environment. To magnify the mechanical effects, the cantilever is driven optically from dc across its resonance frequency, and the amplitude and phase of its oscillation are acquired by an optical beam deflection method and a lockin amplifier. We show that radiation pressure and photothermal effects can be distinguished through the cantilever’s frequency response. Furthermore, in a radiation pressure dominant regime, our measurement of the radiation force agrees quantitatively with the theoretical calculation.

8:12AM F21.00002 Sensitivity Improvement and Cryogenic Application of Scanning Microwave Microscope, HIDEYUKI TAKAHASHI, YOSHINORI IMAI, ATSUTAKA MAEDA, Department of Basic Science, the University of Tokyo — The technique to probe the spatial distribution of electric properties has been more important in modern material science. Scanning near-field microwave microscope (SMM) can be a powerful tool to study inhomogeneous materials. Recently we have developed scanning tunneling/microwave microscope (STM/SMM) with high sensitivity[1,2]. The SMM probe is a modified coaxial resonator whose resonant frequency is 10.7 GHz and Q-factor is 1200-1300 at room temperature. It is applicable to measurements at cryogenic environment. By downsizing the resonator probe, we achieved stable operation down to liquid helium temperature. Q-factor is enhanced to 2000-3000 below 77 K. As an example of application of our STM-SMM, we present the study on inhomogeneous iron-based superconductor KFe2Se2. We successfully observed the characteristic mesoscopic phase separation of the metallic phase and the semiconducting phase by two different scanning modes; constant current mode and constant Q-factor mode. The spatial resolution is no worse than 200nm, which is comparable to curvature radius of a probe tip.

2 J. Lee et al., Appl. Phys. Lett. 97, 183111 (2010).

8:24AM F21.00003 Subsurface Imaging with the Scanning Microwave Microscope, JOSEPH KOPANSKI, LIN YOU, JONATHAN MICHELSOn, EMILY Hitz, YAW OBENG, Semiconductor and Dimensional Metrology Division, National Institute of Standards and Technology, BACK END OF THE LINE RELIABILITY & METROLOGY PROJECT TEAM — The scanning microwave microscope (SMM) forms images from the reflected amplitude and phase of an incident RF (~ 2.3 GHz) signal. The reflected signal is a function of the properties of the tip-sample contact, but can also be influenced by buried interfaces and subsurface variations of the sample permittivity. This mechanism allows limited imaging of conductors buried within dielectrics, voids within metal, or multiple metal layers with different permittivity. Subsurface SMM data acquisition modes include passive and various active data acquisition modes. The theory of sub-surface imaging with SMM and COMSOL multi-physics simulations of specific situations will be presented. Measurements of specifically designed test structures and correlation with simulations show the sensitivity and resolution of the technique applied to imaging subsurface metal lines embedded in dielectric. Applications include metrology for back end of the line (BEOL) multi-level metallization and three-dimensional integrated circuits (3D-ICs).

8:36AM F21.00004 Advances in imaging and quantification of electrical properties at the nanoscale using Scanning Microwave Impedance Microscopy (sMIM), STUART FRIEDMAN, YONGLIANG YANG, OSKAR AMSTER, Primenano, Inc — Scanning Microwave Impedance Microscope (sMIM) is a mode for Atomic Force Microscopy (AFM) enabling imaging of unique contrast mechanisms and measurement of local permittivity and conductivity at the 10’s of nm length scale. Recent results will be presented illustrating high-resolution electrical features such as sub 15 nm Moiré patterns in Graphene, carbon nanotubes of various electrical states and ferro-electrics. In addition to imaging, the technique is suited to a variety of metrology applications where specific physical properties are determined quantitatively. We will present research activities on quantitative measurements using multiple techniques to determine dielectric constant (permittivity) and conductivity (e.g. dopant concentration) for a range of materials. Examples include bulk dielectrics, low-k dielectric thin films, capacitance standards and doped semiconductors.

1 Funded in part by DOE SBIR DE-SC0009586
8:48AM F21.00005 Analytical quantitative theory of RF-SPM for nanocarbon electronics 1. SLAVA V. ROTKIN, Lehigh University, Department of Physics and Center for Advanced Materials and Nanotechnology — Among a variety of Scanning Probe Microscopy (SPM) tools RF- or microwave-SPM has recommended itself as a versatile characterization tool, recently demonstrated capability to map electronic properties of nanocarbon materials non-destructively and with nanometer resolution. The transparent theory of RF-SPM sensing mechanism is however lacking, mostly limited to numerical or empirical solutions, especially when studying low-dimensional quantum objects, such as nanotubes/nanowires (NT/NW), where the classical description is often invalid. One-dimensional electronic structure of the NT/NW, weak screening of Coulomb interaction and finite e-e compressibility were successfully taken into account to provide an analytic form of its quasi-stationary (due to low RF frequency of the excitation) selfconsistent response. SPM tip response function was, in turn, efficiently analyzed in multipole series, and non-perturbatively diagrammatically summed in the sense of the Random Phase Approximation. Resulting theory shows transparently the physics of RF-SPM sensing mechanism, simultaneously allowing a quantitative analysis of recent RF-SPM data on nanotube electronic devices [E. Seabron, S. MacLaren, X. Xie, SV. Rotkin, JA. Rogers, WL. Wilson, unpublished].

1 Support by AFOSR (# FA9550-11-1-0185) is acknowledged.

9:00AM F21.00006 Ferromagnetic Resonance detection using stroboscopic magneto optical Kerr effect, SEUNGHA YOON, NIST - Natl Inst of Stds & Tech, and University of Maryland, TAKAHIRO MORIYAMA, NIST - Natl Inst of Stds & Tech, and Kyoto University, ROBERT MICHAEL, NIST - Natl Inst of Stds & Tech — Ferromagnetic resonance (FMR) is a powerful method for measuring the magnetic properties of ferromagnets. A number of related optical techniques have become popular, including time-resolved magneto-optical Kerr effect (TR-MOKE) microscopy and Brillouin light scattering (BLS). In this presentation we describe a new, stroboscopic method of measuring FMR based on the magneto-optical Kerr effect (MOKE). We use a polarized telecommunications fiber laser (wavelength = 1550 nm) and a fiber modulator driven at a frequency of interest (1 GHz to 10 GHz) to create pulsed, linearly polarized light incident on a CoFeB thin film sample. Precession in the sample is driven via a coplanar waveguide in the sample holder while the reflected light is split by a polarization beam splitter and detected by a balanced detector. As the magnetic field is swept, oscillations in the Kerr angle and in the intensity mix to produce a DC resonance signal. The spectra are Lorentzian, with a superposition of symmetric and anti-symmetric shapes that depends on the phase of the optical and microwave signals. In the presentation, we will also discuss phase sensitive measurements with this technique as well as the advantages over other FMR techniques.

9:12AM F21.00007 Time-resolved scanning tunneling microscopy for studies of nanoscale magnetization dynamics, SEBASTIAN LOTH, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — The time resolution of the scanning tunneling microscope can be boosted greatly by use of electronic pump probe measurement schemes. Pulse shaping of the input pulses can even overcome bandwidth limitations of the instrument and enables sub-nanosecond time resolution [1]. In this talk we will focus on applications of this technique for measurements of fast spin dynamics in nanomagnets. We use the probe tip of a low-temperature STM to arrange magnetic atoms into arrays of our own design. Thin insulating films decouple the atoms from the supporting metallic substrate so that the nanostructures show quantum-magnetic properties with discrete spin states. The time-domain information gained in pump probe spectroscopy quantifies the spin relaxation between metastable spin states [2]. It enables isolating the interaction between the nanomagnet and its environment. In particular, we find that the magnetic atoms of a spin-polarized STM tip interact significantly with the surface even at moderate tunneling conditions. This interaction acts analogously to a highly localized magnetic field. It depends exponentially on the tip-nanomagnet distance and can reach a strength of several tesla. We use this atomically localized magnetic field to control the spin state mixing of a nanomagnet in an avoided level crossing of low-energy spin states [3]. Furthermore, pump probe spectroscopy enables non-local measurements of magnetic states and highlights pathways to design and control magnetism at the single atom level.


9:48AM F21.00008 A low temperature ultrahigh vacuum scanning tunneling microscope with high-NA optics to probe optical interactions at the atomic scale, HAIGANG ZHANG, Argonne National Laboratory, Argonne, IL 60439, JOSEPH SMERDON, University of Central Lancashire, Lancashire, UK, OZGUN SUZER, HGST, a Western Digital Company, San Jose, CA 95135, HEATH KERSELL, Ohio University, Athens, OH 45701, JEFFREY GUEST, Argonne National Laboratory, Argonne, IL 60439 — The optical and photophysical properties of single molecules/atoms, defects, and nanoscale structures at surfaces hinge on structure at the atomic scale. In order to characterize and control this structure and unravel these correlations, we are developing a low temperature (LT) laser-coupled ultrahigh vacuum (UHV) scanning tunneling microscope (LT Laser UHV STM) based on the Pan-style STM scanner with integrated high-numerical-aperture (NA) optics for single particle spectroscopy measurements under the STM tip. Using slip-stick inertial piezo steppers, the sample stage can be coarsely translated in X and Y directions. For optical measurements, high-NA optics behind and above the sample focus laser excitation on and collect photons emitted from the tip-sample junction. The STM is cooled by a liquid helium bath surrounded by a liquid nitrogen jacket for operation near 5 K; two separate ultrahigh vacuum chambers are used for sample preparation and STM measurements, respectively. We will describe our progress in demonstrating this instrument and plans for experiments studying the correlation between structure and optical function in nanoscale systems.

1 U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences

10:00AM F21.00009 Metal-Insulator Phase transition of VO2 nano crystals studied by near-field nanoscopy, YOHANNES ABATE, Georgia State University — Near-field dipolar plasmon interactions of multiple infrared antenna structures in the strong coupling limit are studied using scattering-type scanning near-field optical microscope (s-SNOM) and theoretical finite-difference time-domain (FDTD) calculations. We monitor in real-space the evolution of plasmon dipolar mode of a stationary antenna structure as multiple resonantly matched dipolar plasmon particles are closely approaching. Interparticle separation, length and polarization dependent studies show that the cross geometry structure favors strong interparticle charge-charge, dipole–dipole and charge–dipole Coulomb interactions in the nanometer scale gap region, which results in strong field enhancement in cross-bowties and further allows these structures to be used as polarization filters. The nanoscale local field amplitude and phase maps show that due to strong interparticle Coulomb coupling, cross-bowtie structures redistribute and highly enhance the out-of-plane (perpendicular to the plane of the sample) plasmon near-field component at the gap region relative to ordinary bowties. Preliminary results on using VO2 film to tune infrared plasmon antenna resonances will be presented.
10:12AM F21.00010 Determination of the dielectric function of materials with scattering-type scanning near field optical microscopy. PENG XU, T.J. HUFFMAN, M.M. QAZILBASH, College of William and Mary, INHAE KWAK, AMLAN BISWAS, University of Florida —. In apertureless scattering-type near field optical and infrared microscopy has been widely employed for imaging a variety of systems at the nanoscale including semiconductor nanostructures, organic bio-systems, and phase coexistence during metal-insulator transitions. In apertureless, scattering-type near field infrared microscopy, one can measure both the near field amplitude and phase. To obtain the complex dielectric function of the material at nanometer length scales from the measured amplitude and phase, the inverse problem of near field interaction needs to be solved.

We employed the lightning rod model[1] to analyze the near field interaction and obtain the dielectric function numerically. We present results for near-field infrared measurements on transition metal oxides including those that exhibit optical contrast due to coexisting phases. [1] A. S. McLeod et al., Phys. Rev. B 90, 085136 (2014)

1This work was supported by the National Science Foundation

10:24AM F21.00011 Generalized method of eigenoscillations for near-field optical microscopy. BOR-YUAN JIANG, Univ of California - San Diego, LINGFENG ZHANG, Boston University, ANTONIO CASTRO NETO, National University of Singapore, DIMITRI BASOV, MICHAEL FOGLER, Univ of California - San Diego — Electromagnetic interaction between a sub-wavelength particle (the “probe”) and a material surface (the “sample”) is studied theoretically. The interaction is shown to be governed by a series of resonances (eigenoscillations), corresponding to surface polariton modes localized near the probe. The resonance parameters depend on the dielectric function and geometry of the probe, as well as the surface reflectivity of the material. Calculation of such resonances is carried out for several axisymmetric particle shapes (spherical, spheroidal, and pear-shaped).

For spheroids an efficient numerical method is proposed, capable of handling cases of large or strongly momentum-dependent surface reflectivity. The method is applied to modeling near-field spectroscopy studies of various materials. For highly resonant materials such as aluminum oxide (by itself or covered with graphene) a rich structure of the simulated signal is found, including multi-peak spectra and nonmonotonic approach curves. These features have a strong dependence on physical parameters, e.g., the probe shape. For less resonant materials such as silicon oxide the dependence is weaker, and the spheroid model is generally applicable.

10:36AM F21.00012 Cryogenic Near-Field Microscopy in Correlated Electronic Systems. ADRIAN GOZAR, Brookhaven National Laboratory — We present results on the performance of a scattering-based scanning near-field optical microscope. The instrument was designed for measuring nano-scale complex dielectric properties of materials in a variable-temperature environment. The setup has a 20 - 30 nm spatial resolution with sample temperatures in the 10 - 300 K range. Spectral operation is in the infrared to visible and 0.1 - 1 THz regions. We illustrate these capabilities with results in graphene and ultra-thin sub-surface oxide films.

10:48AM F21.00013 Radiation pressure excitation of Low Temperature Atomic Force & Magnetic Force Microscope (LT-AFM/MFM) for Imaging. OZGUR KARCII, UMIT CELIK, NanoMagnetics Instruments Ltd., AHMET ORAL, Middle East Tech Univ, NANOMAGNETICS INSTRUMENTS LTD. TEAM, MIDDLE EAST TECH UNIV TEAM — We describe a novel method for excitation of Atomic Force Microscope (AFM) cantilevers by means of radiation pressure for imaging in an AFM for the first time. Piezo excitation is the most common method for cantilever excitation, but it may cause spurious resonance peaks. A fiber optic interferometer with 1310 nm laser was used both to measure the deflection of cantilever and apply a force to the cantilever in a LT-AFM/MFM from NanoMagnetics Instruments. The laser power was modulated at the cantilever’s resonance frequency by a digital Phase Lock Loop (PLL). The force exerted by the radiation pressure on a perfectly reflecting surface by a laser beam of power P is F = 2P/c. We typically modulate the laser beam by ~ 800 µW and obtain 10nm oscillation amplitude with Q ~ 8,000 at 2.5x10^-4 mbar. The cantilever’s stiffness can be accurately calibrated by using the radiation pressure. We have demonstrated performance of the radiation pressure excitation in AFM/MFM by imaging a hard disk sample between 4-300K and Abrikosov vortex lattice in BSCCO single crystal at 4K to for the first time.

Tuesday, March 3, 2015 8:00AM - 10:24AM - Session F22 DCMP: Transport and Theory of Non-Fermi liquids

8:00AM F22.00001 ABSTRACT WITHDRAWN

8:12AM F22.00002 Kondo Effects in Single Layer Transition Metal Dichalcogenides. MICHAEL PHILLIPS1, VIVEK AJI2, University of California, Riverside — Inversion symmetry breaking and strong spin orbit coupling in two dimensional transition metal dichalcogenides leads to interesting new phenomena such as the valley hall and spin hall effects. They display optical circular dichroism and the ability to generate excitation with valley specificity. In this talk we report on the consequences of these properties on correlated states in hole doped systems focusing on the physics of the screening of magnetic impurities. Unlike typical metals, the breaking of inversion symmetry leads to the mixing of a triplet component to the Kondo cloud. Using a variational wave function approach we determine the nature of the many body state. With the ground state in hand we analyze the excitations generated by valley discriminating perturbations.

1Graduate Student
2Advisor / Principal Investigator

8:24AM F22.00003 Non-Fermi-liquid behavior and anomalous suppression of Landau damping in layered metals close to ferromagnetism. SAM RIDGWAY, CHRIS HOOLEY, Univ of St Andrews — We analyse the low-energy physics of nearly ferromagnetic metals in two spatial dimensions using the functional renormalization group technique. We find a new class of low-energy fixed point, at which the fermionic (electron-like) excitations are non-Fermi-liquid ($\epsilon_f = T/6$) and the magnetic fluctuations exhibit an anomalous Landau damping whose rate vanishes as $\Gamma_q \sim |q|^{1/3}$ in the low-$|q|$ limit. We discuss the physical nature of this fixed point, and highlight its possible applicability to experiments on UGe$_2$ and related compounds.

8:36AM F22.00004 Stable non-Fermi liquid phase of itinerant spin-orbit coupled ferromagnets. YASAMAN BAHRI, ANDREW POTTER, University of California, Berkeley — Direct coupling between gapless bosons and a Fermi surface results in the destruction of Landau quasiparticles and a breakdown of Fermi liquid theory. Such a non-Fermi liquid phase arises in spin-orbit coupled ferromagnets with spontaneously broken continuous symmetries due to strong coupling between rotational Goldstone modes and itinerant electrons. These systems provide an experimentally accessible context for studying non-Fermi liquid physics. Possible examples include low-density Rashba coupled electron gases, which have a natural tendency towards spontaneous ferromagnetism, or topological insulator surface states with proximity-induced ferromagnetism. Crucially, unlike the related case of a spontaneous nematic distortion of the Fermi surface, for which the non-Fermi liquid regime is expected to be masked by a superconducting dome, we show that the non-Fermi liquid phase in spin-orbit coupled ferromagnets is stable.
temperature- and angle-dependent in-plane and out-of-plane magnetoresistance measurements in the ultra-quantum limit on graphite. Our experiments reveal a rich structure, though the complicated phase transitions, suggesting more researches should be carried out to understand the mysterious transitions. We performed transport measurements in the quantum limit of graphite between 22T and 53T. Recently, another unexpected high-field transition was observed around 75T. The relative simple band structure at high fields, we establish the phase diagram of graphite in its ultra-quantum limit. Our results imply the existence of a topologically-protected chiral Fermi surface – an interacting, scale invariant, non-Fermi liquid phase found in quadratic semimetals which has been recently suggested to be realized in strongly correlated pyrochlore iridate systems. We develop a kinetic equation formalism to describe the d.c. transport properties, which are dominated by collisions, and consider the shear viscosity η as a model transport coefficient. The ratio of shear viscosity to entropy density η/s is a measure of the strength of interaction between the excitations of a quantum fluid. As a consequence of the quantum critical nature of the system, η/s is a universal number and we find it to be consistent with a bound proposed from gauge-gravity duality.

9:36AM F22.00009 Transport in two-dimensional disordered semimetals, MICHAEL KNAP, Harvard University, JAY D. SAU, University of Maryland, BERTRAND I. HALPERIN, EUGENE DEMLER, Harvard University — We theoretically study transport in two-dimensional semimetals. Typically, electron and hole puddles emerge in the transport layer of these systems due to smooth fluctuations in the potential. We calculate the electric response of the electron-hole liquid subject to zero and finite perpendicular magnetic fields using an effective medium approximation and a complimentary mapping on resistor networks. In the presence of smooth disorder and in the limit of weak electron-hole recombination rate, we find small but finite overlap of the electron and hole bands an abrupt upturn in resistivity when lowering the temperature but no divergence at zero temperature. We discuss how this behavior is relevant for several experimental realizations and introduce a simple physical explanation for this effect.

9:48AM F22.00010 Phase diagram of a semimetal in the magnetic ultra-quantum limit, ALDO ISIDORI, FRANK ARNOLD, Royal Holloway, University of London, ERIK KAMPERT, Hochfeld-Magnetlabor Dresden, BEN YAGER, MATTHIAS ESCHRIG, JOHN SAUNDERS, Royal Holloway, University of London — Semimetals like graphite have recently received compelling interest as they not only are able to host topologically non-trivial phases but also can be driven into the ultra-quantum limit by magnetic fields now achievable in modern-day laboratories. Thus, they provide insight into quantum-Hall physics and the physics of massless Dirac fermions in three dimensions. They also represent ideal model systems for studying magnetic-field driven density wave instabilities, as the onset field for such collective excitations is suppressed in semimetals. Using pulsed high-magnetic fields up to 60 T applied to a single crystal of natural Tanzanian graphite, we find a series of field-induced phase transitions into collinear charge-density wave states resulting from enhanced interactions between the lowest four Landau levels. By analysing magneto-transport data and calculating the renormalized Landau level structure at high fields, we establish the phase diagram of graphite in its ultra-quantum limit. Our results imply the existence of a topologically-protected chiral edge state at high fields supporting both charge and spin currents.

1We acknowledge the support of the HLD-HZDR, member of the European Magnetic Field Laboratory (EMFL), the Hubbard Theory Consortium, and the Engineering and Physical Science Research Council (EPSRC Grant Nos. EP/H048375/1 and EP/J010618/1)
8:00AM F23.00001 Ammonium Azide under High Pressure — a combined Theoretical and Experimental Study1, HARRY RADOUSKY, JONATHAN CROWHURST, JOSEPH ZAUG, Lawrence Livermore National Laboratory, BRADLEY STEELE, AARON LANDERVILLE, IVAN OLEYNIK, University of South Florida — Efforts to synthesize, characterize and recover novel polynitrogen energetic materials have driven attempts to subject high nitrogen content precursor materials (in particular metal and non-metal azides) to elevated pressures. Here we present a combined theoretical and experimental study of the high pressure behavior of ammonium azide (NH₄N₃). Using density functional theory we have considered the relative thermodynamic stability of the material with respect to two other crystal phases, namely trans-tetrazene (TTZ), and also a novel material, hydronitrogen solid (HNS) of the form (NH₃)₄. Our calculations demonstrate that the HNS becomes stable only at pressures much higher (89.4 GPa) than previously predicted (36 GPa). Our Raman spectra are consistent with earlier reports up to lower pressures, and at higher pressures, while some additional subtle behavior is observed (e.g. mode splitting) there is again no evidence of a phase transition to either TTZ or the HNS.

1Funded by NSF and Research Board of University of Illinois

8:12AM F23.00002 ABSTRACT WITHDRAWN —

8:24AM F23.00003 Calculations and experimental studies of bis-triaminoguanidium azotetrazolate (TAGzT) under high pressure — I.G. BATYREV, R.C. SAUSA, US Army Research Laboratory — Nitrogen-rich organic compounds may offer distinct advantages over conventional energetic materials for applications relating to gas generators, low-sensitivity propellants, and additives to pyrotechnics and explosives. We have performed plane-wave, density functional theory calculations of TAGzT, an energetic, nitrogen-rich salt, up to 40 GPa, and report the pressure dependences of polarizability, x-ray diffraction patterns, and dipole moments. These results are compared to those we obtain experimentally from Raman Spectroscopy,1 and x-ray diffraction analysis and infrared spectroscopy. Our results suggest TAGzT does not undergo any phase transitions within this pressure range. Mulliken and Hirshfeld population analysis of TAGzT at ambient and high pressure yields the change of charge distribution with an increase in pressure. We report and discuss this trend at the meeting. Also, we report trends in the pressure-induced modifications of both bond lengths and angles of TAGzT, and reveal how hydrogen bonding contributes to the stability of TAGzT under pressure.1 K.D. Behler, J.A. Ciezak-Jenkins, R.C. Sausa, J. Phys. Chem A. 117(8), 1737 (2013)

8:36AM F23.00004 Many-body Green’s function calculations of optical properties of LiF in extreme conditions1, CATALIN D. SPATARU, LUKE SHULENBURGER, Sandia National Labs, LORIN X. BENEDICT, Lawrence Livermore National Labs — We present Density Functional Theory (DFT) + quasiparticle (G0W0) + Bethe-Salpeter calculations of the real and imaginary parts of the long-wavelength dielectric function of LiF between ambient pressure and P= 5 Mbars. While the optical absorption spectrum is predicted to show dramatic pressure-dependent features above the optical gap, the index of refraction well below the gap is shown to exhibit the same trends as that seen in both DFT calculations and experiment: a linear increase with \( P \). This increase does not result from a decrease in the band gap, but rather follows from the increase in oscillator strength which counteracts a smaller increase in band gap with \( P \). Our calculations also suggest that the index of refraction (for visible and near-UV light) of the higher-\( T \) B2-phase should be close enough to that of the B1 (ambient crystalline) phase that a transition from B1 to B2 is not likely to present a substantial change in index. These findings may be of interest to researchers who use LiF as a window material in dynamic compression experiments.

1SNL is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Co., for the U.S. DOE’s NNSA under contract DEAC04-94AL85000. Work at LLNL was performed under the auspices of the U.S. DOE under Contract No. DE-AC52-07NA27344.

8:48AM F23.00005 Strongly correlated valence electrons and core-level chemical bonding of Lithium at terapascal pressures, ANGUANG HU, FAN ZHANG, Defence Research and Development Canada at Suffield Research Centre — As the simplest pure metal, lithium exhibits some novel properties on electrical conductivity and crystal structures under high pressure. All-electron density functional theory simulations, recently developed by using the linear combination of localized Slater atomic orbitals, revealed that the bandwidth of its valence bands remains almost unchanged within about 3.5 eV even up to a terapascal pressure range. This indicates that the development from delocalized to strongly correlated electronic systems takes place under compression, resulting in metal-semiconductor and superconductivity transitions together with a sequence of new high-pressure crystal phases, discovered experimentally. In contrast to the valence bands, the core-level bands become broadening up to about 10 eV at terapascal pressures. It means the transformation from chemical non-bonding to bonding for core electrons. Thus, dense lithium under compression can be characterized as core-level chemical bonding and a completely new class of strongly correlated materials with narrow bands filled in s-electron shells only.
9:00AM F23.00006 Equation of state, thermodynamic and transport properties in liquid indium and iron under high pressure¹, HUAMING LI, YONGLI SUN, College of Physics and Optoelectronics, Taiyuan University of Technology, MO LI, School of Materials Science and Engineering, Georgia Institute of Technology — We apply a general equation of state of liquid [1] to study thermodynamic properties in liquid indium and iron under high temperature and high pressure. In particular, density, isothermal bulk modulus, and internal pressure are then analyzed in liquid indium and iron. Molar volume of molten indium is calculated along the isothermal line with good precision comparing with the known data from experiments in an externally heated diamond anvil cell. For liquid indium at given parameters, density anomaly, i.e. the molar volume, is observed along certain isobaric paths. In liquid iron, the entropy scaling law of self-diffusion coefficient and viscosity under high pressure (up to 350 GPa) and high temperature (up to 8000 K) are investigated. Comparisons are made with experimental data and other EOS models for liquid iron.

¹Shanxi Provincial government (“100-talents program”) and National Natural Science Foundation of China (NSFC) under grant No. 11204200.

9:12AM F23.00007 Stable Xenon Nitride at High Pressures, YUNWEI ZHANG, FENG PENG, YANMING MA, State Key Lab of Superhard Materials, Jilin University — Nitrogen is the most abundant element on Earth and exists as inert N₂ molecules in the atmosphere. Noble gas nitrates are missing in nature because N₂ molecules do not interact with noble gases at ambient conditions, greatly impeding the understanding of physics and chemistry of such nitrates. We report here a pressure-induced chemical reaction of N₂ with xenon predicted using a swarm-structure searching calculation as implemented in the CALYPSO code [1-2]. This reaction leads to the formation of a hitherto unexpected Xe nitride at megabar pressure accessible to high-pressure experiments. The high-pressure phase with a hypervalent state of Xe by accepting unprecedented Xe-N covalent bonds appears to be the most stable stoichiometry. The Xe bonding situation in this new phase is substantially different from earlier high-pressure examples of ionic Xe bonding or van der Waals interactions.


9:24AM F23.00008 The phase diagram of solid hydrogen at high pressure: A challenge for first principles calculations¹, SAM AZADI, MATTHEW FOULKES , Imperial College London — We present comprehensive results for the high-pressure phase diagram of solid hydrogen. We focus on the energetically most favorable molecular and atomic crystal structures. To obtain the ground-state static enthalpy and phase diagram, we use semi-local and hybrid density functional theory (DFT) as well as diffusion quantum Monte Carlo (DMC) methods. The closure of the band gap with increasing pressure is investigated utilizing quasi-particle many-body calculations within the GW approximation. The dynamical phase diagram is calculated by adding proton zero-point energies (ZPE) to static enthalpies. Density functional perturbation theory is employed to calculate the proton ZPE and the infra-red and Raman spectra. Our results clearly demonstrate the failure of DFT-based methods to provide an accurate static phase diagram, especially when comparing insulating and metallic phases. Our dynamical phase diagram obtained using fully many-body DMC calculations shows that the molecular-to-atomic phase transition happens at the experimentally accessible pressure of 374 GPa. We claim that going beyond mean-field schemes to obtain derivatives of the total energy and optimize crystal structures at the many-body level is crucial.

¹This work was supported by the UK engineering and physics science research council under grant EP/I030190/1, and made use of computing facilities provided by HECTOR, and by the Imperial College London high performance computing centre.

9:36AM F23.00009 Novel chemistry of matter under high pressure, MAOSHENG MIAO, Beijing Computational Science Research Center — The periodicity of the elements and the non-reactivity of the inner-shell electrons are two related principles of chemistry, rooted in the atomic shell structure. Within compounds, Group I elements, for example, invariably assume the +1 oxidation state, and their chemical properties differ completely from those of the p-block elements. These general rules govern our understanding of chemical structures and reactions. Using first principles calculations, we demonstrate that under high pressure, the above doctrines can be broken. We show that both the inner shell electrons [1] and the outer shell empty orbitals [2] of Cs and other elements can involve in chemical reactions. Furthermore, we show that the quantized orbitals of the enclosed interstitial space may play the same role as atomic orbitals, an unprecedented view that led us to a unified theory for the recently observed high-pressure electride phenomenon [3].


9:48AM F23.00010 Multi-center semi-empirical quantum models for carbon under extreme thermodynamic conditions¹, NIR GOLDMAN, Lawrence Livermore Natl Lab — We report on the development of many-body density functional tight binding (DFTB) models for carbon accurate over thousands of GPa and tens of thousands of Kelvin. DFTB holds promise as a fast quantum simulation approach that can yield several orders of magnitude increase in computational efficiency over Kohn-Sham Density Functional Theory (DFT) while retaining most of its accuracy. However, standard DFTB can yield large errors for materials under high pressures and temperatures, where electrons can become delocalized. Here, we overcome these limitations by computing the environmental dependence of the DFTB Hamiltonian matrix elements directly from DFT. We include these results in DFTB calculations by either explicitly calculating three-center terms in the Hamiltonian, or by implicitly incorporating them in the diagonal matrix elements. We then determine a three-body repulsive energy for the implicit approach, which yields accurate equation of state and structural delocalized. Here, we overcome these limitations by computing the environmental dependence of the DFTB Hamiltonian matrix elements directly from DFT.

¹This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, and was funded by Laboratory Directed Research and Development grant # 12-ERD-052.

10:00AM F23.00011 Decomposition reactions in RDX at elevated temperatures and pressures¹, IGOR SCHWEIGERT, US Naval Research Laboratory — Mechanisms and rates of elementary reactions controlling condensed-phase decomposition of RDX under elevated temperatures (up to 2000 K) and pressures (up to a few GPa) are not known. Global decomposition kinetics in RDX below 700 K has been measured; however, the observed global pathways result from complex manifolds of elementary reactions and are likely to be altered by elevated temperatures. Elevated pressures can further affect the condensed-phase kinetics and compete with elevated temperatures in promoting some elementary reactions and suppressing others. This presentation will describe density functional theory (DFT) based molecular dynamics simulations of crystalline and molten RDX aimed to delineate the effects of elevated temperatures and pressures on the mechanism of initial dissociation and the resulting secondary reactions.

¹This work was supported by the Naval Research Laboratory, by the Office of Naval Research, and by the DOD High Performance Computing Modernization Program Software Application Institute for Multiscale Reactive Modeling of Insensitive Munitions.
10:12AM F23.00012 Atomistic picture of the shock to deflagration transition in a solid explosive: ultra-fast chemistry under non-equilibrium, MITCHELL WOOD, MATHEW CHERUKARA, Materials Engineering, Purdue University, EDWARD KOBERT, Theoretical Division, Los Alamos National Lab, ALEJANDRO STRACHAN, Materials Engineering, Purdue University — We use large-scale molecular dynamics (MD) simulations to describe the chemical reactions following the shock-induced collapse of cylindrical pores in the high-energy density material RDX. For shocks with particle velocities of 2km/s, we find that the collapse of a 40 nm diameter pore leads to a deflagration wave, resulting in the first atomic-level description of this process. Pore collapse leads to ultra-fast, multi-step chemical reactions that occur under non-equilibrium conditions. The formation of exothermic product molecules within a few picoseconds of the pore collapse prevents the nanoscale hot spot from quenching. Within 30 ps, a local deflagration wave develops which propagates at speeds of ~ 0.25 km/s and consists of an ultra-thin reaction zone of only ~ 5 nm, thus involving large temperature and composition gradients. These results provide insight into the initiation of detonation, which is critical to understanding the performance and safety of this class of materials.

10:24AM F23.00013 Electride-like phases at extreme compression: towards bridging the gap between theory and experiment1, STANIMIR BONEV, Lawrence Livermore National Laboratory — The transformation of materials into electride-like structures under the application of extreme pressure has attracted a lot of interest recently. Theoretical studies have predicted the existence of low-coordinated crystal phases, where the conduction electrons are localized in the interstitial atomic regions, for a number of elements at high density. Most of these works have been limited to static lattice calculations. The pressures where such transformations are projected to occur are accessible in dynamically-driven experiments, but at elevated temperatures. In this talk I will discuss the temperature dependence of electride structures, both solids and liquids, as well as the requirements for their accurate simulation.

1This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

10:36AM F23.00014 The effect of core level crossing on the high-pressure equation of state of osmium, JOHN WILLS, Los Alamos Natl Lab — The equation of state of the 5d transition metal osmium has been studied with a combination of experiment and theory at pressures up to 500 GPa. The experimental results show a c/a ratio increasing by approximately 1 percent over this pressure range and displaying anomalies at pressures near 180 GPa and near 400 GPa. We have use all-electron fully relativistic density functional theory (DFT) calculations to study the cold equation of state and structural parameters of osmium at pressures up to 500 GPa, using one LDA and two GGA functionals. The increase in the c/a ratio agrees well with experiment, and we find anomalies, although less extreme, near the experimentally observed pressures. We find that the high pressure anomaly coincides with the crossing and hybridization of the 4f(7/2) and 5p(3/2) semi-core levels. In this talk we discuss the theoretical results and methodology and the possible implication for the equations of state of the 5d transition and actinide metals.

10:48AM F23.00015 Dynamic compression experiments and first-principles simulations on liquid deuterium above the melt boundary to investigate the insulator-to-metal transition1, T.R. MATTSSON, M.D. KNUDSON, M.P. DESJARLAIS, R.W. LEMKE, K.R. COCHRANE, M.E. SAVAGE, D.E. BLISS, Sandia National Laboratories, Albuquerque, NM; J.K. ISA, A. BECKER, R. REDMER, Institute of Physics, University of Rostock, Germany. — Important phenomena at high pressure, for example in planetary science, occur at conditions that cannot be reached in shock impact experiments. Different techniques have therefore been developed at Sandia’s Z-machine. One new approach is shock-ramp loading. The accelerator delivers a two-step current pulse that accelerates the electrode, creating a well-defined shock, and subsequently produces ramp compression from the shocked state. The technique makes it possible to achieve cool (1000-2000 K), high pressure (above 300 GPa), high compression states (10-15 fold) in hydrogen, thus allowing experimental access to the region of phase space where hydrogen is predicted to undergo a first-order phase transition from an insulating molecular liquid to a conducting atomic fluid. Knowing the behavior of hydrogen under these conditions is of pivotal importance to understanding the physics of giant planets. We will survey theoretical predictions for the liquid-liquid insulator-to-metal transition in hydrogen and present the results of experiments on Z.

1Sandia is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

Tuesday, March 3, 2015 8:00AM - 11:00AM — Session F24 DMP: Superconducting Quantum Devices and Josephson Junctions 203AB - Laura Adams, Harvard University

8:00AM F24.00001 Direct measurements of the current-phase relation in long-range spin-triplet SFS Josephson junctions, DAVID HAMILTON, DALE VAN HARLINGEN, Univ of Illinois - Urbana, YIXING WANG, NORMAN BIRGE, Michigan State University — We present direct measurements of the current-phase relation (CPR) of Josephson junctions which use multiple ferromagnetic layers to generate long-range spin-triplet pair correlations. Using a phase-sensitive Josephson interferometry technique, we obtain the phase and temperature dependence of this spin-triplet supercurrent. We also demonstrate the use of an inductive shunt to enhance this technique at higher critical currents. Our data suggest that the current-phase relation of these junctions is harmonic in character. Further measurements are planned in order to determine the ground state phase shift of these junctions.

8:12AM F24.00002 Parity conservation in a Cooper-pair transistor, DAVID VAN WOERKOM, ATTILA GERESEI, SEBASTIAN RUBBERT, ANTON AKHMEROV, LEO KOUWENHOVEN, Delft Univ of Tech — In a small superconducting island, hosting an even number of electrons, all charge carriers form Cooper pairs, defining the ground state of the Cooper-pair transistor (CPT). An additional, unpaired electron can only occupy a higher energy level, determined by the superconducting order parameter. This even-odd (parity) energy difference makes the CPT a very sensitive charge detector as well as a prototype superconducting qubit, whose coherence relies on the conservation of the parity of the island. Here we report parity conservation in a niobium-based superconductor, NbTiN, for the first time. NbTiN is a popular superconductor since it can sustain high parallel and perpendicular magnetic fields which is often a requirement for hybrid devices. The parity conversation resulted in the first 2e-periodicity measurements in a non-Aluminium CPT. The highest reported parity lifetime ever, which was longer than one minute, was measured. The parity lifetime didn’t saturate down to a base temperature of 12mK, showing state-of-the-art device shielding of thermal photons. We show that our CPT is magnetic field compatible, opening new possibilities for coupling spin degrees of freedom to superconducting circuits and qubits and for topological superconductivity, enabling qubits based on Majorana fermions.
entirely of magnetic-field compatible materials, offering new opportunities for hybrid experiments combining microwave circuits with polarized spin ensembles. This flux-qubit like behaviour results from non-sinusoidal current-phase relations in the nanowire Josephson elements. These hybrid microwave circuits are made of conventional superconductor/ferromagnet (S/F) systems since long-range spin-triplet correlations (LRTCs) were predicted. Despite the many breakthroughs so far in this field, the ability to control the triplet generation reliably still needs to be realized before these devices can be used in technological applications. One possible direction to control the state in such structures is to manipulate the magnetizations of the various F layers within, specifically to switch between colinear and non-colinear directions between the layers. In this work, we report on the progress made to control LRTC generation in such a way.

Supported by the DOE-BES under grant DE-FG-02-06ER46341.

1Supported by Northrop Grumman Corporation and by IARP under SPAWAR contract N66001-12-C-2017.

8:36AM F24.00004 Control of triplet supercurrent in superconductor/ferromagnet hybrid systems , WILLIAM MARTINEZ, W.P. PRATT, JR., NORMAN O. BIRGE, Michigan State University — A lot of excitement has been generated in superconductor/ferromagnet (S/F) systems since long-range spin-triplet correlations (LRTCs) were predicted. Despite the many breakthroughs so far in this field, the ability to control the triplet generation reliably still needs to be realized before these devices can be used in technological applications. One possible direction to control the state in such structures is to manipulate the magnetizations of the various F layers within, specifically to switch between colinear and non-colinear directions between the layers. In this work, we report on the progress made to control LRTC generation in such a way.

Supported by the DOE-BES under grant DE-FG-02-06ER46341.

8:48AM F24.00005 Fabrication and characterization of single domain magnetic Josephson . MAZIN KHASAWNEH, BETHANY NIEDZIELSKI, ERICH GINGERICH, REZA LOLOEE, WILLIAM PRATT, JR, NORMAN BIRGE, Michigan State Univ — A nice effect that can be observed in Ferromagnetic (F) Josephson junctions is the crossover from a standard Josephson junction (0-junction) to a “π-junction” as a function of the thickness of the F layer, dp. This observation is interesting not only from the scientific point of view but also from a practical point of view, as it could be used in cryogenic memory, for example. In this work we are fabricating and measuring micron-scale Josephson junctions containing a soft magnetic material such as NiFe. Such junctions exhibit clear switching of the single-domain magnetic element as a function of applied field. We will report on our recent progress.

1Northrop Grumman

9:00AM F24.00006 Wireless Josephson Junction Arrays , LAURA ADAMS, Harvard University — We report low temperature, microwave transmission measurements on a wireless two-dimensional network of Josephson junction arrays composed of superconductor-insulator-superconductor tunnel junctions. Unlike their biased counterparts, by removing all electrical contacts to the arrays and superfluous microwave components and interconnects in the transmission line, we observe new collective behavior in the transmission spectra. In particular we will show emergent behavior that systematically responds to changes in microwave power at fixed temperature. Likewise we will show the dynamic and collective response of the arrays while tuning the temperature at fixed microwave power. We discuss these spectra in terms of the Berezinskii-Kosterlitz-Thouless phase transition and Shapiro steps. We gratefully acknowledge the support Prof. Steven Anlage at the University of Maryland and Prof. Allen Goldman at the University of Minnesota.

1Physics and School of Engineering and Applied Sciences

9:12AM F24.00007 ABSTRACT WITHDRAWN —

9:24AM F24.00008 $8\pi$-periodic Josephson effects in a quantum dot / quantum spin-Hall josephson junction system , HOI-YIN HUI, CMT-C, Univ of MD, College Park, JAY SAU, CMT-C and JQI, University of Maryland — Josephson junctions made of conventional $s$-wave superconductors display $2\pi$ periodicity. On the other hand, $\pi$-periodic fractional Josephson effect is known to be a characteristic signature of topological superconductors and Majorana fermions [1]. Zhang and Kane have shown that Josephson junctions made of topological superconductors are $8\pi$-periodic if interaction is used to avoid dissipation [2]. Here we present a general argument for how time-reversal symmetry and Z2 non-trivial topology constrains the Josephson periodicity to be $8\pi$. We then illustrate this through a microscopic model of a quantum dot in a quantum spin-hall Josephson junction.

1Work supported by NSF-JQI-PFC, LPS-CMTC and Microsoft Q

9:36AM F24.00009 Superconducting-semiconducting nanowire hybrid microwave circuits , G. DE LANGE, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, P.O. Box 5046, 2600 GA Delft, The Netherlands, B. VAN HECK, Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands, A. BRUNO, D. VAN WOERKOM, A. GEREDE, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, P.O. Box 5046, 2600 GA Delft, The Netherlands, S. R. PLISSARD, E. P. A. M. BAKKERS, Eindhoven University of Technology, 5612 MB Eindhoven, The Netherlands, A. R. AKHMEROV, L. DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, P.O. Box 5046, 2600 GA Delft, The Netherlands — Hybrid superconducting-semiconducting circuits offer a versatile platform for studying quantum effects in mesoscopic solid-state systems. We report the realization of hybrid artificial atoms based on Indium-Arsenide nanowire Josephson elements in a circuit quantum electrodynamics architecture. Transmon-like single-junction devices have gate-tunable transition frequencies. Split-junction devices behave as transmons near zero applied flux and as flux qubits near half flux quantum, wherein states with oppositely flowing persistent current can be driven by microwaves. This flux-qubit like behaviour results from non-sinusoidal current-phase relations in the nanowire Josephson elements. These hybrid microwave circuits are made entirely of magnetic-field compatible materials, offering new opportunities for hybrid experiments combining microwave circuits with polarized spin ensembles and Majorana bound states.

1We acknowledge funding from Microsoft Research and the Dutch Organization for Fundamental Research on Matter (FOM).
9:48 AM F24.00010 An Ultra-Sensitive Electrometer based on the Cavity-Embedded Cooper-Pair Transistor

This work was supported by the NSF under Grant No. DMR-1104821, by the ARO under Contract No, W911NF-13-1-0377 and by AFOSR/DARPA under Agreement No. FA8750-12-2-0339.

1This work was supported by the UC Scholars Program

10:00AM F24.00011 Microwave Resonant Activation Results in Hybrid MgB2/I/Pb and MgB2/I/Sn Josephson Junctions with Low to Moderate Damping

The reflected wave is amplified by both SLUG and HEMT amplifiers before its phase is measured. Results of recent measurements on the cCPT will be compared with theoretical predictions.

10:12AM F24.00012 Improved tunable microstrip SQUID amplifier for the Axion Dark Matter xExperiment (ADMX)

We have demonstrated that the phase of the reflected wave from the cCPT can be measured with high accuracy. The results of recent measurements on the cCPT will be compared with theoretical predictions.


We have fabricated Josephson junctions by using a focused helium ion beam to irradiate a narrow barrier in the plane of a 25 mm thick Y-Ba-Cu-O film. We have measured the critical current of these junctions as a function of magnetic field and temperature. Our results are consistent with theoretical predictions.

10:36AM F24.00014 Transition from superconducting-normal metal to superconducting-insulating barrier in focused helium beam YBCO Josephson junctions

We report measurements of the Josephson tinctor transition (MIT) in high-temperature superconductors, planar Y-Ba-Cu-O Josephson junctions. The junctions were made by irradiation of a 1 nm barrier with a focused helium ion beam. Our data show that the MIT occurs at a temperature of about 1 K.


We have developed a model based on the Stewart-McCumber and Ambegaokar-Halperin models that includes the effect of self-field effects. Our model shows good agreement with experimental measurements.

This work was supported by the UC Scholars Program
8:00AM F25.00001 Hole motion in the Hubbard model. B. MORITZ, SLAC National Accelerator Laboratory, Y. WANG, C.J. JIA, Stanford University and SLAC National Accelerator Laboratory, C.-C. CHEN, Argonne National Laboratory, M. VAN VEENENDAAL, Argonne National Laboratory and Northern Illinois University, T. P. DEVEREAUX, Stanford University and SLAC National Accelerator Laboratory, K. WÖHLFELD, University of Warsaw and SLAC National Accelerator Laboratory — The motion of a single hole in the half-filled two-dimensional Hubbard model is not fully understood, despite the fact that it constitutes a crucial first step in unravelling the doping evolution of the electronic properties. Here we unambiguously show, using anglical-particle-hole breakup calculations, that the bandwidth renormalization is determined by a complex interplay between (i) the strong coupling of a hole to magnons and (ii) the strongly renormalized, but effectively free, next-nearest-neighbor hopping resulting from additional delocalization pathways. By studying the changes in the hole dynamics in the one-to-two-dimensional crossover regime we comment on applicability of the spin-charge separation ansatz and the spin density wave dispersion picture in the single-particle dynamics of the two-dimensional Hubbard model.

8:12AM F25.00002 Spectral properties of the two-dimensional Hubbard model with next-nearest-neighbor hopping near the Mott transition. MASANORI KOHNO, International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Japan — The single-particle spectral properties of the two-dimensional Hubbard model with next-nearest-neighbor hopping near the Mott transition are investigated using cluster perturbation theory [1]. Based on the consideration of how the next-nearest-neighbor hopping shifts the spectral-weight distribution, the spectral features are explained by tracing the origins back to those of the one-dimensional and two-dimensional Hubbard models [1-3]. From this viewpoint, various anomalous features observed in hole-doped and electron-doped cuprate high-temperature superconductors, such as the pseudogaps in different momentum regimes between hole-doped and electron-doped cuprates, are collectively explained as properties of a two-dimensional system with next-nearest-neighbor hopping near the Mott transition.

8:24AM F25.00003 Origin of the quasiparticle dispersion kinks in Bi-2212 determined from angle-resolved inelastic electron scattering\(^1\). SEAN VIG, ANSHUL KOGAR, Univ of Illinois - Urbana, VIVEK MISHRA, MIKE NORMAN, Argonne National Laboratory, GENDA GU, Brookhaven National Laboratory, PETER ABBAMONTE, Univ of Illinois - Urbana — The kink features in low energy photoemission and ARPES measurements in cuprate superconductors have been extensively studied using angle-resolved photoemission spectroscopy (ARPES). The existence of these kinks is a signature of a renormalization of the fermionic quasiparticles due to coupling to some bosonic collective mode at a scale related to the kink energy. In this talk, we will present angle-resolved inelastic electron scattering studies of the bosonic collective excitations in optimally doped Bi\(_2\)Sr\(_2\)Ca\(_{x}\)Cu\(_{2+x}\)O\(_{2+y}\). Performing a 2D momentum parameterization of these modes, we reconstruct the complete dynamical susceptibility, \(\chi(q,\omega)\), which we use to perform a one-loop self energy correction to the quasiparticle dispersion. The result reproduces well the dispersion observed with ARPES, indicating that these excitations are the origin of the observed kinks. I will discuss the implications of our study for phonon vs. spin fluctuation interpretation of these effects.

\(^1\)This work was supported as part of the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science

8:36AM F25.00004 Ultrafast quenching of electron-boson interaction and superconducting gap in a cuprate superconductor. WENTAO ZHANG, CHOOKYU HWANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA, CHRISTOPHER SMALLWOOD, TRISTAN MILLER, GREGORY AFFELDT, Department of Physics, University of California, Berkeley, California 94720, USA, KOSHI KURASHIMA, Department of Applied Physics, Tohoku University, Sendai 980-8579, Japan, CHRISSJOZWIACKI, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA, HIROSHI EISAKI, Electronics and Photonics Research Institute, National Institute of Advanced Industrial Science and Technology, Ibaraki 305-8568, Japan, TADASHI ADACHI, Department of Engineering and Applied Sciences, Sophia University, Tokyo, Japan, YOJI KOIKE, Department of Applied Physics, Tohoku University, Sendai 980-8579, Japan, JUNG-HAI LEE, LANZARA ALESSANDRA, Department of Physics, University of California, Berkeley, California 94720, USA — Ultrafast spectroscopy makes it possible to track similarities and correlations that are not evident in equilibrium. Time- and angle-resolved photoemission measurements on cuprate high-temperature superconductor reveals that below the superconductor’s critical temperature, ultrafast excitations trigger a synchronous decrease of electron self-energy and superconducting gap. In contrast, electron-boson coupling is unresponsive to ultrafast excitations above the superconductor’s critical temperature and in the metallic state of a related material. These findings open a new pathway for studying transient self-energy and correlation effects in solids.

8:48AM F25.00005 Calculation of RIXS spectra of cuprates using band structure parameters. YIFEI SHI, ISRAEL KLIICH, University of Virginia, DAVID BENJAMIN, EUGENE DEMLER. Harvard University — We explore the quasi particle theory to study the Resonant Inelastic X-ray Scattering(RIXS) by using the band structure parameters. We use both the determinant method(D. Benjamin, I. Kliich and E. Demler, Phys. Rev. Lett. 112, 247002(2014)) and the expansion in the core-hole potential. The methods are applied to the (Ca\(_1-x\)La\(_x\)\(_2\))Ba\(_2\)Cu\(_3\)O\(_y\) system with next-nearest-neighbor hopping near the Mott transition.

9:00AM F25.00006 Nernst Effect in HTC cuprate from BDW. CHUNXIAO LIU, University of Maryland College Park — The pseudogap regime in low hole doped high \(T_c\) cuprate superconductors exhibits peculiar experimental signatures like the detection of enhanced negative signals for Hall, Seebeck and Nernst coefficients. It has been suggested that some of these phenomena can be understood in terms of a competition between a bond density wave order and superconductivity. In this work, we theoretically studied the Nernst effect using a mean-field quasi-particle model with \(Q_1 = (0, 2\pi r /3)\) and \(Q_2 = (2\pi r /3, 0)\). By employing semi-classical Boltzmann dynamics, we have shown that the thermoelectric coefficient depends linearly on the absolute value of order parameter for small values of the induced gap and the contribution mainly comes from the small area of hot spot.

9:12AM F25.00007 Electronic structure of La\(_2\)CuO\(_4\) within self-consistent GW approximation. SANGKOOK CHOI, Rutgers University, Piscataway, NJ, USA, ANDREY KUTÉPOV, Ames Laboratory, Ames, IA, USA, KRISTJAN HAULE, Rutgers University, Piscataway, NJ, USA, MARK VAN SCHILFGAARDE, King’s college, London, UK, GABRIEL KÖTLIAR, Rutgers University, Piscataway, NJ, USA — La\(_2\)CuO\(_4\), the parent compound of the high-temperature superconductor, is a classic strongly-correlated material. We present a first-principles study on the excitations spectrum of La\(_2\)CuO\(_4\) within the self-consistent GW approximation based on full-potential linearized augmented-plane-wave methods. We compare the results of the Quasiparticle (QP) self-consistency and the fully self consistent approach. We find that the spin-polarized self-consistent GW calculation succeed in predicting the insulating ground state and anti-ferromagnetic superordering. It also describes charge-transfer character of the top of the valence band and reproduce the experimental spectral function well, including the weight of the copper d and the position of the lanthanum levels, but it overestimates the bandgap by 75%. We comment on the implications of our results for the implementation of GW+DMFT in a one shot, QP, and fully self consistent version.
9:24AM F25.00008 Strong Correlation of Electron Saddle Point Singularities to the Anomalous Isotope Effect in Zr, Nb, Sn, and YBa2Cu3O7. GUANG-LIN ZHAO, Physics Department, Southern University and A&M College — Anomalously small isotope effect in some high and low Tc superconductors such as Zr, Nb, Sn, and YBa2Cu3O7 (YBCO) created a great challenge for understanding. It has been shown by experiments and first-principles calculations that there exist extended saddle point singularities in the electronic structures of these materials. In this work, a new methodology is further implemented by integrating first-principles calculations of electronic structures of the materials into the theory of many-body physics for superconductivity. The aim is to seek a unified methodology to calculate the electronic and superconducting properties of these materials. It is demonstrated from first-principles that the extended saddle point singularities in Zr, Nb, Sn, and YBCO strongly correlate to the anomalous isotope effect in these superconductors. However, there still exist some differences between the calculated and experimental results that require further research work.

3The work was funded in part by NSF LASIGMA Project (Award No. EPS-1003897, NSF2010-15-RII-SUBR) and by AFOSR (Award No. FA9550-09-1-0367).

9:36AM F25.00009 Resonant tunneling of fluctuation Cooper pairs: Shapiro steps above superconducting critical temperature. ALEXEY GALDA, Materials Science Division, Argonne National Laboratory, ALEXANDER MEL’NIKOV, Institute for Physics of Microstructures, Russian Academy of Sciences, VALERII VINOKUR, Materials Science Division, Argonne National Laboratory — Superconducting fluctuations have proved to be an irreducible source of information about microscopic and macroscopic material parameters that could be inferred from experiments. According to common wisdom, the effect of thermodynamic fluctuations in the vicinity of the superconducting transition temperature, Tc, is to round off all of the sharp corners and discontinuities, which otherwise would have been expected to occur at Tc. Here we report the current spikes due to radiation-induced resonant tunneling of fluctuation Cooper pairs between two superconductors which grow even sharper and more pronounced upon approach to Tc. This striking effect offers an unprecedented tool for direct measurements of fluctuation Cooper pairs’ lifetime, which is key to our understanding of the fluctuation regime, most notably to nature of the pseudogap state in high temperature superconductors. Our finding marks a radical departure from the conventional view of superconducting fluctuations as blurring and rounding phenomenon.

9:48AM F25.00010 Inhomogeneities in a strongly correlated d-wave superconductors in the limit of strong disorder. DEBMALYA CHAKRABORTY, Indian Institute of Science Education and Research-Kolkata, Mohanpur Campus, India-741252, RAJDEEP SENARMA, Department of Theoretical Physics, Tata Institute of Fundamental Research, Mumbai-400005, India, AMIT GHOSAL, Indian Institute of Science Education and Research-Kolkata, Mohanpur Campus, India-741252 — The complex interplay of the strong correlations and impurities in a high temperature superconductor is analyzed within a Hartree-Fock-Bogoliubov theory, augmented with Gutzwiller approximation for taking care of the strong electronic repulsion. The inclusion of such correlations is found to play a crucial role in reducing inhomogeneities in both qualitative and quantitative manner. This difference is comprehended by investigating the underlying one-particle “normal states” that includes the order parameters in the Hartree and Fock channels in the absence of superconductivity. This amounts to the renormalization of disorder both on the lattice sites and also on links. These two components of disorder turn out to be spatially anti-correlated through self-consistency. Interestingly, a simple pairing theory in terms of these normal states is shown to show how disorder modifies the superconducting gap and reduces disorder. This effect puts a limit on long-range superconductivity, while fluctuations can persist to higher temperature. BCS-type model calculations are used to show how disorder modifies the superconducting gap and reduces Tc. Some ideas of how to recuperate a higher Tc from superconducting fluctuations are discussed.

10:00AM F25.00011 Effects of thermal disorder on electronic structure, electron-phonon coupling and spin-fluctuations in high-Tc cuprates, THOMAS JARLBORG, DPMC, University of Geneva, CH1211 Geneva 4 — The superconducting Tc’s are estimated from the values of electron-phonon and spin-phonon coupling in typical high-Tc cuprates. It is shown that the couplings are peaked for just a few q-vectors because of the 2-dimensional Fermi surface shape. The influence of few severe spin-phonon modes compensates the low electronic density-of-states, which allows for a high Tc. [1] Thermal disorder at moderately high temperature perturbs the strongly correlated modes through incoherent potential fluctuations of the Madelung terms, and electronic structure calculations show that the effective spin-phonon coupling suffers from lattice disorder. This effect puts a limit on long-range superconductivity, while fluctuations can persist to higher temperature. BCS-type model calculations are used to show how disorder modifies the superconducting gap and reduces Tc. Some ideas of how to recuperate a higher Tc from superconducting fluctuations are discussed.


10:12AM F25.00012 Pairing glue at finite temperature in high-temperature superconductors. A. REYMBAUT, RQMP, Phys. Dept. Université de Sherbrooke, QC J1K 2R1, G. SORDI, Phys. Dept. HTC, Royal Holloway, U. London, TW20 0EX, D. BERGERON, P. SEMIN, M. CHARLESBOIS, RQMP, Phys. Dept. Université de Sherbrooke, QC J1K 2R1, A.-M.S. TREMBLAY, RQMP, Phys. Dept. Université de Sherbrooke, QC J1K 2R1, K. CIFAR, ON M5G 1Z8, (2014). — Superconductivity has been documented in the weak to intermediate correlation regime, the strong-correlation limit is still largely unexplored. One of the best ways to access the frequencies relevant for the unconventional pairing dynamics present in doped Mott insulators is to study the anomalous spectral function associated with the frequency-dependent Gorkov function. Already studied at zero temperature,[2-4] that anomalous spectral function is difficult to obtain at finite temperature when one needs maximum entropy continuation methodology.[5] Indeed, this method requires a non-negative spectral function. In this talk we present the solution to this problem. Then we show our results for the Hubbard model on a 2x2 cluster solved with Cluster Dynamical Mean Field Theory (CDMFT) using Continuous-Time Quantum Monte-Carlo (CTQMC) in the hybridization expansion as an impurity solver.


10:24AM F25.00013 DMRG simulations of a 3 band Hubbard model for the cuprates. STEVEN WHITE, University of California, Irvine, DOUGLAS SCALAPINO, University of California, Santa Barbara — While both the hole and electron doped cuprates can exhibit d2̃ – 2̃-wave superconductivity, the local distribution of the doped carriers is known to be significantly different with the doped holes going primarily on the O sites while the doped electrons go on the Cu sites. Here we report the results of a density-matrix-renormalization-group calculation for a three-orbital conventional superconductivity has been documented in the weak to intermediate correlation regime, the strong-correlation limit is still largely unexplored.[1] One of the best ways to access the frequencies relevant for the unconventional pairing dynamics present in doped Mott insulators is to study the anomalous spectral function associated with the frequency-dependent Gorkov function. Already studied at zero temperature,[2-4] that anomalous spectral function is difficult to obtain at finite temperature when one needs maximum entropy continuation methodology.[5] Indeed, this method requires a non-negative spectral function. In this talk we present the solution to this problem. Then we show our results for the Hubbard model on a 2x2 cluster solved with Cluster Dynamical Mean Field Theory (CDMFT) using Continuous-Time Quantum Monte-Carlo (CTQMC) in the hybridization expansion as an impurity solver.


10:24AM F25.00013 DMRG simulations of a 3 band Hubbard model for the cuprates, STEVEN WHITE, University of California, Irvine, DOUGLAS SCALAPINO, University of California, Santa Barbara — While both the hole and electron doped cuprates can exhibit d2̃ – 2̃-wave superconductivity, the local distribution of the doped carriers is known to be significantly different with the doped holes going primarily on the O sites while the doped electrons go on the Cu sites. Here we report the results of a density-matrix-renormalization-group calculation for a three-orbital model of a CuO2 lattice. In addition to the asymmetric dependence of the intra-unit-cell occupation of the Cu and O for hole and electron doping, we find important differences in the longer range spin and charge correlations. As expected, the pairwise response has an d2̃ – 2̃-like structure for both the hole and electron doped systems.

10:36AM F25.00014 DMFT+FLEX approach to unconventional superconductivity. MOTOHARU KITATANI, NAOTO TSUJI, HIDEO AOKI, Department of Physics, University of Tokyo — We propose to combine the dynamical mean field theory (DMFT) with the fluctuation exchange approximation (FLEX) to investigate strongly correlated systems and especially to obtain a phase diagram for d-wave superconductors such as the cuprates, which seems inaccessible to the DMFT due to the pair-breaking effective pairing interaction, so that the method can describe anisotropic pairing along with the local correlation effect that is important in Mott physics. We have applied the formalism to the two-dimensional repulsive Hubbard model to obtain superconducting transition temperature. The result does indeed exhibit a Tc-dome structure. We have traced back the origin of the dome to the local vertex correction from DMFT that gives a filling-dependent effect on the FLEX self-energy.
10:48AM F25.00015 Quantum oscillation signatures of spin-orbit interactions controlling the residual nodal bilayer-splitting in underdoped high-$T_c$ cuprates, NEIL HARRISON, Los Alamos National Labs, ARKADY SHEKHTER, National High Magnetic Field Laboratory, Tallahassee — We investigate the origin of the small residual nodal bilayer-splitting in the underdoped high-$T_c$ superconductor YBa$_2$Cu$_3$O$_{6.1}$-$x$ using the results of recently published angle-resolved quantum oscillation data [Sebastian et al., Nature 511, 61 (2014)]. A crucial clue to the origin of the residual bilayer-splitting is found to be provided by the anomalously small Zeeman-splitting of some of the observed cyclotron orbits. We show that such an anomalously Zeeman-splitting (or small effective $g$-factor) for a subset of orbits can be explained by spin-orbit interactions, which become significant in the nodal regions as a result of the vanishing bilayer coupling. The primary effect of spin-orbit interactions is to cause quasiparticles traversing the nodal region of the Brillouin zone to undergo a spin flip. We suggest that the Rashba-like spin-orbit interactions, naturally present in bilayer systems, have the right symmetry and magnitude to give rise to a network of coupled orbits consistent with experimental observations in underdoped YBa$_2$Cu$_3$O$_{6.1}$-$x$. This work is supported by the DOE BES proposal LANLF100, while the magnet lab is supported by the NSF and Florida State.

Tuesday, March 3, 2015 8:00AM - 11:00AM –
Session F26 DCP: Focus Session: At the Interface of Molecules and Materials I

8:00AM F26.00001 Tunable and responsive plasmonic properties of metal oxide nanocrystals, DELIA MILLIRON, The University of Texas at Austin — Degenerately doped metal oxide semiconductors, like ITO, exhibit plasmonic resonance near and mid-infrared wavelengths tunable by varying their composition. Nanocrystals of many such materials have now been synthesized and are emerging that leverage the responsiveness of their localized surface plasmon resonance (LSPR) to electronic charging and discharging. For example, electrochromic glass that can dynamically control heat loads in buildings is under development. In biological systems, plasmonic oxide nanocrystals can act as active sensors, where changes in their optical absorption indicates biochemical redox has occurred. Nonetheless, significant fundamental questions remain open regarding the nature of the infrared optical response in these doped oxides. Doping impurities influence the optoelectronic properties beyond simply donating free carriers. For example, the distribution of Sn in ITO was found to dramatically influence the line shape of the LSPR and the effective electron mobility. In addition, by post-synthetically modifying carrier concentrations (through photodoping or electrochemical doping), we have observed that aliovalent doping and electronic doping each modify LSPR spectra, providing access to a broad range of tunable optical properties. Heterogeneous broadening, uncovered by single nanocrystal spectroscopy, also contributes to ensemble line shapes, complicating direct interpretation of LSPR spectra. Finally, the possibility of electric field enhancement by metal oxide LSPRs is critically examined to suggest what future applications might be on the horizon.

8:36AM F26.00002 Tunable Plasmonic Nanoparticles with Catalytically Active High-Index Facets, HAO JING, University of South Carolina, NICOLAS LARGE1, Northwestern University, QINFENG ZHANG, University of South Carolina, PETER NORDLANDER, Rice University, HUI WANG, University of South Carolina — Noble metal nanoparticles have been of tremendous interest due to their intriguing size- and shape-dependent plasmonic and catalytic properties. Combining tunable plasmon resonances with superior catalytic activities on the same metallic nanoparticle, however, has long been challenging because nanoplasmonics and nanocatalysis typically require nanoparticles in two drastically different size regimes. Here, we demonstrate that creation of high-index facets on subwavelength metallic nanoparticles provides a unique approach to the integration of desired plasmonic and catalytic properties on the same nanoparticle. Through site-selective surface etching of metallic nanocuboids whose surfaces are dominated by low-index facets, we have controllably fabricated nanorice and nanodumbbell shaped particles, which exhibit drastically enhanced catalytic activities arising from the catalytically active high-index facets abundant on the particle surfaces. The nanorice and nanodumbbell particles also possess appealing tunable plasmonic properties that allow us to gain quantitative insights into nanoparticle-catalyzed reactions with unprecedented sensitivity and detail through time-resolved plasmon-enhanced spectroscopic measurements.

1 Past affiliation: Rice University

8:48AM F26.00003 Protected Noble-Metal Clusters at the Transition from Molecules to Materials, ROBERT L. WHETTEN, University of Texas, San Antonio — Protected noble-metal clusters are found at a molecular level of definite composition and structure up to a size of 145-165 metal atoms. Curiously, this size-range is also where several key signatures of metallic character begin to converge. These substances have been of great interest for many application-areas in the past couple decades, but the understanding of their structure and bonding, remarkable self-selection, electronic structure and optical properties has only recently started to reach a fundamental or molecular level of definition. This presentation emphasizes this recent progress and also outlines the prospects for extending the molecular domain of metallurgy well beyond the 200- atom range, thanks to advances in experimental & theoretical methods.

9:24AM F26.00004 ABSTRACT WITHDRAWN —

10:00AM F26.00005 Rich Information on Quantum States and Ways to Calculate It in The Absorption Spectra of Au$_{144}$ Gold Cluster Compound, XOCHITL LOPEZ-LOZANO, ROBERT L. WHETTEN, Department of Physics & Astronomy, The University of Texas at San Antonio, HANS-CHRISTIAN WEISSKER, Aix-Marseille Univ., CNRS, CInaM — In recent decades, the prevalent view has been that noble-metal clusters of intermediate size necessarily have smooth optical absorption spectra of low information content in the near-IR, VIS and near-UV regions. At most, one expects a broad, smooth localized surface plasmon resonance feature. Recently, we demonstrate that, in contrast to the commonly held view, the optical absorption of the most widely applied gold cluster, the thiolate-protected Au$_{144}$ cluster, exhibits a rich spectrum of bands that are individually visible over the entire near-IR, VIS and near-UV regions (1.0-4.0 eV), demonstrating high information content related to the quantum size effects which distinguish the nanoparticles from the bulk materials. In the calculation, the result is sensitive to the details of the structure. In the present work, we systematically compare the different structures actually used to date. We studied aspects like symmetry, geometry and type of ligands. In particular, we discuss the effect of their differences on the optical absorption spectra as well as how the theoretical methodology influences the final results.
Calculations and the Classical Picture of Charge Oscillations, HANS-CHRISTIAN WEISSKER, CNRS - CINAM, Centre Interdisciplinaire de Nanoscience de Marseille, XÓCHITL LÓPEZ-LOZANO, Department of Physics and Astronomy — The University of Texas at San Antonio One UTSA Circle, San Antonio, TX 78249 — The localized surface-plasmon resonance (LSPR) in metal clusters corresponds to a collective charge oscillation of quasi-free electrons of the metal. We use the real-time formulation [1] of time-dependent density-functional theory (TDDFT) with pseudopotentials to study the correspondence and differences of the quantum calculations with the classical picture. By means of animations, we discuss the real-time evolution of the electronic density for different geometries. While there is a clear correspondence between the overall picture of a charge oscillation and the actual dynamic in quantum-sized clusters, the situation is much more intricate owing to quantum effects and the atomistic inhomogeneity of the cluster. A fine pattern is present over the volume of the cluster even at moments of zero overall polarization. The difference between Ag and Au is clearly visible. Finally, we discuss the question of collective vs. molecular-like transitions; even for single transitions, the dynamics of the total density can be similar to the picture of a charge oscillation.

Interdisciplinaire de Nanoscience de Marseille, XÓCHITL LÓPEZ-LOZANO, Department of Physics and Astronomy — The University of Texas at San Antonio


[3] López-Lozano, X.; Barron, H.; Mottet, C.; Weissker,
8:36AM F27.00002 Two-Dimensional Line Shapes in Electronic-Vibrational Spectroscopy as a Measure of Correlated Spectral Dynamics of Electronic and Vibrational Degrees of Freedom.

NICHOLAS LEWIS, HUI DONG, THOMAS OLIVER, GRAHAM FLEMING, University of California, Berkeley — 2D optical spectroscopies in many different frequency regimes have been useful to study the correlated spectral behavior for many different types of system degrees of freedom. The slope of the center-line of a feature in 2D electronic and 2D infrared spectroscopy has been shown to provide detailed information about the correlation functions that describe the system-bath coupling for the system degrees of freedom. Recently, we have demonstrated a new spectroscopic technique, 2D electronic-vibrational spectroscopy, that is capable of directly measuring the correlation between spectral motion of the electronic and vibrational degrees of freedom. Here we demonstrate that the center-line slope of a 2DEV resonance can be directly related to the correlation function for the vibrational degrees of freedom on the electronic excited state. We show experimentally that this can be observed in 2DEV spectra of the dye DTTCI. Finally, we show how 2DEV spectra can be used to directly measure the strength of system-bath coupling for the vibrational degrees of freedom on the electronic excited state versus those on the electronic ground state.

1K. Kwac and M. Cho, J. Phys. Chem. A 107, 5903
2T.A.A. Oliver, N.H.C. Lewis and G.R. Fleming, PNAS 111, 0927

8:48AM F27.00003 Femtosecond Stimulated Raman Spectroscopy by Six-Wave Mixing. ANDREW MORAN, University of North Carolina — Knowledge of the structural changes that accompany photochemical reactions has motivated the development of a wide variety of time-resolved vibrational spectroscopies. For example, a technique known as femtosecond stimulated Raman spectroscopy (FSSR) has yielded important insights into numerous photochemical processes in the past 10-15 years. Simultaneous probing of all resonances in the fingerprint region of the vibrational spectrum and sensitivity to dynamics on the 100-fs time scale are the primary selling points for the FSSR technique. Despite its utility, FSSR is challenged by a large background of residual laser light and lower-order nonlinearities. In this talk, I will introduce a newly developed FSRS experiment in which five laser beams are used to eliminate the background of residual laser light and lower-order nonlinearities present in the traditional three-beam FSRS geometry. Applications to photoinduced reactions in triiodide and heme proteins will be discussed. It is envisioned that this approach will be useful for investigating photoinduced dynamics in a wide variety of condensed phase systems.

9:24AM F27.00004 Quantum Process Tomography by 2D Fluorescence Spectroscopy. LEONARDO A. PACHON, Institute of Physics, University of Antioquia. Department of Chemistry and Chemical Biology, Harvard University. — Characterization of quantum dynamics is one of the most important steps toward the implementation of any quantum technology and therefore, it is of fundamental relevance. Traditionally, dynamics are studied for particular initial preparations and hence, only partial information about the underlying physical processes is obtained. To overcome this drawback, a variety of proposals based on spectroscopic techniques have been suggested. Quantum Processes Tomography allows for the experimental reconstruction of the dynamics regardless the initial condition. Despite the success of QTP, the spectroscopic techniques they are based on require large samples to enhance the non-linear signal. Hence, particular features of the dynamics and realistic time scales are hidden by the incoherent average over the large structural and electronic heterogeneity. Based on recent progress on non-linear spectroscopies using collinear phase-modulated ultra-short pulses, which is suitable for single molecule spectroscopy, a formulation of single molecule QPT with classical light is provided here. This technique is applied to recover the dynamics of a model dimer. The single molecule character of this technique predicts longer coherence times than those techniques based on the phase-matching condition.

9:36AM F27.00005 Ultrafast 2D Fluorescence Spectroscopy using Spectrally Entangled Photon Pairs. MICHAEL RAYMER, University of Oregon — We propose entangled photon-pair two-dimensional fluorescence spectroscopy (EPP-2DFS) to probe the nonlinear electronic response of molecular systems. [1] The method, inspired by results in [2], uses a technique from quantum optics—a separated two-photon (Franson) interferometer, which generates time-delayed packets of time-frequency-entangled photon pairs. This interferometer is incorporated into the framework of a fluorescence-detected 2D optical spectroscopic experiment [3]. The continuous stream of entangled photons are phase-modulated in the interferometer, and used to excite a two-photon-absorbing sample, whose excited-state population is selectively detected by simultaneously monitoring the sample fluorescence and the transmitted exciting fields. In comparison to standard classical 2DFS techniques using coherent laser pulses and standard pulse-scanning sequences, advantages of this scheme include the suppression of uncorrelated background signals, the suppression of diagonal 2D spectral features, the enhancement and narrowing of off-diagonal spectral cross-peaks that contain information about electronic coupling, and the possibility for enhancement of simultaneous time- and frequency resolution, including spectral selectivity within an inhomogeneously broadened distribution. These effects arise from the properties of parametric down-conversion light source, which effectively creates a different interaction-scanning protocol than in standard laser-pulse scanning. We numerically simulate the EPP-2DFS observable for the case of an electronically coupled molecular dimer. The EPP-2DFS spectrum is greatly simplified in comparison to its standard classical 2D counterpart. Our results indicate that EPP-2DFS can provide previously unattainable resolution to extract model Hamiltonian parameters from electronically coupled molecular dimers.


10:12AM F27.00006 Surface Sum Frequency Generation of III-V Semiconductors1. ZHENYU ZHANG, JISUN KIM, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA, RAMI KHOURY, Department of Chemistry, Louisiana State University, Baton Rouge, LA, E.W. FLUMMEL, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA, LOUIS HABER, Department of Chemistry, Louisiana State University, Baton Rouge, LA — Optical sum frequency generation (SFG) is a well-established technique for surface and interface studies but its use has been limited mainly to centrosymmetric materials so far. Here, we demonstrate that femtosecond broadband SFG spectroscopy has the ability to identify surface molecular vibrations on the archetypical non-centrosymmetric semiconductor GaAs (001), in which the bulk SFG signal typically dominates over surface SFG contributions. Azimuthal angle dependence of the second order SFG nonlinear response from GaAs (001) surface in the reflection geometry in vacuum for all eight polarization combinations are detected and analyzed. The results agree with and extend upon previous second harmonic generation (SHG) studies and phenomenological analysis. In addition, carbon monoxide and methanol are employed as molecular-markers on the GaAs (001) surfaces. The C-O stretching mode of carbon monoxide and the methyl group stretching modes of methanol are clearly observed even though the bulk contribution dominates the SFG signal. Coherent heterodyne interference is proposed as the mechanism for the surface signal enhancement. Two other zinc blende type III-V semiconductors, GaP and GaSb, are also studied and compared.

1Funded by EFRC
10:24AM F27.00007 Probing Molecular Organization and Electronic Dynamics at Buried Organic Interfaces, SEAN ROBERTS, University of Texas at Austin — Organic semiconductors are a promising class of materials due to their ability to mold the charge transport capabilities of semiconductors with many of the processing advantages of plastics. In thin film organic devices, interfacial charge transfer often comprises a crucial step in device operation. As molecular materials, the density of states within organic semiconductors often reflect their intermolecular organization. Truncation of the bulk structure of an organic semiconductor at an interface with another material can lead to substantial changes in the density of states near the interface that can significantly impact rates for interfacial charge and energy transfer. Here, we will present the results of experiments that utilize electronic sum frequency generation (ESFG) to probe buried interfaces in these materials. Within the electric dipole approximation, ESFG is only sensitive to regions of a sample that experience a breakage of symmetry, which occurs naturally at material interfaces. Through modeling of signals measured for thin organic films using a transfer matrix-based formalism, signals from buried interfaces between two materials can be isolated and used to uncover the interfacial density of states.

10:36AM F27.00008 Stimulated Second Harmonic Generation for High-Sensitivity Interfacial Spectroscopy and Imaging, AARON GOODMAN, Department of Physics and Astronomy, Massachusetts Institute of Technology, WILLIAM TISDALE, Department of Chemical Engineering, Massachusetts Institute of Technology — Second-order nonlinear optical interactions such as sum- and difference-frequency generation are widely used for bioimaging and as selective probes of interfacial environments. However, inefficient nonlinear optical conversion often leads to poor signal-to-noise ratios and long signal acquisition times. Here, we demonstrate the dramatic enhancement of weak second-order nonlinear optical signals via stimulated sum- and difference-frequency generation. We present a conceptual framework to quantitatively describe the interaction and show that the process is highly sensitive to the relative optical phase of the stimulating field. To emphasize the utility of the technique, we demonstrate stimulated enhancement of second harmonic generation (SHG) from bovine collagen-I fibrils. Using a stimulating pulse fluence of only 3 nJ/cm², we obtain an SHG enhancement of > 10⁴ relative to the spontaneous signal. The stimulated enhancement is greatest in situations where spontaneous signals are the weakest - such as low laser power, small sample volume, and weak nonlinear susceptibility - emphasizing the importance of this technique for improving signal-to-noise ratios in biological imaging and interfacial spectroscopy.

Tuesday, March 3, 2015 8:00AM - 11:00AM — Session F28 GMAG DMP: Focus Session: Pyrochlores and Spinels 205 - Christopher Wiebe, University of Winnipeg

8:00AM F28.00001 From Spin Glass to Spin Liquid Ground States in Molybdate Pyrochlores, BRUCE GAULIN, LUCY CLARK, Department of Physics and Astronomy, McMaster University, GORAN NILSEN, Institute Laue-Langevin, EDWIN KERMARREC, Department of Physics and Astronomy, McMaster University, GEORG EHlers, Oak Ridge National Laboratory, KEVIN KNIGHT, ISIS Rutherford Appleton Laboratory, ANDREW HARRISON, Diamond Light Source, PAUL ATTFIELD, University of Edinburgh — The rare earth molybdate pyrochlores are a well-studied family of geometrically frustrated magnetic materials and in particular, the spin glass ground state in Y₄,M₂O₇ is of interest. Here we will present a study of the Lu-based analogue Lu₄,M₂O₇, which displays a transition to a spin glass state at T_g = 16 K and an unusual T^3 dependence of low temperature heat capacity. Our neutron scattering studies reveal a build-up of diffuse elastic magnetic scattering and the collapse of the inelastic magnetic scattering into the acoustic line at T_g. Furthermore we will show that Lu₄,M₂O₇ can be topochemically substituted for N³⁺, which consequently oxidizes the molybdenum cations and drives down their spin quantum number from Mo⁷⁺ to Mo⁵⁺. This new n oxide phase shows an absence of magnetic order despite strong antiferromagnetic exchange and the persistence of inelastic neutron scattering down to low energy scales. Our results on the oxynitride Lu₄,M₂O₇:N₂ are consistent with a gapless spin liquid, which highlights the significant role of quantum fluctuations [1]. [1] L Clark et al., Phys. Rev. Lett 113, 117201 (2014)

8:12AM F28.00002 Partially ordered state in stoichiometric Yb₂T₂O₇, KATE ROSS, Colorado State University, EDWIN KERMARREC, JONATHAN GAUDET, BRUCE GAULIN, McMaster University — The nature of the magnetic state below a first order transition at T_c = 265 mK in the Quantum Spin Ice Yb₂T₂O₇ is hotly debated. It has been proposed as a Quantum Spin Liquid (QSL) ground state, but some studies find evidence for long range ferromagnetic order; results seemingly vary from sample to sample. We will present low temperature neutron measurements on a polycrystalline sample of Yb₂T₂O₇ that is known to be stoichiometric. Our measurements reveal 1) there is a change of intensity at nuclear Bragg positions upon warming which does not occur sharply at T_c, and which involves an ordered moment size of \sim 1.1μB (58% of the saturation moment) and 2) the inelastic excitations below T_c suggest the presence of dispersive modes coexisting with incoherent low energy fluctuations. The data will be compared to Yb₂Sm₂O₇, which shows nearly identical behavior via inelastic neutron scattering. Our results suggest that the ground state in nominally pure Yb₂T₂O₇ and Yb₂Sm₂O₇ is not a conventionally ordered ferromagnet, but instead involves only partial polarization of the magnetic moments coexisting with a disordered component, a situation reminiscent of the partially polarized QSL called the Coulomb Ferromagnetic phase.

1Supported by NSERC of Canada

8:24AM F28.00003 Neutron spectroscopic study of Crystal-field excitation in Yb₂(Ti₂₋ₓYₓ)O₇₋ₓ , JONATHAN GAUDET, DALINI MAHARAJ, EDWIN KERMARREC, McMaster University, GARRETT GRANROTH, Oak Ridge National Lab, KATE ROSS, John Hopkins University, HANNA DABOWSKA, BRUCE GAULIN, McMaster University — Among the rare-earth titanate pyrochlores, Yb₂Ti₂O₇ has attracted much attention as a potential realization of a quantum spin ice [1]. While strong quantum effects are absent in classical spin ice compounds, they are thought to be significant in Yb₂Ti₂O₇ because of an ordering of Ti^3+ sites. A significant sample dependence in the low temperature heat capacity has been reported and attributed to an excess of Yb⁺³ (“stuffing”) in the structure [2]. Our measurements, carried out on two well-characterized samples with different levels of stuffing, allow us to discuss the impact of such disorder on the CEF levels. [1] K.A. Ross, L. Savary, B.D. Gaulin, L. Balents, Physical Review X, 1(2), 021002, (2011). [2] K.A. Ross, Th. Proffen, H.A. Dabkowska, J.A. Quilliam, L.R. Yaraskavitch, J.B. Kycia and B.D. Gaulin, Phys. Rev. B 86, 17442

8:36AM F28.00004 What is going on in Yb₂Ti₂O₇? , LUDOVIC JAUBERT, OIST, OWEN BENTON, OIST, JAPAN, MICHEL GINGRAS, University of Waterloo, Canada, JAAN OITMAA, UNSW, Australia, JEFF RAU, University of Waterloo, Canada, NIC SHANNON, OIST, Japan, RAJIV SINGH, UC Davis, USA — Yb₂Ti₂O₇ has become an excellent example of the complexity of frustrated magnets, showing properties of a spin liquid, dimensional reduction, ferromagnetism and multiple phase transitions. In this talk, we shall bring together many of these aspects into one general theoretical framework, showing how competing orderings can be aligned to explain several experimental features observed in bulk measurements (Hostel et al. PRB 2014) and neutron scattering (Chang et al. Nature Comm. 2012).
8:48AM F28.00005 Frozen Spin Ice Ground States in the Pyrochlore Magnet Tb$_2$Ti$_2$O$_7$, KATHARINA FRITSCH, Helmholtz-Zentrum Berlin für Materialien und Energie — The ground state nature of the candidate spin liquid pyrochlore magnet Tb$_2$Ti$_2$O$_7$ has remained a puzzle for over 15 years. Despite theoretical expectations of magnetic order below 1 K based on classical Ising-like Tb$^3+$ spins, early μSR and neutron scattering experiments showed no long range order down to 50 mK [1,2]. This motivated two theoretical scenarios to account for the apparently disordered ground state: a quantum spin ice scenario in which the classical spin order is suppressed by virtual crystal field excitations that renormalize the antiferromagnetic exchange [3], or a scenario arising from a yet to be observed structural distortion creating a non-magnetic singlet ground state [4]. I will discuss our time-of-flight neutron scattering measurements on Tb$_2$Ti$_2$O$_7$ that reveal a glassy spin ice ground state, characterized by frozen antiferromagnetic short range order and the formation of a $\sim 0.08$ meV energy gap in its spin excitation spectrum at the ($1/2,1/2,1/2$) quasi-ordering wave vectors. A new $H - T$ phase diagram for Tb$_2$Ti$_2$O$_7$ in [110] magnetic field will be presented[6]. I will further discuss recent experiments on slightly off-stoichiometric Tb$_{2+x}$Ti$_{2-x}$O$_7$-$y$ samples, which also display the same gapped spin ice correlations at ($1/2,1/2,1/2$) wave vectors.


9:24AM F28.00006 Magnetoelastic excitations in Tb2Ti2O7 in applied magnetic field, MARTIN RUMINY, MICHEL KENZELMANN, TOM FENNELL, Paul Scherrer Institut — The key puzzle in Tb$_2$Ti$_2$O$_7$ is how the expected long-range magnetic order and/or structural phase transition are suppressed, resulting in the stabilization of the spin liquid phase [1]. This spin liquid phase supports spin ice-like powerlaw correlations [2,3,4], and an array of anomalous magnetoelastic properties (see e.g. [5]). Recently we have discovered a microscopic coupling between the magnetic and lattice fluctuations, which form a hybrid propagating excitation with both spin and phonon components [6,7]. Using inelastic neutron scattering, we have now explored the effect of an applied magnetic field on the magnetoelastic coupling. I will show how these experiments cast light not only on the coupling between spins and phonons in Tb$_2$Ti$_2$O$_7$, but also on other unexplained phenomena in Tb$_2$Ti$_2$O$_7$, such as the field induced long-range antiferromagnetic order [8].


9:36AM F28.00007 The ground state of the Er$_3$Ti$_4$O$_7$ pyrochlore XY antiferromagnet: Energetic vs. order-by-disorder selection, JEFFREY G. RAU, University of Waterloo, SYLVAIN PETIT, LLB, CEA-CNRS, CEA-Saclay, MICHEL J. P. GINGRAS, University of Waterloo — Conclusive evidence of order by disorder is rare in real materials. One of the strongest cases presented, Er$_3$Ti$_4$O$_7$, is a microscopic coupling between the magnetic and lattice fluctuations, which form a hybrid propagating excitation with both spin and phonon components [6,7]. Using inelastic neutron scattering, we have now explored the effect of an applied magnetic field on the magnetoelastic coupling. I will show how these experiments cast light not only on the coupling between spins and phonons in Tb$_2$Ti$_2$O$_7$, but also on other unexplained phenomena in Tb$_2$Ti$_2$O$_7$, such as the field induced long-range antiferromagnetic order [8].


9:48AM F28.00008 Inelastic light scattering measurements of structural phase coexistence in ferrimagnetic spinel Mn$_3$O$_4$, SAMUEL GLEASON, TAYLOR BYRUM, ALEXANDER THALER, GREGORY MACDOUGALL, S. LANCE COOPER, Univ of Illinois - Urbana — The ferrimagnetic spinel Mn$_3$O$_4$ has a number of functional properties, e.g., magnetodielectricity, that are ascribed to a coupling between the spins and lattice of this material. Such a coupling is manifested in the symmetry-lowering structural distortion that occurs when Mn$_3$O$_4$ magnetically orders at $T = 33$ K. A recent x-ray diffraction study of polycrystalline Mn$_3$O$_4$ found that this distortion is not fully realized, i.e., the high-symmetry and low-symmetry structures coexist below $T = 33$ K due to strains from lattice mismatch. To extend this work, we use variable-pressure and variable-magnetic-field inelastic light scattering spectroscopy to study structural phase coexistence in single crystals of Mn$_3$O$_4$. We confirm the coexistence of tetragonal (high-symmetry) and orthorhombic (low-symmetry) phases below $T = 33$ K. Furthermore, we demonstrate that the application of hydrostatic pressure suppresses the tetragonal phase, while the application of magnetic field can bolster this phase. These results indicate that microscopic descriptions of functional behavior in Mn$_3$O$_4$ should consider effects due to structural phase coexistence. [2]

[1] Research was supported by the U.S. Department of Energy under Award DE-FG02-07ER46453. T. Byrum was partially supported by the National Science Foundation under Grant Number DGE-1144245.

10:00AM F28.00009 Neutron scattering investigation of magnetic phases in Mn$_3$O$_4$ with field applied away from the easy axis, ALEXANDER THALER, ALEXANDER ZAKJEVSKI, BRIAN NGUYEN, YEWON GIM, University of Illinois - Urbana, ANNE FARWICK, Xavier University, ADAM ACZEL, Oak Ridge National Laboratory, S. LANCE COOPER, GREGORY MACDOUGALL, University of Illinois - Urbana — Mn$_3$O$_4$ is an orbital ordered, magnetically frustrated spinel with strong spin-lattice coupling, which exhibits a series of low temperature magnetic and structural transitions. Recent data shows that the structural phases are radically different with applied field at several different angles to the easy axis. We will present data suggesting that the field-temperature phase diagram of this material is radically altered by varying the applied field direction.

2This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under award number DE-FG02-07ER46453.
10:12AM F28.00010 \( \mu \)SR study of real space magnetic phase separation in \( \text{Mn}_2\text{O}_4 \)\(^1\) \( \ldots \) ALEXANDER ZAKJEVS KII, ALEXANDER THALER, DALMAU REIG-\( \text{P} \)LESSIS, ISAAC BRODSKY, YE WON GIM, University of Illinois - Urbana, ADAM ACZEL, Oak Ridge National Laboratory, S. LANCE COOPER, GREGORY MACDOUGALL, University of Illinois - Urbana — The material \( \text{Mn}_2\text{O}_4 \) is a magnetically frustrated spinel which exhibits three distinct magnetic transitions below 42 K. Recent work has shown that the lowest of these is accompanied by an orthorhombic structural distortion, implying strong magneto-elastic coupling. Magnetic force microscopy (MFM) measurements indicate a substantial region of phase coexistence below this transition, with domain walls that order on the mesoscale. It is further suggested that a tradeoff in ordered volume with field may play a role in the recent quantum phase transition reported in this material. To follow up on these ideas, we have performed a series of zero- and transverse-field muon spin rotation measurements on single-crystal \( \text{Mn}_2\text{O}_4 \). The zero-field data clearly show the co-existence of ordered and disorder volumes, consistent with MFM results. Here we report these data, and further attempts to vary the ordered volume with applied field. We will discuss both zero- and transverse-field results within the context of the current understanding of the material.

\(^1\)This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under award number DE-FG02-07ER46453.

10:24AM F28.00011 Quantum Criticality in \( \text{FeSc}_2\text{S}_4 \) \( \ldots \) DANIEL ISH, University of California - Santa Barbara, LEON BALENTS, Kavli Institute for Theoretical Physics — Despite possessing a local spin 2 moment on the iron site and a Curie-Weiss temperature of 45 K, the site spinon \( \text{FeSc}_2\text{S}_4 \) does not magnetically order down to 50mK. Previous theoretical work by Chen and Balents advanced an explanation for this observation in the form of the \( J_2-\lambda \) model which places \( \text{FeSc}_2\text{S}_4 \) close to a quantum critical point on the disordered side of a quantum phase transition between a Néel ordered phase and a “Spin-Orbital Liquid” in which spins and orbitals are entangled, quenching the magnetization. We present new theoretical studies of the optical properties of the \( J_2-\lambda \) model, including a computation of the dispersion relation for the quasiparticle excitations and the form of the collective response to electric field. We argue that the latter directly probes a low energy excitation continuum characteristic of quantum criticality, and that our results reinforce the consistency of this model with experiment.

10:36AM F28.00012 Competition between the inter- and intra-sublattice interactions in \( \text{Yb}_2\text{V}_2\text{O}_7 \) \( \ldots \) ZHILING DUN, Department of Physics and Astronomy, University of Tennessee, JIE MA, HUIBO CAO, TAO HONG, MASA AKI MATA-SUDA, Quantum Condensed Matter Division, Oak Ridge National Laboratory, YIMING QIU, JOHN COPLEY, NIST Center for Neutron Research, JINGUANG CHENG, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, MINSEONG LEE, EUN SANG CHOI, National High Magnetic Field Laboratory, Florida State University, STEVE JOHN STON, Department of Physics and Astronomy, University of Tennessee, Knoxville, HAI DONG ZHOU, Department of Physics and Astronomy, University of Tennessee, Knoxville, National High Magnetic Field Laboratory, Florida State University — We studied single crystals of \( \text{Yb}_2\text{V}_2\text{O}_7 \) using dc and ac susceptibility measurements, elastic and inelastic neutron scattering measurements, and linear spin wave theory. The experimental data shows a ferromagnetic ordering of \( \text{V}^{4+} \) ions at 70 K, a short-range ordering of \( \text{Yb}^{3+} \) ions below 40 K, and finally a long-range non-collinear ordering of \( \text{Yb}^{3+} \) ions below 15 K. With external magnetic field oriented along the [111] axis, the Yb-sublattice experiences a spin flop transition related to the “three-in-one-out” spin structure. By modeling the spin wave excitations, we extract the Hamiltonian parameters. Our results confirm that although the extra inter-sublattice Yb-V interactions dramatically increases the Yb ordering temperature to 15 K, the intra-sublattice Yb-Yb interactions, based on the pyrochlore lattice, still stabilize the Yb ions’ non-collinear spin structure and spin flop transition.

10:48AM F28.00013 Quantum spin state in a spin-1/2 breathing pyrochlore antiferromagnet \( \ldots \) KENTA KIMURA, Osaka University, SATORU NAKATSUJI, The University of Tokyo, TSUYOSHI KIMURA, Osaka University — A pyrochlore lattice antiferromagnet consisting of corner-sharing tetrahedra of magnetic ions has attracted much attention because the inherent geometrical frustration often leads to exotic magnetism such as quantum spin liquid [1]. The key building unit of pyrochlore magnet is a single spin tetrahedron. Thus, a material composed of a spin-tetrahedral unit is expected to provide important insights on physics of full pyrochlore lattice. Moreover, it may show exotic magnetism based on the unique properties of the single tetrahedron associated with the spin chirality. However, no spin-1/2 regular tetrahedral system has been reported to date. In this study, we report the characterization of a new Yb-based material \( \text{Ba}_3\text{Yb}_2\text{Zn}_5\text{Si}_11 \) [2]. This material is identified as a model system of a pseudospin-1/2 quantum antiferromagnet on breathing pyrochlore lattice characterized by an alternating array of small and large Yb tetrahedra. Despite antiferromagnetic interactions \( J \sim 7 \) K, a large amount of magnetic entropy (25%) remains at 0.38 K, indicating that each small Yb tetrahedron forms a unique doubly degenerate singlet state.


Tuesday, March 3, 2015 8:00AM - 11:00AM — Session F29 GMAG DMP FIAP: Focus Session: Spin-Orbit Effects 206A - Weigang Wang, University of Arizona

8:00AM F29.00001 Optical probe of spin-orbit fields in metallic magnetic structures \( \ldots \) MOHAMMAD MONTAZERI, PRAMEY UPADHYAYA, GUOQIANG YU, KIN L. WONG, MURONG LANG, YABIN FAN, PEDRAM KHALILI AMIRI, ROBERT N. SCHWARTZ, KANG L. WANG, Dep. of Electrical Engineering, University of California, Los Angeles — We report a novel self-consistent optical approach based on magneto-optical Kerr effect to directly and quantitatively probe the spin-orbit fields of magnetic devices with 1um diffraction limited spatial resolution. The optical probe is exemplified by investigating the spin-orbit fields in a magnetic stack of Ta(5 nm)/CoFeB(1.1 nm)/MgO(2.0 nm)/TaOx with enhanced perpendicular anisotropy. Both field-like and damping-like contributions were measured independently and their coefficients are quantified at \( 3.3 \times 10^{-2} \) and \(-2.0 \times 10^{-6}\) Oe/A cm\(^{-2}\), respectively. A detailed comparison with standard transport technique is presented in which a very good agreement were found. Our results establish the relevance of the optical methods for studying spin-orbit torque related physics. We acknowledge the support from the National Science Foundation (DMR-1411085) and the FAME Center, one of the six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA.
We study the interaction between two localized magnetic moments in the presence of the Rashba spin-orbit coupling and obtain expressions for the interaction,

\[
\mathbf{\mathbf{J}} = \mathbf{J}_1 + \mathbf{J}_2 + \mathbf{J}_3
\]

where \( \mathbf{J}_1 \) contains the RKKY, Dzyaloshinsky-Moriya, as well as a tensor part, viz.,

\[
\mathbf{J}_1 = J_1 \mathbf{S}_1 \cdot \mathbf{S}_2
\]

We will treating the nonmagnetic impurity scattering in the self-consistent Born approximation with ladder-type vertex corrections, we calculate the Rashba torques as deterministic magnetic reversal of perpendicularly magnetized square dots via in-plane dc and/or pulsed currents. We believe that integration of two emerging magneto-ionic gates into prototype spintronic devices will be discussed. In collaboration with U. Bauer, A. J. Tan, S. Emori, L. Yao, and S. van Dijken.

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**References**


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**8:12AM F29.00002 Detection of inverse Rashba-Edelstein effect at Cu/Bi interface using lateral spin valves**, MIREN ISASA, CIC nanogune, San Sebastián, Spain, M. CARMEN MARTINEZ-VELARTE, Universidad Zaragoza, Zaragoza, Spain, ESTITXU VILLAMOR, CIC nanogune, San Sebastián, Spain, LUIS MORELLÓN, Universidad Zaragoza, Zaragoza, Spain, JOSE M. DE TERESA, Universidad Zaragoza-CSIC, Zaragoza, Spain, MANUEL R. IBARRA, Universidad Zaragoza, Zaragoza, Spain, LUIS E. HUESO, FELIX CASANOVA, CIC nanogune, San Sebastián, Spain; IKERBASQUE, Bilbao, Spain — The spin-orbit coupling (SOC) can be exploited to generate and detect pure spin currents, which are key elements in the field of spintronics. One important example is the spin Hall effect. A novel SOC phenomenon, the inverse Rashba-Edelstein effect (IREE), is attracting a large interest. IREE arises from the Rashba coupling that appears at interfaces or surface states (SSs), leading to the conversion of a 3D spin current into a 2D charge current. An interesting system to study the IREE is thus the SS of a semimetal such as Bi. In this work [1], we study the spin-to-charge conversion in Bi using a device based on a lateral spin valve (LSV) geometry. We demonstrate a spin-to-charge current conversion in the LSV. The analysis of the obtained results leads us to argue that the spin-to-charge conversion occurs at the Cu/Bi interface, therefore detecting IREE. Moreover, we evaluate the IREE length, which characterizes the spin-to-charge conversion ratio, as a function of temperature. This ratio changes sign at a certain temperature threshold (125 K), in excellent agreement with the experimental observation of a change in the type of carriers that dominate the electronic transport in Bi.

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**9:12AM F29.00005 Perpendicular Magnetization Switching via Current induced Spin-Orbit Torques on Flexible Substrate**, OUKJAE LEE, LONG YOU, JAEWON JANG, VIVEK SUBRAMANIAN, SAYEEF SALAHUDDIN, UC Berkeley, UC BERKELEY TEAM — Implementation of perpendicularly magnetized thin films and of electrically functional devices on flexible substrates may offer new degree of freedom such as strain effect on the ultrathin magnetic films with a strong spin orbit coupling. Moreover the flexibility has advantages in applications with bendable, stretchable and/or mobile environment. In this talk we present the magnetic characteristics of ultrathin multilayers with a sufficient PMA that were grown on a flexible plastic substrate by dc/rf magnetron sputtering. In addition we fabricate cross-Hall bar devices and demonstrate fully deterministic magnetic reversal of perpendicularly magnetized square dots via in-plane dc and/or pulsed currents. We believe that integration of two emerging technologies promises new spintronic devices that can be utilized in arbitrary surface geometries and be worked in ultra small dimensions.

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**9:24AM F29.00006 Microscopic calculation of Rashba spin-orbit torques**, JUNJI FUJIMOTO, Osaka University, HIROSHI KOHNO, Nagoya University — We study current-induced spin-orbit torques (Rashba torques) in a two-dimensional Rashba ferromagnet, which may model the interface of the ferromagnetic — heavy and paramagnetic metals. Using the linear response theory and the Green’s function method and treating the nonmagnetic impurity scattering in the self-consistent Born approximation with ladder-type vertex corrections, we calculate the Rashba torques as functions of magnetization direction, strength of the spin-orbit coupling, and the chemical potential. It is found that the Rashba torques are independent of the direction of the magnetization for a parabolic dispersion in good metals, whereas they show a clear angular dependence for a tight-binding model. We will discuss our results comparing with other theoretical calculations [C. O. Paucar, X. Wang, M. Chshiev and A. Manchon, Appl. Phys. Lett. 102, 252403 (2013), K.-S. Lee, et al, arXiv:1409.8540] and the recent experiments.
Both lattice and spin subsystems.

To the lattice subsystem, we show that this novel extension enables the exchange of angular momentum and leads to the mutual thermalization of lattice vibrations. Using MD-SD simulations, we investigate the effect of these terms on the spin-lattice relaxation in BCC iron. By coupling a conventional spin-orbit coupling. These interactions are modeled in terms of the local magnetic anisotropies that arise as a consequence of the symmetry breaking due to relaxation process. To circumvent this drawback, we extend the conventional MD-SD approach by incorporating additional interaction terms that characterize coordinate-dependent exchange interaction, which allows the dynamic exchange of energy between the lattice and spin subsystems; however such exchange-effect of magnetism into the atomistic simulations of transition metals. The coupling between the atomic and spin degrees of freedom is established via a polarizer [1,2,3]. In this work, I will first present recent theoretical investigations on the spin-orbit torque that emerges at the interface between a topological insulator and a ferromagnetic metal. The ability to measure spin structure on the nanometer scale has attracted substantial interest for a long time. Spin-polarized scanning tunneling microscopy (SPSTM) is an excellent tool for studying fundamental aspect of magnetism at atomic scale. We combine a low temperature STM equipped with a vector magnet and a spin-polarizable tip, to probe superconductors with strong spin-orbit coupling, such as Pb, which is emerging as a platform for engineering topological superconductivity [1]. We observe anisotropic tunneling conductance between tip and substrate as a function of the angle of applied in-plane magnetic field. This finding suggests that SPSTM may provide a tool to locally measure spin-orbit coupling, even in non-magnetic substrates. [1] S. Nadj-Perge, I.K. Drozdov, J. Li, H. Chen, S. Jeon, J. See, A.H. Macdonald, B.A. Bernevig, A. Yazdani, Science 346, 602 (2014)


Spin-orbit-induced relaxation in combined molecular and spin dynamics simulations of BCC iron1, DILINA PERERA, The University of Georgia, MARKUS EISENBACH, Oak Ridge National Laboratory, DON NICHOLSON, University of North Carolina at Asheville, JUNQI YIN, University of Tennessee, G. MALCOLM STOCKS, Oak Ridge National Laboratory, DAVID P. LANDAU, The University of Georgia — The combined molecular and spin dynamics (MD-SD) method has emerged as a powerful tool for integrating the effect of magnetism into the atomistic simulations of transition metals. The coupling between the atomic and spin degrees of freedom is established via a coordinate-dependent exchange interaction, which allows the dynamic exchange of energy between the lattice and spin subsystems; however such exchange-based coupling alone cannot facilitate the transfer of angular momentum between the two subsystems. This results in an unrealistic depiction of the spin-lattice relaxation process. To circumvent this drawback, we extend the conventional MD-SD approach by incorporating additional interaction terms that characterize spin-orbit coupling. These interactions are modeled in terms of the local magnetic anisotropies that arise as a consequence of the symmetry breaking due to lattice vibrations. Using MD-SD simulations, we investigate the effect of these terms on the spin-lattice relaxation in BCC iron. By coupling a conventional thermostat to the lattice subsystem, we show that this novel extension enables the exchange of angular momentum and leads to the mutual thermalization of both lattice and spin subsystems.

1Research supported by the Center for Defect Physics, an U.S. Department of Energy, Energy Frontier Research Center.
8:00AM F30.00001 First-principles analysis of a Dzyaloshinskii-Moriya driven magnetic structure in a monolayer Cr on W(110). STEFAN BLÜGEL, BERND ZIMMERMANN, TIMO SCHENK, MARCUS HEIDE, YURYI MOKROUSOV, GUSTAV BİHLMAYER, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — The observation of a chiral magnetic spin spiral in a magnetic Mn monolayer on a W(110) substrate has opened a new vista in low-dimensional magnetism [1] with possible applications in spintronics. The origin was explained by the occurrence of the Dzyaloshinskii-Moriya interaction (DMI), which occurs due to the presence of a structure inversion-asymmetry. In this talk, we turn our attention to a monolayer Cr on W(110) [2]. We show by DFT calculations, that the DMI is so strong that it creates a non-collinear spin-spiral ground state, with excellent agreement to spin-polarized STM experiments [3]. We determine a considerable inhomogeneity of the spin spiral by means of a micromagnetic model. We compare our results to the systems Mn and Fe on W(110), where the direction of the spiral and period length are different. We present a minimal tight binding model [4] and show that indeed the sign and strength of the DMI reveals a non-trivial dependence on the electronic structure.


8:12AM F30.00002 Majorana bound state in a magnetic biskyrmion. GUANG YANG, RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Japan, DANIEL LOSS, Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — Magnetic skyrmion, recently discovered [1] in thin film dipolar ferromagnet with uniaxial anisotropy, is a highly mobile nanoscale topological spin texture. We show that a magnetic skyrmion in proximity to an s-wave superconductor supports a zero-energy Majorana bound state in its core. The Majorana bound state can be manipulated through driving the motion of the magnetic skyrmion by electric current. We discuss the realization of non-Abelian statistics of such Majorana bound states.


8:24AM F30.00003 ABSTRACT WITHDRAWN

8:36AM F30.00004 Unraveling skyrmion spin texture using resonant soft x-ray scattering. SUJOY ROY, Lawrence Berkeley National Laboratory — The recent discovery of skyrmions, that were originally predicted in context of high energy physics, in magnetic materials has sparked tremendous interest in the research community due to its rich physics and potential in spintronics applications. Skyrmions have an unusual spin texture that manifests as magnetic knot and can be easily moved around. Understanding the fundamental physics and mechanisms for controlling their dynamical properties presents important scientific challenges. So far experimental verifications of the skyrmions in magnetic systems have come from neutron scattering and Lorentz transmission electron microscopy (TEM) measurements. In this talk we report the first observation of the skyrmions using resonant soft x-ray scattering. We have used soft x-rays tuned to the Cu L3 edge to diffract off the skyrmion lattice in a multiferroic Cu2OSeO3 compound. We show that in Cu2OSeO3 there exist two skyrmion lattices arising due to the two inequivalent Cu-O sublattices that have two different magnetically active d-orbitals. The two skyrmion sublattices are mutually rotated with respect to each other. The angle of rotation could be changed by an external magnetic field, thereby indicating possible existence of a new phase. We have also studied skyrmion spin texture in an ultra-thin Fe/Gd multilayer that shows perpendicular anisotropy. The Fe/Gd sample exhibits a near perfect aligned stripe phase. Within a small range of temperature and magnetic field we observe a hexagonal scattering pattern due to skyrmion bubbles. Analysis of the scattering pattern suggests that the skyrmion lattice unit cell contains two skyrmions. The skyrmion state is also revealed by Lorentz TEM images. The near room temperature discovery of skyrmion in a technology relevant material is a significant step towards using skyrmions in magnetic devices.

1Work at LBNL was supported by the Office of Basic Energy Sciences of the U.S. Department of Energy (Contract No. DE-AC02-05CH11231).

9:12AM F30.00005 X-ray microscope Imaging of skyrmions in Ultrathin Films with Strong Dzyaloshinskii-Moriya Interaction. SEONGHOON WOO, MIT, BENJAMIN KRUGER, MATHIAS KLÄUI, University of Mainz, PETER FISCHER, Lawrence Berkeley National Laboratory, GEOFFREY BEACH, MIT, MIT COLLABORATION, UNIVERSITY OF MAINZ COLLABORATION, LAWRENCE BERKELEY NATIONAL LABORATORY COLLABORATION — Spin textures stabilized by the Dzyaloshinskii-Moriya interaction (DMI) have been of considerable recent interest due to extraordinary static and dynamic behaviors derived from their topological nature. It has recently been shown that DMI can also manifest in buried ultrathin sputtered film stacks. Here we examine magnetic bubble domains in submicron patterned dots with strong DMI. We use magnetic transmission X-ray microscopy to image the evolution of the magnetization configuration as a function externally applied fields. We imaged a series of [Pt(3nm)/Co(0.9nm)/Co(0.9nm)/Co(0.9nm)] x 15, where the DMI is strong, and [Pt(3nm)/Co(0.9nm)/Pt(3nm)] x 15 stacks, where DMI is small enough due to symmetric structure, and 15 repeats were used to enhance XMCD contrast. We observed that the size of domain can be significantly narrower for the case of strong DMI and micromagnetic modeling confirmed the observation. We also imaged that magnetic bubbles can be easily nucleated and controlled using external fields in micrometersize-patterns. The static stability of bubbles for the same cases were tested using external bias field, showing skyrmionic bubble has larger bubble-collapse field by the factor of two. Other qualitative and quantitative measurements will also be presented.

9:24AM F30.00006 Skyrmions in quasi-2D chiral magnets with broken bulk and surface inversion symmetry1. JAMES ROWLAND, Ohio State University, SUMILAN BANERJEE, Ohio State University and Weizmann Institute of Science, MOHIT RANDERIA, Ohio State University — Most theoretical studies of skyrmions have focused on chiral magnets with broken bulk inversion symmetry, stabilized by easy-axis anisotropy [1]. Recently, we considered 2D systems with broken surface inversion [2] and showed that skyrmion crystals are more stable than in 3D, pointing out the importance of easy-plane anisotropy. In the present work we investigate quasi-2D systems which break both bulk and surface inversion symmetry. The Landau-Ginzburg free energy functional thus contains two Dzyaloshinskii-Moriya terms of strength $D_D$ and $D_R$ arising from Dresselhaus and Rashba spin-orbit coupling respectively. We trace the evolution of the phase diagram as $D_D/D_R$ is varied, and find that skyrmions are increasingly destabilized with respect to the cone phase as $D_D$ increases relative to $D_R$. We find an evolution from vortex-like skyrmions in the pure Dresselhaus limit to hedgehog-like skyrmions in the pure Rashba limit. We discuss the relevance of these results to existing experiments and the prospects of tuning the ratio of Dresselhaus and Rashba spin-orbit coupling via film thickness and strain. [1] M. Wilson et al., PRB 89, 094411 (2014). [2] S. Banerjee, J. Rowland, O. Ertan, and M. Randeria, PRX 4, 031045 (2014).

1Supported by NSF DMR-1410364 (J.R. and M.R.) and DOE-BES DE-SC0005035 (S.B.)
9:36AM F30.00007 Anisotropic Magnetoresistance in the Layered Chiral Helimagnet Cr$_{1/3}$Nb$_2$S$_6$, ALEXANDER BORINSTEIN, University of Colorado Boulder, NIRMAL GHIMIRE, DAVID MANDRUS, University of Tennessee, Oak Ridge National Laboratory, DAVID PARKER, Oak Ridge National Laboratory, MINHYEA LEE, University of Colorado Boulder — We study the magnetotransport properties and the low temperature specific heat in a highly anisotropic helimagnet Cr$_{1/3}$Nb$_2$S$_6$. We compare the dependence of both measurements on field orientation: within the crystallographic plane and normal to it. In transport measurements, the current always remains within the crystallographic ab-plane. We find a three times larger reduction in the resistivity when the magnetization is saturated normal to the plane compared to within the plane. This discrepancy occurs below 50 K $< T_C < 130$ K. In the same temperature range, an unusual field dependence of the Hall Effect is also observed. From first principles calculations, we connect the changes in resistivity to modification of the density of states dependent on the direction of spin polarization. The Sommerfeld constant for both spin orientations is discussed in relation to the transport behavior.

9:48AM F30.00008 Fermi Surface Induced Scalar Chiral Stripes in the Kondo Lattice Model on a Square Lattice, RYO OZAWA, Department of Applied Physics, University of Tokyo, KIPTON BARROS, GIA-WEI CHERN, SHI-ZHEN LIN, Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, MASAFUMI UDAGAWA, YUKITOSHI MOTOME, Department of Applied Physics, University of Tokyo, CRISTIAN BATISTA, Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory — The stability and controllability of emergent nano/mesoscale spin structures are one of the central issues for spintronics. The possibility of stabilizing non-coplanar spin structures in chiral magnets (e.g. skyrmion crystals) is opening a new avenue for controlling transport properties with small magnetic fields. An electron moving in a loop picks up a Berry phase proportional to the net scalar spin chirality of the underlying spin configuration that is enclosed by the loop. In other words, the scalar spin chirality acts as an effective magnetic field that couples to the electronic orbital motion. By solving the Kondo lattice model on a square lattice, we will show that mesoscale chiral stripes emerge in the vicinity of a Lifshitz transition of the Fermi surface. Our unbiased results are obtained by applying a novel algorithm which allows for very efficient simulations based on Langevin dynamics.

10:00AM F30.00009 Magnetoresistance measurements in a chiral magnet CrNb$_2$S$_6$ subject to locally applied magnetic field, YU MATSUMOTO, Osaka Prefecture Univ., YUSUKE KOUSAKA, JUN AKIMITSU, Aoyama Gakuin Univ., SADAUFUMI NISHIHARA, KATSUYA INOUE, Hiroshima Univ., ROBERT STAMPS, Univ. of Glasgow, ALEXANDER S. OVCHINIKOV, Ural Federal Univ., JUN-ICHIRO KISHINE, The Open Univ. of Japan, YOSHIHIKO TOGAWA, Osaka Prefecture Univ. — CrNb$_2$S$_6$ is one of interesting magnetic materials with structural chirality, wherein chiral magnetic orders are formed as a consequence of the competition between Heisenberg exchange and antisymmetric Dzyaloshinsky-Moriya (DM) interactions. Interestingly, a chiral helimagnetic order appears as the ground state at zero magnetic field, while it transforms into a chiral spin soliton lattice, a spin superlattice of forced ferromagnetic regions partitioned by a soliton with $2\pi$ rotation of spin magnetic moments, in the presence of magnetic field applied perpendicular to the chiral structural axis [1]. In this work, we have investigated the magnetoresistance (MR) in a micro-fabricated single crystal of CrNb$_2$S$_6$ by means of the standard ac transport measurement. We have found that the MR exhibits a hysteresis behavior during the magnetic field cycle, although a continuous negative MR is observed in a bulk single crystal [2]. In the presentation, we will show the MR changes induced by locally applied magnetic field and discuss their properties in terms of the macroscopic coherence of the chiral spin soliton lattice.

10:12AM F30.00010 Meron crystals and skyrmion fractionalization in chiral magnets, AVADH SAXENA, SHI-ZENG LIN, CRISTIAN D. BATISTA, Los Alamos National Lab — The recent discovery of skyrmions in chiral magnets, e.g. MnSi, has triggered enormous interest due to their huge potential for spintronics. Unlike magnetic domain walls, skyrmions can be manipulated with very small electric currents, thus rendering them as prime candidates for novel information storage devices with much lower power consumption. Here we study the equilibrium phase diagram of ultrathin chiral magnets with an easy-plane anisotropy $A$. The triangular skyrmion lattice phase that is obtained for $A = 0$ evolves through different structural phase transitions upon increasing $A$, which are related to the compact packings of disks with two different radii. Meanwhile, the topological charge of a skyrmion decreases continuously and we call this process skyrmion fractionalization. For a strong easy-plane anisotropy, a meron-antimeron crystal is stabilized. Akin to the case of skyrmions, the resulting merons can be manipulated with external current, and they behave like particles. Meron charge can be measured in transport experiments or by direct imaging of meron motion. Our work demonstrates that symmetric magnetic anisotropy can be used as a knob for tuning the topological character of the emergent mesoscale particles as well as the nature of the crystal that they form.

10:24AM F30.00011 Theory of electromagnons in CuO, KUN CAO, FELICIANO GIUSTINO, Department of Materials, University of Oxford, PAOLO RADAELLI, Clarendon Laboratory, Department of Physics, University of Oxford — Recently, an electromagnon excitation was found in the multiferroic phase of CuO for electric field parallel to the [101] direction, with excitation energy $\sim 3$ meV. We performed symmetry analysis to show that the experimentally measured electromagnon cannot be explained by the exchange-striction mechanism. We then studied the CuO electromagnons using ab-initio calculations and effective model simulations. The experimentally measured electromagnon was found to originate from the Dzyaloshinskii-Moriya interaction, with the magnon part corresponding to a phason mode. We further predict that a new high-energy electromagnon with selection rule $E-II$ [010] should also exist in the multiferroic phase of CuO, due to the exchange-striction mechanism.

10:36AM F30.00012 Wave Equation of Three-Dimensional Skyrmion Line, JUNICHI IWASAKI, Dept. of Applied Physics, Univ. of Tokyo, CHRISTOPH SCHUTTE, Institut für Theoretische Physik, Universität zu Köln, NAOTO NAGAOSA, RIKEN Center for Emergent Matter Science and Dept. of Applied Physics, Univ. of Tokyo — Magnetic skyrmion is a particle in magnets, which is now regarded as one of the most promising candidate for information carrier in future memory devices. In the bulk of chiral magnets, skyrmions form lines along the applied magnetic field. Previous studies report that extra energy is required to create skyrmion lines. Here, we raise a more fundamental question: how does the wave propagates in these one-dimensional “strings”? Surprisingly, the numerical simulation reveals that the waves propagating in positive and negative directions are different. This asymmetric feature is described by magnon contribution, which has, in general, $k$-linear term in its dispersion relation under the Dzyaloshinskii-Moriya interaction. Starting from the action of the spin system in chiral magnets, we derive the wave equation of the skyrmion line.

10:48AM F30.00013 Thermalization and dynamic phase transition of quantum spins\(^1\), MEHRTASH BABADI, Institute for Quantum Information and Matter, California Institute of Technology, Pasadena, CA 91125, EUGENE DEMLER, MICHAEL KNAP, Department of Physics, Harvard University, Cambridge, MA 02138 — We develop a controlled field theoretic technique for studying far-from-equilibrium dynamics of interacting quantum spins. This is achieved by combining the Majorana fermion representation of spins and 1/N expansion of the two-particle irreducible effective action (2PI-EA). We use the technique to study the relaxation dynamics of quantum spin spirals in the Heisenberg model. The non-equilibrium magnetization and spin correlations are found by solving the Kadannoff-Baym and Bethe-Salpeter equations resulting from the 1/N expansion of the 2PI-EA to the next-to-leading order. In three dimensions, we identify a dynamic phase transition in the steady state magnetization for spiral states near the Neél order. We further find a dynamical stabilization of the initial out-of-plane ordering instability in the course of the relaxation dynamics, in contrast to the linear response analysis.

\(^1\)MB was supported by IQM, an NSF Physics Frontiers Center. MK an ED acknowledge support from Harvard-MIT CUA, ARO-MURI Quism program, ARO-MURI on Atomtronics, as well as the Austrian Science Fund (FWF) Project No. J 3361-N20.
Tuesday, March 3, 2015 8:00AM - 11:00AM –
Session F31 GMAG DMP FIAP: Focus Session: Spin-Dependent Phenomena in Semiconductors: Defects in Diamond and SiC  207A - Michael Flatte, University of Iowa

8:00AM F31.00001 Nuclear magnetic resonance of external protons using continuous dynamical decoupling with shallow NV centers1. CHARLES DE LAS CASAS, KENICHI OHNO, DAVID D. AWSCHALOM, Institute for Molecular Engineering, University of Chicago — The nitrogen vacancy (NV) center in diamond is a paramagnetic defect with excellent spin properties that can reside within a few nanometers of the diamond surface, enabling atomic-scale magnetic resonance sensing of external nuclear spins. Here we use rotating frame longitudinal spin relaxation ($T_1^L$) based sensing schemes, known as Continuous Dynamical Decoupling (CDD), to detect external nuclear spins with shallow NV centers (<5 nm from the surface). Distinguishing neighboring nuclear spins from each other requires the NV center be near enough to create differences in the hyperfine shifts and coupling strengths of the nuclei. However, spin coherence time and consequently the sensitivity of dynamical decoupling techniques degrade sharply as NVs become shallower. We use strong continuous driving to overcome this fast decoherence and detect an ensemble of external nuclear spins using a single shallow NV center with a short $T_2$ (<2μs) at magnetic fields as high as 0.5 Tesla. The increased sensitivity of this method relative to pulsed dynamical decoupling techniques demonstrates the benefits of CDD for sensing with very shallow NV centers.

1This work was supported by DARPA, AFOSR, and the DIAMANT program.

8:12AM F31.00002 High-field optically detected magnetic resonance of a single nitrogen-vacancy center in diamond. VIKTOR STEPANOV, CHATHURANGA ABEYWARDANA, FRANKLIN CHO, RANA AKIEL, SUSUMU TAKASHI, University of Southern California — A nitrogen-vacancy center (NV) in diamond is a promising candidate for fundamental investigation of spin physics and applications to quantum information processing and quantum sensing because of its remarkable properties such as long lived coherence, superb photostability and capability to detect a single NV center using an optically detected magnetic resonance (ODMR) technique. Here, we discuss a platform to investigate a NV center at high magnetic fields. We will present the development of a high-field ODMR system consisting of a high-frequency excitation component, superconducting magnet, NV detection system, microscope system and sample stage. We also discuss ODMR and double electron-electron resonance measurements of a single NV center at high magnetic fields.

8:24AM F31.00003 Fast Room-Temperature Phase Gate on a Single Nuclear Spin in Diamond2. S. SANGTAWESIN, T.O. BRUNDAGE, J.R. PETTA, Department of Physics, Princeton University — Nuclear spins support long lived quantum coherence due to weak coupling to the environment, but are difficult to rapidly control using nuclear magnetic resonance as a result of the small nuclear magnetic moment. We demonstrate a fast ~ 500 ns nuclear spin phase gate on a $^{14}$N nuclear spin qubit intrinsic to a nitrogen-vacancy center in high purity diamond [1]. This phase gate is achieved by utilizing electron-nuclear hyperfine interaction. By driving off-resonant Rabi oscillations on the electronic spin, we can generate an arbitrary phase gate on the nuclear spin. We also demonstrate that repeated applications of $\pi$-phase gates can bang-bang decouple the nuclear spin from the environment, locking the spin state for up to 140 μs.


2Research was supported by the Sloan and Packard Foundations, the National Science Foundation through awards DMR-0819860 and DMR-0846341, and the Army Research Office through PECASE award W911NF-08-1-0189.

8:36AM F31.00004 Quantum control of orbital and spin dynamics in diamond using ultrafast optical pulses1. F. JOSEPH HEREMANS2, Institute for Molecular Engineering, University of Chicago — Optically addressable spin defects in solid-state materials have shown great potential for applications ranging from metrology to quantum information processing. Many of these experiments require a detailed understanding of the full Hamiltonian dynamics in order to develop precise quantum control. Here we use picosecond resonant optical pulses to investigate the coherent orbital and spin dynamics of the nitrogen-vacancy (NV) center in diamond, over timescales spanning six orders of magnitude. We implement an ultrafast optical pump-probe technique to study the NV center’s orbital-doublet, spin-triplet excited state [1]. These experiments reveal dynamics on femtosecond to nanosecond timescales due to the interplay between the ground and excited state orbital levels. This all-optical technique also provides a method to dynamically control the spin state of the NV center by harnessing the excited state structure. Through studying the spin dynamics of the NV center with coherent pulses of light, we are able to rotate the spin state on sub-nanosecond timescales. Furthermore, by tuning the excited-state spin Hamiltonian with an external magnetic field, we demonstrate arbitrary-axis spin rotations through controlled unitary evolution of the spin state. Extending this to the full excited-state manifold, we develop a time-domain quantum tomography technique to precisely map the NV center’s excited state Hamiltonian. These techniques generalize to other systems and can be a powerful tool in characterizing and controlling qubits in other optically addressable spin systems.


1This work is supported by the AFOSR and NSF.

2In collaboration with L.C. Bassett, D.J. Christie, C.G.Yale, G. Burkard, B.B. Buckley, and D.D. Awschalom

9:12AM F31.00005 Electron spin lifetimes in 1e14 cm$^{-3}$ proton irradiated SiC3. KYLE MILLER, JOHN COLTON, Brigham Young University, SAM CARTER, Naval Research Lab — Silicon vacancies created by irradiation with protons or electrons in 4H silicon carbide (SiC) are potential spintronic devices. In our experiments, electron spin states are polarized with 870 nm laser light, and we manipulate the spins with resonant microwaves at 10.47 GHz and a magnetic field of 350 mT. Spin states are detected by the change in photoluminescence from the silicon defects, and lifetimes are calculated through optically detected spin resonance and electron spin echo. We have measured $T_2$ lifetimes in 1e14 cm$^{-3}$ proton irradiated SiC to be about 16 μs at various temperatures, fairly independent with temperature. Future plans include studying how defect density will impact spin lifetimes.

3Partially funded by NSF (Grant No. REU PHY1157078)
Spin states of the silicon vacancy in silicon carbide

MICHELE BOCKSTEDTE, University of Salzburg, Austria, and University Erlangen-Nuernberg. Germany, FELIX SCHUETZ, University Erlangen-Nuernberg, Germany — SiC as a semi conductor fulfills all necessary requirements for implementing qubits via defect electron spins, such as the silicon vacancy, the di-vacancy or a complex of a silicon vacancy and a nitrogen impurity. The spin-selective fluorescence in contrast to the prototypical NV-center in diamond operates in the spectral range favorable for telecom applications.

Spin-manipulation of the intrinsic centers was demonstrated even at room temperature. For the silicon vacancy in SiC inter system crossings (ISCs) from high to yet unknown low spin states govern the spin-relaxation. By DFT and a DFT-based multi-reference Hamiltonian we analyze the spin physics of the defect. In 4H SiC distinct luminescence lines are obtained for the inequivalent defect sites in agreement with experiment. Our result thus establishes an assignment of the lines to the sites. Owing to the spin (S=3/2) and a stronger electron-phonon coupling in the excited state, we find ISCs distinct from the NV-center.

1 J. R. Weber et al., PNAS 107, 8513 (2010).

Near unity optical spin polarization of 20Si nuclei in silicon carbide

WENHAO HU, MICHAEL E. FLATTÉ, Department of Physics and Astronomy, University of Iowa — Recently, a decoherence-free subspace (DFS) system has been predicted in the substitutional nickel spin center of diamond [1]. Here we describe our investigations of substitutional transition metal dopants in 3C silicon carbide using density functional theory in the SGGA approximation. We used a 64-atom supercell for the silicon carbide host, inserted a dopant atom (Ni or Cr) at a single carbon or a single silicon site. The atomic positions were allowed to relax with a force precision of 0.1 mRy/a.u. The Heisenberg exchange coupling energy J was calculated as a function of hydrostatic strain. An antiferromagnetic-ferromagnetic transition can be seen in nickel spin centers at certain strains. A model of two spatially separated spins can be used to explain the dependence of J on the atomic separation. By applying a magnetic field, we predict two of the triplet states can be split off so as to create a DFS. Strain modulation and resonant microwave can be exploited to manipulate the qubit.

Finally, the experimental feasibility of our scheme is evaluated.


This work was supported by an AFOSR and NSF.

Tight-Binding Model for Exchange Interaction Between Transition Metal Dopants in Diamond and SiC

VICTORIA R. KORTAN, CÜNEYT SAHIN, MICHAEL E. FLATTÉ, Optical Science and Technology Center & Department of Physics and Astronomy, University of Iowa — Diamond and SiC are wide-band-gap semiconductors with long-lived spin lifetimes [1,2] and promising for quantum information technology device design. Spin initialization, manipulation and readout has already been demonstrated for the NV center in diamond [3] and the vacancy in SiC [4]. Transition metal spin centers offer additional benefits in tetrahedral hosts due to the crystal field splitting of the d-states into localized and extended states. For example, the application of strain in diamond allows switching between two spin states of a single Ni dopant [5]. Here we use a spds* tight-binding model including spin-orbit interaction to describe transition metal spin centers in diamond and 3C-SiC as well as the NV center in diamond and divacancy in 3C-SiC. The energy levels for an isolated dopant are taken from experiment, when available, and density functional theory calculations otherwise. We calculate and compare the wavefunctions of these spin centers, as well as the strength of the exchange interaction between pairs of them.


This work was supported by an AFOSR MURI.

Isolation and Control of Spins in Silicon Carbide with Millisecond-Coherence Times

DAVID J. CHRISTLE, ABRAM L. FALK, PAOLO ANDRICH, PAUL V. KLIMOV, DAVID D. AWSCHALOM, Institute for Molecular Engineering, University of Chicago, JAWAD UL HASSAN, NGUYEN T. SON, ERIK JANZÈN, Department of Physics, Chemistry and Biology, Linköping University, TAKESHI OHSHIMA, Japan Atomic Energy Agency — The elimination of defects from silicon carbide (SiC) has facilitated its move to for implementing qubits via defect electron spins, such as the silicon vacancy, the di-vacancy or a complex of a silicon vacancy and a nitrogen impurity. The spin-selective fluorescence in contrast to the prototypical NV-center in diamond operates in the spectral range favorable for telecom applications.

Spin-manipulation of the intrinsic centers was demonstrated even at room temperature. For the silicon vacancy in SiC inter system crossings (ISCs) from high to yet unknown low spin states govern the spin-relaxation. By DFT and a DFT-based multi-reference Hamiltonian we analyze the spin physics of the defect. In 4H SiC distinct luminescence lines are obtained for the inequivalent defect sites in agreement with experiment. Our result thus establishes an assignment of the lines to the sites. Owing to the spin (S=3/2) and a stronger electron-phonon coupling in the excited state, we find ISCs distinct from the NV-center.

1 J. R. Weber et al., PNAS 107, 8513 (2010).

This work was supported by an AFOSR MURI.

Funding by NSF, AFOSR MURI, and the Knut & Alice Wallenberg Foundation is gratefully acknowledged.

10:24AM F31.00011 Two-dimensional nanoscale imaging of gadolinium spins via scanning probe relaxometry with a single spin in diamond. MATTHEW PELLICCIONE, BRYAN MYERS, LAETITIA PASCAL, ANAND DAS, ANIA JAVICH, University of California, Santa Barbara — Spin-labeling of molecules with paramagnetic ions is an important approach for determining molecular structure, however current ensemble techniques lack the sensitivity to detect few isolated spins. In this talk, we demonstrate two-dimensional nanoscale imaging of paramagnetic gadolinium compounds using scanning relaxometry of a single nitrogen vacancy (NV) center in diamond. Gadopentenate dimeglumine attached to an atomic force microscope tip is controllably interacted with and detected by the NV center, by virtue of the fact that the NV exhibits fast relaxation in the fluctuating magnetic field generated by electron spin flips in the gadolinium. We demonstrate a reduction in the T1 relaxation time of the NV center by over two orders of magnitude, probed with a spatial resolution of 20 nm, limited by thermal drift in ambient conditions. We discuss the importance of mitigating drift to reach truly nanoscale imaging and present progress towards cryogenic scanning magnetometry, along with utilizing chemically functionalized tips to gain greater control over the Gd distribution on the tip. Our result exhibits the viability of the technique for imaging individual spins attached to complex nanostructures or biomolecules, along with studying the magnetic dynamics of isolated spins.

10:36AM F31.00012 Coherent Control of a Nitrogen-Vacancy Center Spin Ensemble with a Diamond Mechanical Resonator1, F. GUO, E.R. MACQUARRIE, T.A. GOSAVI, A.M. MOEHLLE, N.R. JUNGWIRTH, S.A. BHAVE, G.D. FUCHS, Cornell University — In contrast to the traditional coherent control of the nitrogen vacancy (NV) center in diamond’s triplet spin state with ac magnetic fields, we recently demonstrated that gigahertz-frequency lattice strain resonant with the m_s=+1 to -1 spin state splitting can also be used to drive spin transitions.1 We present coherent spin control over NV center ensembles with a bulk-mode mechanical microresonator that generates large amplitude ac stress within the diamond substrate. Using these structures, we mechanically drive coherent Rabi oscillations between the +1 and -1 states. We also accurately model the Rabi dephasing with a combination of a spatially inhomogeneous mechanical driving field and magnetic noise from a fluctuating spin bath. Understanding mechanically driven dynamics in spin ensembles could have applications in sensing and quantum optomechanics where interactions can be enhanced by the number of mechanical modes for quantum transitions, thus closing the loop on NV center ground state spin control and enabling the creation of a coherent Δ-system within the NV center ground state.

We gratefully acknowledge support from the ONR.


10:48AM F31.00013 Recursive polarization of nuclear spins in diamond at arbitrary magnetic field. DANIELA PAGLIERO, ABDELGHANI LARAOUI, JACOB HENSHAW, CARLOS MERILES, CUNY-City College of New York — We introduce an alternate route to dynamically polarize the nuclear spin host of nitrogen-vacancy (NV) centers in diamond. Our approach articulates optical, microwave and radio-frequency pulses to recursively transfer spin polarization from the NV electronic spin. Using two complementary variants of the same underlying principle, we demonstrate nitrogen nuclear spin initialization approaching 80% at room temperature both in ensemble and single NV centers. Unlike existing schemes, our approach does not rely on level anti-crossings and is thus applicable at arbitrary magnetic fields. This versatility should prove useful in applications ranging from nanoscale metrology to sensitivity-enhanced NMR.

Tuesday, March 3, 2015 8:00AM - 10:48AM –
Session F32 GMAG DMP: Focus Session: Manganeses

8:00AM F32.00001 Domain walls in improper ferroelectrics as functional oxide interfaces. MANFRED FIEBIG, Department of Materials, ETH Zurich, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland — The coexistence of magnetic and electric order in multiferroics and the resulting magnetoelectric coupling have triggered an immense research interest. The most prominent mechanisms promoting magnetic and ferroelectric order, however, tend to be mutually exclusive. As a result, multiferroics are an inherently source of “unusual” ferroelectricity. In many cases the ferroelectric state is improper, i.e., induced by the ordering of a different parameter like magnetism or strain. This secondary nature can lead to properties not normally found in ferroelectrics. In my talk I will discuss consequences for the ferroelectric domain walls of various multiferroics. For example, in magnetically induced ferroelectrics like MnWO4 or TbMnO3 the electric polarization within the wall is expected to rotate instead of passing through zero, as in conventional displaceable ferroelectrics. This affects the distribution and propagation of the ferroelectric domains. In addition, a magnetic-field-induced rotation can reversible charge and discharge the domain walls. In strain-induced ferroelectrics like SrMnO3 the interplay of strain and oxygen vacancies leads to a polar state in which domain walls act as insulating boundaries to the conducting domains which therefore acts as nano-capacitors.

8:36AM F32.00002 Neutron Scattering Studies of Magnetic Structure and Excitations in Na5/8Mn2O3, ROBIN CHISNELL, NIST Center for Neutron Research, XIN LI, XIAOHUA MA, MIT, DONG SU, Brookhaven National Laboratory, LEI LIU, SHUYE PING ONG, HAILONG CHEN, ALEXANDRA TOUMAR, MIT, JUAN-CARLOS IDROBO, Oak Ridge National Laboratory, YUECHUAN LEI, MIT, JIANMING BAI, FENG WANG, Brookhaven National Laboratory, JEFFREY LYNN, NIST Center for Neutron Research, YOUNG LEE, GERBRAND CEDER, MIT — Na5/8Mn2O3 (TM=transition metal) materials consist of alternating layers of Na and TM ions with the TM ions arranged on a geometrically frustrated triangular lattice. Na can be easily and reversibly removed from these materials, making them of interest for application in rechargeable batteries and allowing for exploration of their rich phase diagrams as a function of Na concentration. Na ordering is an important factor in ground state selection, and is driven by electrostatic interactions in many Na1−xTMO2 systems. The series Na5/8Mn2O3 differs in that Na ordering is driven by a cooperative Jahn-Teller effect, due to the coexistence of Jahn-Teller active Mn3+ and non-active Mn4+ ions. We have recently shown the existence of a charge stripe ordering a in the material Na5/8Mn2O3 [1]. At low temperatures a magnetic stripe order also develops. We present neutron diffraction and inelastic scattering measurements and examine the details of the magnetic structure and excitations in the magnetic stripe ordered phase. [1] X. Li et al. Nature Mater. 13, 586 (2014)

8:48AM F32.00003 Scanning Tunneling Microscopy of Bilayer La2−2xSr1+x2Mn2O7 Single Crystals1, LEUJEN CHEN, XINZHOU TAN, SEONG HEON KIM, JEEHOON KIM, J.-S. ZHOU, J.B. GOODENOUGH, ALEX DE LOZANNE, University of Texas at Austin — We employed a spin-polarized scanning tunneling microscope to image the (001) surface topography and spectroscopy in La2−2xSr1+x2Mn2O7 (x=0.32, 0.40 & 0.52) single crystals below the Curie temperature. As the doping is increased from x=0.3 to x=0.5 the spins arrange themselves in antiferromagnetic, ferromagnetic, in-plane and out-of-plane configurations. From local density of states (LDOS) maps, we observed a charge density wave with a wavelength of about 1.6 nm along the tetragonal a or b axes in the x=0.32 sample, which is known to be ferromagnetic with spins perpendicular to the surface. On the other hand, the x=0.52 crystal is expected to be type A antiferromagnetic with spins parallel to the surface, which is confirmed by our LDOS maps.

1Supported by NSF grants DMR-0810119 and DMR-1122603.
9:00AM F32.00004 Inhomogeneity driven giant magneto-resistance in compressed LaMnO₃.
MARIA BALDINI, HPsynC, Carnegie Inst of Washington, TAKAKI MURAMATSU, Carnegie Inst of Washington, MOHAMMAD SHERAFATI, Department of Physics, University of Missouri, HO-KWANG MAO, Carnegie Inst of Washington, LORENZO MALAVASI, Department of Chemistry and INSTM, University of Pavia, PAOLO POSTORINO, Department of Physics, University of Rome "Sapienza", SASHI SATPATHY, Department of Physics, University of Missouri, VIKTOR STRUZHINKIN, Carnegie Inst of Washington — CMR in rare-earth manganites has been intensively studied over the past decades. However, the mechanism underlying the CMR is still not completely clarified. Up to now, CMR was only observed in doped manganites suggesting that the presence of mixed valence Mn ions is an essential ingredient of the CMR phenomenon. Since its discovery, phase separation has been established yet [1-5]. We performed high pressure transport measurement varying temperature and magnetic field in a pure compound LaMnO₃, and observe CMR at around 32 GPa. This result leaves aside many ambiguities inherent to compounds with complex chemical composition. We used pressure to modify the material’s property and to clarify in a clean way the role played by phase separation. We found that pressure induces the formation of a mixed phase which consists of two components: an insulating one with Jahn Teller distortion and a metallic one without distortion. The volume fraction of the metallic phase grows with pressure and the CMR is observed just below the percolation threshold. The experimental results are well reproduced by theoretical calculations and percolation theory.

9:12AM F32.00005 Polaron-Mediated Spin Correlations in Metallic and Insulating La₁₋ₓAₓMnO₃. JOEL HELTON, US Naval Academy, DANIEL PAJEROWSKI, YIMING QIU, YANG ZHAO, NIST Center for Neutron Research, DMITRY SHULYATEV, YAKOV MUKOVSKII, National University of Science and Technology "MISiS", GEORGII BYCHKOV, SERGEI BARILO, Belarus Academy of Sciences, JEFFREY LYNN, NIST Center for Neutron Research — Neutron spectroscopy measurements reveal short-range spin correlations near and above the ferromagnetic-paramagnetic phase transition in manganite materials of the form La₁₋ₓAₓMnO₃ (A=Ca, Sr, or Ba), including samples with an insulating ground state as well as colossal magnetoresistive samples with a metallic ground state. Quasielastic magnetic scattering is revealed that forms clear ridges running along the [100]-type directions in momentum space. A simple model consisting of a conduction electron hopping between spin polarized Mn ions that becomes self-trapped after a few hops captures the essential aspects of this magnetic component of the scattering. We associate this scattering component with the magnetic part of diffuse polarons, as we observe a temperature dependence similar to that of the diffuse nuclear scattering arising from individual polarons.

9:24AM F32.00006 Unexpected nanoscale metamagnetic transition in a colossal magnetoresistance manganite¹. LINGJIA SHEN, ELIZABETH BLACKBURN, ALEXANDER. T. HOLMES, EDWARD. M. FORGAN, Univ of Birmingham, UK, SEBASTIAN MUEHLBAUER, Forschungsneutronenquelle Heinz Maier-Leibnitz, Technische Universität München, Garching, Germany, ANDRE HEINEMANN, German Engineering Materials Science Centre, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — Intrinsic inhomogeneities, both on the nanometer and micrometer scale, are crucial to the phase separation seen in the colossal magnetoresistance (CMR) manganite manganites. The origin of these inhomogeneities has been an open question for the past decade [1, 2], but they clearly play an important role. To investigate these inhomogeneities, we have studied Pr₀.₇Ca₀.₃MnO₀.₉₇Ga₀.₀₃O₃ using small angle neutron scattering in fields up to 16 T. In zero field at ~220 K, there is a transition to a charge/orbital ordered (CO/OO) paramagnet, as in Pr₁₋ₓCaₓMnO₃ [3]. At 150 K, the CO/OO phase is destroyed by applying a field of 6 T, and we find that above this field, nanoscale inhomogeneities undergo a separate, uncoupled, metamagnetic transition. We have also explored metamagnetic avalanches at low temperature [4] in this material, and a possible link between the avalanches and the magnetic nanoscale phases will be illustrated. [1] E. Dagotto et al. Phys. Reports 344, 1-153 (2001). [2] K. H. Ahn et al. Nature, 428, 401 (2004). [3] Y. Tomioka et al. Phys. Rev. B 53, R1689 (1996). [4] C. Voille et al. Physical Review B, 68, 224412 (2003).

¹This research is supported by the EPSRC grant EP/J016977/1 and Chinese Scholarship Council.

9:36AM F32.00007 Tunable metamagnetic transitions in double-perovskite EuₓCoMnO₃ single crystals. HWAN YOUNG CHOI, NARA LEE, Yonsei Univ, M.S. SEO, S.Y. PARK, Division of Materials Science, Korea Basic Science Institute, Daejeon 305-806, South Korea, Y.J. JO, Department of Physics, Kyungpook National University, Daegu 702-701, South Korea, Y.J. CHOI, Yonsei Univ — Double perovskite single crystals of EuₓCoMnO₃ were first synthesized using flux method and their magnetic properties were investigated. Magnetic field dependence of magnetization reveals a metamagnetic transition in as-grown crystals. Controlling valences of magnetic ions in different gas annealing conditions leads to the complete change of shapes and locations of metamagnetic transitions in the isothermal magnetization. This remarkable variation originates from the formation of magnetic clusters with different valences of magnetic ions.

9:48AM F32.00008 Spin excitations used to uncover the nature of the magnetically ordered ground state of Pr₀.₅Ca₀.₅MnO₃. RUSSELL EWINGS, TOBY PERRING, ISIS Pulsed Muon & Neutron Source, OLGA SIKORA, Department of Physics, National Taiwan University — We have used time-of-flight inelastic neutron scattering to measure the spin wave spectrum of the canonical half-doped manganite Pr₀.₅Ca₀.₅MnO₃, in its magnetic and orbitally ordered phase. Comparison of the data, which cover multiple Brillouin zones and the entire energy range of the excitations, with several different models shows that only the CE-type ordered state provides an adequate description of the magnetic ground state. We are able to rule out the Zener polaron and magnetic dimer models as magnetic ground states of the system, the former on the basis of gross features of the observed spin wave spectrum and the latter due to subtle discrepancies between the calculated and observed structure factors at certain positions in reciprocal space.

10:00AM F32.00009 A Combined Density Functional Theory and Monte Carlo Study of Manganites for Magnetic Refrigeration. ROMI KOROTANA, GIUSEPPE MALLIA, ZSOLT GERCSI, NICHOLAS HARRISON, Imperial College London — Perovskite oxides are considered to be strong candidates for applications in magnetic refrigeration technology, due to their remarkable properties, in addition to low processing costs. Manganites with the general formula RₓA₁₋ₓMnO₃, particularly for A=Ca and 0.2 < x < 0.7, undergo a field driven transition from a paramagnetic to ferromagnetic state, which is accompanied by changes in the lattice and electronic structure. Therefore, one may anticipate a large entropy change across the phase transition due to the first order nature. The present work aims to achieve an understanding of the relevant structural, magnetic, and electronic entropy contributions in the doped compound La₀.₇₅Ca₀.₂₅MnO₃. A combination of thermodynamics and first principles theory is applied to determine individual contributions to the total entropy change of the system. Hybrid-exchange density functional (B3LYP) calculations for La₀.₇₅Ca₀.₂₅MnO₃ predict an anti-Jahn-Teller polaron in the localised hole state, which is influenced by long-range cooperative Jahn-Teller distortions. Through the analysis of individual entropy contributions, it is identified that the electronic and vibrational terms have a deleterious effect on the total entropy change.
10:12AM F32.00010 Giant orthorhombic distortions by Cu\textsuperscript{2+} in ferrimagnetic spinel Mn\textsubscript{3}O\textsubscript{4}\textsuperscript{1} 
JAE-HO CHUNG, KEE HWAN LEE, HUN CHANG, IN YONG HWANG, Korea University, HYUN WOOK KANG, SU JAE KIM, SEONGSU LEE, Korea Atomic Energy Research Institute — Mn\textsubscript{3}O\textsubscript{4} is a tetragonal (c > a) spinel that exhibits noncollinear Yafet-Kittel ferrimagnetic ordering at low temperatures. We report large orthorhombic distortions in its ferrimagnetic phase stabilized by a few percent of Cu doping. The orthorhombic strains of the ferrimagnetic phases increased linearly to the doping and reached up to \( \varepsilon \approx 8 \times 10^{-3} \) for \( x = 0.19 \), which is three times larger than the saturated value under external magnetic fields. For high doping (\( x \geq 0.17 \)), the distortions first appeared in the paramagnetic phases and underwent further enhancement simultaneously with the onset of the noncollinear ferrimagnetic ordering. We present the rich magnetostructural phase diagram of Cu\textsubscript{x}Mn\textsubscript{3-x}O\textsubscript{4}, and argue that the dilute \( t_2 \) orbital degeneracy of Cu\textsuperscript{2+} under tetrahedral crystal field breaks the global symmetry and triggers the orthorhombic instability inherent in Mn\textsubscript{3}O\textsubscript{4}.

\textsuperscript{1}This work was supported by the National Research Foundation of Korea through the ARCNEX (NRF-2011-0031933).

10:24AM F32.00011 Magnetic Order and Frustration in Doped Sr\textsubscript{2}Mn\textsubscript{3}As\textsubscript{2}O\textsubscript{5}, CHRISTOPHER GEORGEN, CHIH-WEI CHEN, JIAKUI WANG, EMILIA MOROSAN, Rice University — Crystal structure is often key in dictating a material’s magnetic and physical properties. Two components of crystal structure that can be particularly influential are reduced dimensionality (1D or 2D) or geometric frustration. The layered crystal structure of Sr\textsubscript{2}Mn\textsubscript{3}As\textsubscript{2}O\textsubscript{5}, which crystallizes in the tetragonal I\text{4} /mmm space group, exhibits both these features. This compound is of particular interest because it consists of Fe pnictide-tetrahedral layers that alternate with Cu-O-like octahedral layers. This structure is a promising avenue to study geometric effects in relation to unconventional superconductivity. Here we report a magnetic study of the effects of 3d and 4d transition metal substitutions on the Mn site, with emphasis on the resulting long range and short range order. AC and DC magnetization data provide evidence for spin glass to cluster glass crossover with 4d metal doping, while 3d metal doping suppresses both the magnetic order and glassy state. This can be attributed to half-filled Mn 3d shells in a 2D magnetic structure as suggested by neutron diffraction data and band structure calculations.

10:36AM F32.00012 Spin reorientation and Ce-Mn coupling in antiferromagnetic oxypnictide CeMnAs\textsubscript{O}\textsuperscript{3}, DAVID VAKNIN, QIANG ZHANG, SPENCER PETERSON, KEVIN DENNIS, Ames Laboratory, Iowa State University, WEI TIAN, Oak Ridge National Laboratory — Structure and complex magnetic properties of CeMnAs\textsubscript{O}, a parent compound of the “1111”-type oxypnictides, have been investigated using neutron powder diffraction and magnetization measurements. Whereas there is no structural transition from the P\textsubscript{4}/mmn tetragonal phase below 420 K, CeMnAs\textsubscript{O} undergoes a C-type antiferromagnetic order with Mn\textsuperscript{2+} moments pointing along the c-axis below a relatively high Néel temperature of \( T_N = 345 \) K. Below \( T_{N2} = 35 \) K, two simultaneous transitions occur where the Mn moments reorient to the ab-plane preserving the C-type magnetic order, and Ce moments undergo long-range AFM ordering with moments in the ab-plane. Another transition to a noncollinear magnetic structure occurs below 7 K. We find that CeMnAs\textsubscript{O} primarily falls into the category of a local-moment antiferromagnetic insulator in which the nearest-neighbor interaction (\( J_1 \)) is dominant. The spin reorientation transition driven by the coupling between rare earth Ce and transition metal seems to be common to Mn, Fe and Cr ion, but not to Co and Ni ions in the iso-structural oxypnictides.

\textsuperscript{3}Supported by the Office of Basic Energy Sciences, US-DOE, number DE-AC02-07CH11358.

Tuesday, March 3, 2015 8:00AM - 11:00AM — Session F33 CSWP: Invited Session: Supporting the Recruitment and Retention of Women in Physics 
208 - Zahra Hazari, Florida International University

8:00AM F33.00001 Are you a “physics person”?: Understanding students’ experiences, identities, and beliefs\textsuperscript{1} — GEOFF POTVIN, Department of Physics, and STEM Transformation Institute, Florida International University — For several years, there has been much attention paid to the dearth of women in high school and undergraduate physics. Discussion has centered on various explanatory frameworks as to why women do not pursue physics in college as a career and on their persistence in such pursuits. In this talk, I will summarize efforts by our group to investigate recruitment and persistence issues for women in high school and undergraduate physics. Viewed through the lens of identity, we have repeatedly seen the importance of high school students’ beliefs about their ability to perform well (also known as self-efficacy) and persistence in science fields. In this presentation, I will build from research that suggests men and women draw from different types of experiences when evaluating their self-efficacy. I will demonstrate through a logistic regression analysis that self-efficacy is a positive predictor of success for women and men and persistence in science fields. In this presentation I will build from research that suggests men and women draw from different types of experiences when evaluating their self-efficacy. I will discuss the importance of persistence of women in physics. I will explore how women do that and what they can do to help them succeed. I will also present a variety of ways that women may develop their confidence in their ability to succeed in physics.

\textsuperscript{1}NSF Grant No. 1036617

8:36AM F33.00002 Understanding Women’s Success in Physics through Self-Efficacy — VASHTI SAWTELLE, Michigan State University — The underrepresentation of women in physics has been well documented and is a source of concern for both policy makers and educators. Considerable research has shown a connection between students’ confidence in their ability to perform well (also known as self-efficacy) and persistence in science fields. In this presentation, I will build from research that suggests men and women draw from different types of experiences when evaluating their self-efficacy. I will demonstrate through a logistic regression analysis that self-efficacy is a positive predictor of success for women and men and persistence in science fields. In this presentation I will build from research that suggests men and women draw from different types of experiences when evaluating their self-efficacy. I will discuss the importance of persistence of women in physics. I will explore how women do that and what they can do to help them succeed. I will also present a variety of ways that women may develop their confidence in their ability to succeed in physics.

9:12AM F33.00003 “We’re all unisex anyway”: The persistent discourse of gender neutrality in physics — ALLISON GONSALVES, McGill University — Doctoral physics students have stories about the kinds of actions, behaviours and ways of doing physics that enable them to be recognized as physicists. This presentation will illuminate some of these stories through a lens that scrutinizes how discourses about gender can shape both the stories that students tell and the behaviours they practice to achieve recognition in their field. Through observations, photo-elicitation, and life history interviews, eleven men and women shared stories about their experiences with physics, and the contexts that have enabled or constrained their participation in doctoral physics. The results of this study revealed that recognition was often achieved through the reproduction or reworking of persistent discourses of gender norms. This presentation will explore the particularly persistent discourse of gender neutrality in physics. I will explore how this discourse is constructed, how it can be contested, and how it may be constrained for both men and women students. The construction of physics as gender neutral can pose conflicts of identity for students who feel the need to refigure their gender performances in ways that permit recognition as “physics people.” This presentation will look at two case studies that demonstrate the conflict students experience between expressions of femininity and doing physics against the backdrop of gender neutrality. I will discuss the problematic of gender neutrality, and I will also discuss some of the creative solutions doctoral students adopt to navigate discourses of gender in this neutral terrain.
9:48AM F33.00004 Panel Discussion: Women in Physics Groups with A. Coil, C. Boekema, E. Yitamben, and J. Walrath — Panel Discussion: Women in Physics Groups with A. Coil, University of California; C. Boekema, San Jose State University; E. Yitamben, Purdue University; and J. Walrath, University of Michigan.

Tuesday, March 3, 2015 8:00AM - 11:00AM – Session F34 GERA: Focus Session: Novel Photophysics and Transport Mechanisms for Nanostructured Photovoltaics 210A -

8:48AM F34.00003 Free Charge Carriers in Lead Iodide Perovskites Revealed by Transient Absorption Spectroscopy, MINH TUAN TRINH, XIAOYANG ZHU, Columbia University — Lead iodide perovskites have emerged as the most-promising materials for low-cost thin film photovoltaics and other optoelectronic materials. Much experimental effort has been devoted to understanding fundamental properties and device performances, however the nature of photo-excitation in these materials remains debated. Using transient absorption spectroscopy, we study the dynamics of electrons and holes in photo-excited lead iodide perovskites. We show that, upon excitation with photon energy above the bandgap, hot electrons and holes are created. The e-h pair possess a transient dipole moment, which induces a transient Stark effect seen in subsequent optical transitions by the probe pulse. At high excitation densities, we find that carrier decay is well described by a third-order kinetic process, as expected from Auger recombination of free carriers. We also provide direct evidence for charge carrier traps on the surfaces and excitonic traps below the optical gaps in these materials.

9:00AM F34.00004 Enhanced Multiple Exciton Generation in Amorphous Silicon Nanoparticles1, ANDREI KRYJEVSKI, DEYAN MIHAYLOV, North Dakota State Univ, DMITRI KILIN, University of South Dakota — Multiple exciton generation (MEG) in nm-sized hydrogen-passivated silicon nanowires (NWs), and quasi two-dimensional nanofilms depends strongly on the degree of the core structural disorder as shown by the many-body perturbation theory (MBPT) calculations based on the DFT simulations. Here, we use the HSE exchange correlation functional. In MBPT, we work to the 2nd order in the electron-photon coupling and in the approximate screened Coulomb interaction. We also include the effect of excitons for which we solve Bethe-Salpeter Equation. We calculate quantum efficiency (QE), the average number of excitons created by a single absorbed photon, in 3D arrays of Si29H26 quantum dots, NWs, and quasi 2D silicon nanofilms, all with both crystalline and amorphous core structures. Efficient MEG with QE of 1.3 up to 1.8 at the photon energy of about 3Eg, where Eg is the gap, is predicted in these nanoparticles except for the crystalline NW and film where QE ≃ 1. MEG in the amorphous nanoparticles is enhanced by the electron localization due to structural disorder. The exciton effects significantly red-shift QE(E photon) curves. Nanometer-sized amorphous silicon NWs and films are predicted to have effective MEG within the solar spectrum range.

9:12AM F34.00005 Hot electron-generated plasmon resonance in ultrathin solar absorbers: Theory2, JIANTAO KONG, CHAOBIN YANG, JUAN M. MERLO, MICHAEL J. BURNS, MICHAEL J. NAUGHTON, KRZYSZTOF KEMPA, Boston College — It has been proposed in a simple model calculation that hot electrons excited in a semiconductor can emit plasmons in an adjacent metallic nanostructure at very high rate. Exceeding that of phonon emission [1]. We demonstrate by FDTD simulations and quantum mechanical calculations that an ultrathin solar absorber with a composite metamaterial/plasmonic collector can emit plasmon. The composite collector has a dual function: it is designed to efficiently trap light and it is a plasmonic resonator tuned to absorb the energy of hot electrons, thus “protecting” them from phonon losses. We propose a specific structure where observation of this phenomenon can occur.

1We acknowledge NSF support (CHE-1413614) for method development

2Supported in part by the W.M. Keck Foundation.
9:24AM F34.00006 Electron mediated plasmon resonance in ultrathin solar absorbers: Experiment 1, CHAOBIN YANG, JUAN M. MERLO, AARON H. ROSE, JIANTAO KONG, MICHAEL J. BURNS, KRZYSZTOF KEMP, MICHAEL J. NAUGHTON, Boston College — We describe experimental progress on a hot electron PV structure based on hot electron plasmon protection (HELP) [1] that provides a path to solar efficiency in excess of the Shockley-Queisser limit. It combines hot electron recovery in ultrathin junctions with superabsorption in metamaterial/plasmonic nanosystems and a HELPP plasmon resonance energy transfer (PRET) mechanism. Measurements of optical absorbance (via reflectance and transmittance) of Ag nanopatterns on p- and n-type crystalline and amorphous Si absorbers were performed at incident wavelengths from 350 to 2,500 nm. In samples prepared with Ag nanopatterns with dimensions tuned to provide a resonance near 1,600 nm, we indeed observed such a resonance. We discuss these and other experimental results associated with hot electron facilitated plasmon resonances.

1Supported in part by the W.M. Keck Foundation.

9:36AM F34.00007 Colloidal Nanoparticles for Intermediate Band Solar Cells, MARTON VOROS, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago, GREGELY ZIMANYI, Department of Physics, University of California, Davis — The Intermediate Band (IB) solar cell concept is a promising idea to transcend the Shockley-Queisser limit.[1] Using the results of first principles calculations, we proposed that colloidal nanoparticles (CNPs) are a viable and efficient platform for the implementation of the IB solar cell concept. We focused on CdSe and we showed that intragap states present in the isolated dots with reconstructed surfaces combine to form an IB in arrays of NPs, which is well separated from the valence and conduction band edges. We also showed that in solution such IB may be electron doped using, e.g. decamethylcobaltocene, thus activating an IB-induced absorption process. Our results, together with the recent report of a nearly 9% efficient CNP solar cell[2] indicate that colloidal nanoparticle intermediate band solar cells are a promising platform to overcome the Shockley-Queisser limit.


9:48AM F34.00008 The Molecular Photo-Cell: Quantum Transport and Energy Conversion at Strong Non-Equilibrium, SHIGERU AJISAKA, Department of Chemistry, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel, BOJAN ZUNKOVIC, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Casilla, JONATAN DUBI, Department of Chemistry, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel — The molecular photo-cell is a single molecular donor-acceptor complex attached to electrodes and subject to external illumination. Besides the obvious relevance to molecular photo-volts, the molecular photo-cell is of interest being a paradigmatic example for a system that inherently operates in out-of-equilibrium conditions and typically far from the linear response regime. Moreover, this system includes electrons, phonons and photons, and environments which induce coherent and incoherent processes, making it a challenging system to address theoretically. Here, using an open quantum systems approach, we analyze the non-equilibrium transport properties and energy conversion performance of a molecular photo-cell, including for the first time both coherent and incoherent processes and treating electrons, photons, and phonons on an equal footing. We find that both the non-equilibrium conditions and decoherence play a crucial role in determining the performance of the photovoltaic conversion and the optimal energy configuration of the molecular system.

10:00AM F34.00009 Experimental evidence of enhanced optical absorption in ultra-thin film CdTe PV absorbers via embedded metal nanopatterns, AARON H. ROSE, MICHELLE L. SOLOMON, MICHAEL J. BURNS, MICHAEL J. NAUGHTON, Boston College — We show an increase of optical absorbance in ultra-thin film cadmium telluride solar absorbers by embedded metal nanopatterns (EMN) in the absorber material. Our experimental results are supported by FEM simulations, which also indicate minimal energy loss in the metal. As opposed to locating the metal nanostructures outside of the active region, e.g. at the back or top contact of a solar cell, embedding the structures within the active region gives the greatest absorbance enhancement [1-3]. Previous work has shown a similar increase in absorbance for an amorphous silicon solar medium [1-3], suggesting that EMN is a general light management scheme that can be applied to any thin film photoabsorber. Such light trapping may further yield a viable route to ultra-thin hot electron solar cells [4,5].


10:12AM F34.00010 Broadband Solar Energy Harvesting in Single Nanowire Resonators, YIMING YANG, XINGYUE PENG, STEVEN HYATT, DONG YU, UC Davis — Sub-wavelength semiconductor nanowires (NWs) can have optical absorption cross sections far beyond their physical sizes at resonances frequencies, offering a powerful method to simultaneously lower the material consumption and enhance photovoltaic performance. The degree of absorption enhancement is expected to substantially increase in materials with high refractive indices, but this has not yet been experimentally demonstrated. Here, we show that the absorption efficiency can be significantly improved in high-index NWs, by a direct observation of ~350% performance. The degree of absorption enhancement is expected to substantially increase in materials with high refractive indices, but this has not yet been experimentally demonstrated. Here, we show that the absorption efficiency can be significantly improved in high-index NWs, by a direct observation of ~350% performance. Our results, together with the recent report of a nearly 9% efficient CNP solar cell[2] indicate that colloidal nanoparticle intermediate band solar cells are a promising platform to overcome the Shockley-Queisser limit.

1 Supported by NSF Solar Collaborative under DMR-1035468 and the Center for Advanced Solar Photophysics, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences.

10:24AM F34.00011 Disentangling the roles of free-carrier density and mobility in the performance of CH₃NH₃PbI₃ perovskite films, ELBERT E.M. CHIA, CHAN LA-O-VORAKIAT, M.T. KHUC, R. HASELSBERGER, MARIA-ELISABETH MICHEL-BEYERLE, Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, T. SAUM, HAI BIN SU, Y.M. LAM, School of Materials Science and Engineering, Nanyang Technological University, RUDOLPH A. MARCUS, Noyes Laboratory, California Institute of Technology — Apart from broadband absorption of solar radiation, the performance of photovoltaic devices is governed by two parameters: carrier mobility and carrier density. They indicate how many and how fast the free carriers drift away from the light-harvesting medium before loss mechanisms, such as carrier recombination, occur. However, these parameters are usually entangled as a product. Using time-resolved terahertz spectroscopy, the number density, mobility and quantum yield of charge carriers in a perovskite film have been disentangled. The free carrier recombination mechanisms and rates were determined, and hence the diffusion length. Our results suggest that perovskite-based solar cells can perform well even at low temperatures as long as the three-body recombination has not become predominant.

1 Singapore MOE AcRF Tier 1 (RG 13/12, MOE2014-T1-001-056); Singapore NRF CRP (NRF-CRP4-2008-04); ONR and ARO; A*STAR SERC (1223600006, 1121202012); Danish Council for Strategic Research (CHASOL); BMBF/NTU; NTU Biophysics Center.
2 Current address: Faculty of Science, King Mongkut’s University of Technology Thonburi, Bangkok 10140, Thailand.
10:36AM F34.00012 Bond pathway analysis of NMR spectra for Li$_{1.2}$Mn$_{0.4}$Co$_{0.4}$O$_2$: pristine material. HAKIM IDDIR, BARIS KEY, FULYA DOGAN, JOHN RUSSELL, BRANDON LONG, JAVIER BARENO, JASON CROY, ROY BENEDEK, Argonne National Laboratory — NMR has been applied extensively to lithium ion battery cathode materials, of which layered-layered composites $x$Li$_2$MnO$_3$·(1−$x$)Li$_2$MnO$_2$ and Bond-Pathway-model analysis is applied to elucidate the atomic arrangement and domain structure of this material (in its pristine state, before electrochemical cycling). The simplest structural element of a domain consists of a stripe of composition LiMn$_2$ parallel to an in-layer crystallographic axis in a metal layer of the composite. A simple model of the composite structure may be constructed by a superposition of such stripes in an LiCoO$_2$ background. We show that such a model can account for most of the features of the observed NMR spectra. Support from the Vehicle Technologies Program U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy.

10:48AM F34.00013 Roll-to-Roll Production of Spray Coated N-doped Carbon Nanotube Electrodes for Supercapacitors\textsuperscript{1}, MEHMET KARAKAYA, JINGYI ZHU, ACHYUT RAGHAVENDRA, RAMAKRISHNA PODILA, Clemson University, SAMUEL PARLER, JAMES KAPLAN, Cornell Dubilier Electronics, Inc., APPARAO RAO, Clemson University, CORNELL DUBILIER ELECTRONICS, INC. COLLABORATION — Although nanocarbons are being increasingly used in energy storage, there has been a lack of inexpensive, continuous and scalable synthesis methods. Here we present a scalable roll-to-roll spray coating process for synthesizing supercapacitors from randomly oriented multi-walled carbon nanotubes electrodes on Al foils, which yield high power and energy densities (≈ 700 mW/cm$^2$ and 1 mWh/cm$^2$) and cycle stability (>10000 cycles) on par with Li-ion thin film batteries. Our cost analysis shows that the R2R spray coating process can produce supercapacitors with 10 times the energy density of conventional activated carbon devices at ~ 17% lower cost.

\textsuperscript{1}NSF CMMI SNM Award #1246800

Tuesday, March 3, 2015 8:00AM - 10:48AM — Session F36 GSOFT DBIO: Focus Session: Biofunctionalized Nano-Materials

8:00AM F36.00001 Multi-scale morphology in self-assembly of peptides to proteins via a coarse-grain model\textsuperscript{1}, RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — Self-organizing structures of short peptides (6-7 residues) and proteins (136 residues) are studied by a coarse-grained Monte Carlo simulation. Peptides and proteins are described by coarse-grained chains of residues whose interactions are described by a knowledge-based residue-residue interaction potential that captures the compositional specificity. Large-scale computer simulations are performed to study the structural evolution e.g. aggregation, network, etc. at a range of temperatures and concentrations. A number of local and global physical quantities including structure factor are examined. We find that the residue interactions, concentration, and size of chains are very important in modulating the structure of emerging morphologies in the specified temperature range. Estimates are provided for the effective (fractal) dimension of the assembly over various length scales as a function of temperature.

\textsuperscript{1}This work is supported by the Air Force Research Laboratory.

8:12AM F36.00002 Interaction of Biofunctionalized Nanoparticles with Receptors on Cell Surfaces: MC Simulations, ELENA DORMIDONTTOVA, Physics Department and Institute of Materials Science, University of Connecticut, SHIHU WANG, Chemical Engineering Department, University of Michigan — One of the areas of active development of modern nanomedicine is drug/gene delivery and imaging application of nanoparticles functionalized by ligands, aptamers or antibodies capable of specific interactions with cell surface receptors. Being a complex multifunctional system different structural aspects of nanoparticles affect their interactions with cell surfaces and the surface properties of cells can be different (e.g. density, distribution and mobility of receptors). Computer simulations allow a systematic investigation of the influence of multiple factors and provide a unified platform for the comparison. Using Monte Carlo simulations we investigate the influence of the nanoparticle properties (nanoparticle size, polymer tether length, polydispersity, density, ligand energy, valence and density) on nanoparticle-cell surface interactions and make predictions regarding favorable nanoparticle design for achieving multiple ligand-receptor binding. We will also discuss the implications of nanoparticle design on the selectivity of attachment to cells with high receptor density while ‘ignoring’ cells with a low density of receptors.

8:24AM F36.00003 Prediction of Surface and pH-Specific Binding of Peptides to Metal and Oxide Nanoparticles, HENDRIK HEINZ, TZU-JEN LIN, FATEME SADAT EMAMI, HADI RAMEZANI-DAKHEL, University of Akron, RAJESH NAIK, Air Force Research Laboratory, MARC KNECHT, University of Miami, CAROLE C. PERRY, Nottingham Trent University, YU HUANG, University of California-Los Angeles — The mechanism of specific peptide adsorption onto metallic and oxidative nanostructures has been elucidated in atomic resolution using novel force fields and surface models in comparison to measurements. As an example, variations in peptide adsorption on Pd and Pt nanoparticles depending on shape, size, and location of peptides on specific bounding facets are explained. Accurate computational predictions of reaction rates in C-C coupling reactions using particle models derived from HE-XRD and PDF data illustrate the utility of computational methods for the rational design of new catalysts. On oxidic nanoparticles such as silica and apatites, it is revealed how changes in pH lead to similarity scores of attracted peptides lower than 20\%, supported by appropriate model surfaces and data from adsorption isotherms. The results demonstrate how new computational methods can support the design of nanoparticle carriers for drug release and the understanding of calcification mechanisms in the human body.
8:36AM F36.00004 Aqueous amino acids and proteins near solid surfaces: ZnO, ZnS, Au, and mica, MAREK CIEPLAK, Institute of Physics, Polish Academy of Sciences, Warsaw, Poland — We calculate potentials of the mean force for 20 amino acids in the vicinity of the (111) surface of Au, four surfaces of ZnO, and the (110) surface of ZnS using molecular dynamics simulations combined with the umbrella sampling method. In the case of Au, we compare results obtained within three different force fields: one hydrophobic (for a contaminated surface) and two hydrophilic — with and without polarization of the solid. The properties of water near the surface sensitively depend on the force field. All of these fields lead to good binding with very different specificities and to unlike patterns in the density and polarization of water. We demonstrate that binding energies of dipeptides are distinct from the combined binding energies of their amino acidic components. We show that ZnS is more more hydrophobic than ZnO and that the density profile of water is quite different than that forming near ZnO – it has only a minor articulation into layers. Furthermore, the first layer of water is disordered and mobile. In the case of ZnS, not all amino acids can attach to the surface and when they do, the binding energies are comparable to those found for the surfaces of ZnO (and to hydrogen bonds in proteins) but the nature of the specificity is distinct. The covalent bond with the sulfur atom on cysteine is modeled by the Morse potential. For the hydrophobic Au, adsorption events of a small protein (the tryptophan cage) are driven by attraction to the strongest binding amino acids. This is not so for ZnO, ZnS and for the hydrophilic models of Au – a result of smaller specificities combined with the difficulty for proteins, but sometimes not for single amino acids, to penetrate the first layer of water. Molecular dynamics studies of several proteins near mica with a net charge on its surface indicate existence of two types of states: deformed and unfolded. Using a coarse-grained model, we also study a glassy behavior of protein layers at air-water interfaces. REFERENCES: [1] A. Starzyk and M. Cieplak, Denaturation of proteins near polar surfaces, J. Chem. Phys. 135, 235103 (2011); [2] G. Nawrocki and M. Cieplak, Amino acids and proteins at ZnO-water interfaces in molecular dynamics simulations, Phys. Chem. Chem. Phys. 15, 13628-13636 (2013); [3] G. Nawrocki and M. Cieplak, Interactions of aqueous amino acids and proteins with the (110) surface of ZnS in molecular dynamics simulations, J. Chem. Phys. 140, 095101 (2014); [4] G. Nawrocki and M. Cieplak, Aqueous Amino Acids and Proteins Near the Surface of Gold in Hydrophilic and Hydrophobic Force Fields, J. Phys. Chem. C 118, 12929-12943 (2014); [5] M. Cieplak, D. B. Allen, R. L. Leheny, and D. H. Reich, Proteins at air-water interfaces: a coarse-grained approach, Langmuir (in press).

1Polish National Science Centre; Grant number: 2012/05/B/NZ1/ 00631 and ERA-NET Grant FiberFuel

9:12AM F36.00005 Aptamer functionalized lipid multilayer gratings for label free detection of specific analytes, PLENGCHART PROMMAPAN, Department of Physics, Florida State University, TROY W. LOWRY, Department of Physics and Integrative Nanoscience Institute, Florida State University, DAVID VAN WINKLE, Department of Physics, Florida State University, STEVEN LENHERT, Department of Biological Sciences and Integrative Nanoscience Institute, Florida State University — Lipid multilayer gratings have been formed on surfaces with a period of 700 nm. When illuminated with white light incident at about 50°, these gratings diffract green light perpendicular to their surface. We demonstrate the potential of these gratings as sensors for analytes by monitoring changes in the diffracted light due to the changes in the size and shape of the grating in response to analyte binding. To demonstrate this potential application, a lipid multilayer grating was functionalized with a thrombin binding aptamer. The selectivity of our aptamer functionalized lipid gratings was confirmed both by monitoring the diffracted light intensity and by fluorescence microscopy. Furthermore, the results show that the binding activity between the aptamer and thrombin depends on the relative composition of a zwitterionic lipid (DOTAP) and a cationic lipid (DOTAP). This work shows that nanostructured lipid multilayers on surfaces are a promising nanomaterial for label-free bio-sensing applications.

9:24AM F36.00006 Materials Integration by Nanointaglio, TROY LOWRY, Department of Biological Sciences and Integrative Nanoscience Institute, Department of Physics, Florida State University, AUBREY KUSI-APPIAH, Department of Biological Sciences and Integrative Nanoscience Institute, Florida State University, JINGJIAO GUAN, Department of Chemical and Biomedical Engineering, Florida State University, DAVID VAN WINKLE, Department of Physics, Florida State University, STEVEN LENHERT, Department of Biological Sciences and Integrative Nanoscience Institute, Florida State University — Nanointaglio is a printing process from a microstructured intaglio stamp that in combination with established microarray technology is suitable for heterogeneous materials integration of lipid multilayer micro- and nanostructures. Nanointaglio offers both size dependent functionality and massively parallel materials integration capabilities. The scalable, multi-integrative characteristics of nanointaglio have potential applications in high throughput screening and biosensor arrays.


9:36AM F36.00007 Protein-Polymer Functionalized Nanopatterned Surfaces, HOAYU WANG, PINAR AKCORA, Stevens Inst of Tech — Understanding and controlling the protein interactions with surfaces for biosensors and biomedical implants is a fundamental problem for biocompatible nanomaterial design. Proteins attached in ordered nanopores can exhibit superior biological activities compared to smooth microstructured surfaces. We developed heterogeneous and nanopatterned surfaces decorated with polymer brushes and proteins to control protein fates through elasticity. The heterogeneity of surfaces is controlled with well-defined chemistry, pattern size and geometry, stiffness of polymers and protein types. We will present our recent nanointaglio results on nanopatterned and biofunctionalized flat surfaces and discuss the pattern size effect on protein activity, hence conformation.

9:48AM F36.00008 Air-stable droplet interface bilayers, CHARLES COLLIER, ORNL, ORNL TEAM — Droplet interface bilayers are versatile model membranes useful for synthetic biology and biosensing; however, to date they have been for the most part confined to fluid reservoirs. Here, we demonstrate that when two or more water droplets meet on an oil-infused substrate, they exhibit noncoalescence due to the formation of a thin oil film that gets squeezed between the droplets from the bottom up. We show that when phospholipids are included in the water droplets, a stable droplet interface bilayer forms between the noncoalescing water droplets. As with traditional oil-submerged droplet interface bilayers, we were able to characterize ion transport by incorporating peptides into each droplet. We demonstrate the ability of these air-stable droplet interface bilayers (airDIBs) to incorporate ion channel transport by incorporating peptides into each droplet. We demonstrate the ability of these air-stable droplet interface bilayers (airDIBs) to incorporate ligand-gated ion channels via fusion of microsomes, which enables the biosensing of airborne matter.

10:00AM F36.00009 Interactions of Lysozyme and Azobenzene Derivatives in the Solution and on a Surface, TAO WEI, Lamar University, KATHERINE SHING, Mark Family Department of Chemical Engineering & Materials Science, Los Angeles, CA 90089-1211 — The reversible isomerization of the azobenzene and its derivatives can control protein structure in an aqueous environment with the alternation of visible and UV lights for very promising applications in drug delivery. However, an atomistic description of Aza-molecules and protein amino acid residues is still lacking. In this study we performed atomistic molecular dynamics simulation to study the interactions between a lysozyme molecule and the Azobenzene derivative (in the bulk solution and grafted on the Silica surfaces). Protein structural arrangements (i.e., the shape and secondary structures) and its mobility, as a function of tran/cis ratio in the bulk solution and on the self-assembling monolayer surface’s density and morphology, are systematically investigated.
It was found that the replication process can be electrically monitored by attaching a Klenow fragment of polymerase I to the surface of a carbon nanotube and monitoring the current along the tube [1]. In this talk, we report results from computational studies on DNA polymerase nanocircuits. We have first performed classical molecular dynamics (MD) calculations to get snapshots of different enzymatic stages, particularly the open state (no DNA binding) and the closed state (DNA double helix binding). We then used density functional theory (DFT) and Keldysh non-equilibrium Green’s function (NEGF) formalism to calculate transmission coefficients and currents for each enzymatic state. Our results show that the transmission spectrum and the currents change significantly when the enzyme moves from the open to the closed state. While the initial experiments did not show signal differences between dissimilar bases, the theoretical work in progress is investigating conditions where bases might have distinct signatures, which would allow for DNA sequencing.

10:24AM F36.00011 Graphene under one-dimensional periodic potentials using DNA-assembled parallel nanotubes as a periodic gate array. YONG WU, Univ of California - Riverside, SI-PING HAN, WILLIAM GODDARD, California Institute of Technology, MARC BOCKRATH, Univ of California - Riverside — Graphene under an applied one-dimensional (1D) periodic potential is predicted to show many interesting and unique phenomena such as electron supercollimation and additional Dirac points [1], and some progress has been made in observing graphene in this regime [2]. Here, we use parallel nanotubes assembled using DNA linkers [3] as a back gate to apply periodic or quasi-periodic 1D potentials to graphene layers. The pitch of the nanotube array can be controlled by the linker length which we can vary from 8nm-20nm. We can independently control the periodic potentials using the nanotube array and the carrier density using a top gate to study the transport properties of the system. Our latest results will be discussed.

1. Anisotropic behaviours of massless Diracfermions in graphene under periodic potentials, Nature Physics, C-H Park, Steven Louie
2. Tunable Superlattice in Graphene To Control the Number of Dirac Points, Mandar M. Deshmukh
3. DNA-Linker-Induced Surface Assembly of Ultra Dense Parallel Single Walled Carbon Nanotube Arrays, Nanoletter, Si-ping Han, William Goddard

Tuesday, March 3, 2015 8:00AM - 11:00AM –
Session F37 GQI: Focus Session: Semiconductor Qubits - Topological Qubits, Spin-orbit Effects and Micromagnets

8:00AM F37.00001 Superconducting Edge-Mode Transport in InAs/GaSb Double Quantum Wells. VLAD PRIBIAC, Kavli Institute of Nanoscience, Delft University of Technology — In proximity to a superconductor, topological insulators are predicted to host topological superconductivity, an exotic state of matter that supports Majorana zero-modes. Localized Majorana modes are expected to obey non-Abelian exchange statistics, making them interesting building blocks for topological quantum computing. Here we report supercurrent in the edge modes of Type-II InAs/GaSb quantum wells, a two-dimensional topological insulator (2D TI). By electrostatically-gating the devices we observe superconducting transport in all three regimes of the 2D TI: bulk electrons, edge modes and bulk holes. From superconducting quantum interference measurements, we extract the spatial distribution of the supercurrent in each regime. A clear transition to edge-dominated supercurrent is observed under conditions of high bulk resistivity, which we associate with the 2D topological phase.

8:36AM F37.00002 Quasiparticle parity lifetime of bound states in a hybrid superconductor-semiconductor quantum dot. ANDREW HIGGINBOTTOM, University of Copenhagen, Harvard University, SVEN ALBRECHT, GEDIMINAS KIRSANSKAS, University of Copenhagen, WILLY CHANG, University of Copenhagen, WENCHANG LU, JERRY BERNHOLC, North Carolina State University, PHILIP COLLINS, University of California Irvine — DNA polymerases are important enzymes that replicate DNA molecules with very low error rates – about one error in 10^12 bases. Recently, it was found that the replication process can be electrically monitored by attaching a Klenow fragment of polymerase I to the surface of a carbon nanotube and monitoring the current along the tube [1]. In this talk, we report results from computational studies on DNA polymerase nanocircuits. We have first performed classical molecular dynamics (MD) calculations to get snapshots of different enzymatic stages, particularly the open state (no DNA binding) and the closed state (DNA double helix binding). We then used density functional theory (DFT) and Keldysh non-equilibrium Green’s function (NEGF) formalism to calculate transmission coefficients and currents for each enzymatic state. Our results show that the transmission spectrum and the currents change significantly when the enzyme moves from the open to the closed state. While the initial experiments did not show signal differences between dissimilar bases, the theoretical work in progress is investigating conditions where bases might have distinct signatures, which would allow for DNA sequencing.

1. Anisotropic behaviours of massless Diracfermions in graphene under periodic potentials, Nature Physics, C-H Park, Steven Louie
2. Tunable Superlattice in Graphene To Control the Number of Dirac Points, Mandar M. Deshmukh
3. DNA-Linker-Induced Surface Assembly of Ultra Dense Parallel Single Walled Carbon Nanotube Arrays, Nanoletter, Si-ping Han, William Goddard
We thank financial support by US ARO.

We thank financial support by US ARO and NSF PIF.

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We thank financial support by US ARO and NSF PIF.
factor of ten compared to previous structures. This allows us to bring the nanomagnet closer to the quantum dots, hence increasing the magnetic field gradients by a

Furthermore, we avoid the thick insulating layer between the magnet and the gates by patterning oxidized aluminum

the magnetic field gradients, thus impeding spin rotation speeds in both GaAs [1] and Si [2] quantum dots. In this work, we first reduce the size of the magnet

magnetometry of those improved micromagnets using Hall bars electrostatically defined in an AlGaAs/GaAs two-dimensional electron gas. The gate-voltage

dependent width of the Hall bar enables us to map the averaged magnetic field of the micromagnet, which validates simulations of the inhomogeneous magnetic field profile created by the magnet. We can therefore deduce that our micromagnets can produce magnetic field differences over 200 nm of more than 200 mT.

We selected the material and improved the shape of the micromagnet in order to maximize field gradients and remanence. We perform Hall magnetometry of those improved micromagnets using Hall bars electrostatically defined in an AlGaAs/GaAs two-dimensional electron gas. The gate-voltage dependent width of the Hall bar enables us to map the averaged magnetic field of the micromagnet, which validates simulations of the inhomogeneous magnetic field profile created by the magnet. We can therefore deduce that our micromagnets can produce magnetic field differences over 200 nm of more than 200 mT.


10:24AM F37.00011 Hall magnetometry of micromagnets for single-electron spin qubits, DANY LACHANCE-QUIRON, JULIEN CAMIRAND LEMYRE, LAURENT BERGERON, MICHEL PIORO-LADRIÈRE, Université de Sherbrooke — The coherence time of a single-electron spin can reach tens of milliseconds when placed in the right environment [1]. The electric-dipole interaction between such a single spin and an electric field can be engineered by the inhomogeneous magnetic field of a micromagnet [2]. This effective spin-orbit interaction can be used to manipulate the spin through electric-dipole spin resonance [2], but also to couple a single spin to the electric field of a microwave cavity in the circuit QED architecture [3].

We selected the material and improved the shape of the micromagnet in order to maximize field gradients and remanence. We perform Hall magnetometry of those improved micromagnets using Hall bars electrostatically defined in an AlGaAs/GaAs two-dimensional electron gas. The gate-voltage dependent width of the Hall bar enables us to map the averaged magnetic field of the micromagnet, which validates simulations of the inhomogeneous magnetic field profile created by the magnet. We can therefore deduce that our micromagnets can produce magnetic field differences over 200 nm of more than 200 mT.

10:36AM F37.00011 Hall magnetometry of micromagnets for single-electron spin qubits, DANY LACHANCE-QUIRON, JULIEN CAMIRAND LEMYRE, LAURENT BERGERON, MICHEL PIORO-LADRIÈRE, Université de Sherbrooke — Integrating micrometric size ferromagnets to quantum dots have proven a powerful tool to rotate single spins. In previous approaches, the distance between the magnet and the quantum dots were limiting the magnetic field gradients, thus impeding spin rotation speeds in both GaAs [1] and Si [2] quantum dots. In this work, we first reduce the size of the magnet to improve the field gradients in the dots. Furthermore, we avoid the thick insulating layer between the magnet and the gates by patterning oxidized aluminum gates with a 2 nm thick native oxide. This allows us to bring the nanomagnet closer to the quantum dots, hence increasing the magnetic field gradients by a factor of ten compared to previous structures.


10:48AM F37.00013 High Fidelity Singlet-Triplet S–T+ Qubits in Inhomogeneous Magnetic Fields, CLEMENT WONG, MARK ERIKSSON, SUE COPPERSMITH, MARK FRIESEN, Univ of Wisconsin-Madison — We propose an optimal set of quantum gates for a singlet-triplet qubit in a double quantum dot with two electrons utilizing the S–T+ subspace. Qubit rotations are driven by the applied magnetic field and an orthogonal field gradient provided by a micromagnet. We optimize the fidelity of this qubit as a function of magnetic fields, taking advantage of “sweet spots” where the rotation frequencies are independent of the energy level detuning, providing protection against charge noise. We simulate gate operations and qubit rotations in the presence of quasistatic noise from charge and nuclear spins as well as leakage to nonqubit states, and predict that in silicon quantum dots gate fidelities greater than 99% can be achieved for two nearly-orthogonal rotation axes. Preprint: arXiv:1410.2310

This work was supported in part by NSF, ARO, UW-Madison Bridge Funding, and the Intelligence Community Postdoctoral Research Fellowship Program

Tuesday, March 3, 2015 8:00AM - 11:00AM — Session F38 Gqi: Focus Session: Quantum Error Correction II 212B - Austin Fowler, University of California, Santa Barbara

8:00AM F38.00001 Optimizing the frequency of post-selected quantum error correction in the [[7,1,3]] Steane code, ALI ABU-NADA, BEN FORTESCUE, MARK BYRD, Southern Illinois University Carbondale, SOUTHERN ILLINOIS UNIVERSITY CARBONDALE TEAM — A common assumption in analyses of error thresholds and quantum computing in general is that one applies fault-tolerant quantum error correction (FTQEC) after every logical gate. This, however, is known not to always be optimal if the FTQEC procedure itself can introduce errors. We investigate the effect of varying the number of logical gates between FTQEC operations, and in particular the case where failure of a postselection condition in FTQEC may cause FTQEC to be skipped with high probability. By using a simplified model of errors induced in FTQEC, we derive an expression for the logical error rate as a function of error-correction frequency, and show that in this model the optimal frequency is insensitive to postselection failure probability for a large range of such probabilities. We compare the model to data derived from Monte Carlo simulation for the [[7,1,3]] Steane code.

8:12AM F38.00002 How Often Must We Apply Syndrome Measurements, YAAKOV WEINSTEIN, MITRE — Quantum information is encoded into Quantum Error Correction codes to protect it from decoherence. The detection and correction of possible errors is done via syndrome measurements. Standard quantum fault tolerance approaches assume that syndrome measurements are applied after the implementation of any gate. However, this is resource intensive utilizing much time and many qubits. In this talk we explore whether it is necessary to apply syndrome measurements so often. We examine different syndrome measurement techniques for the [[7,1,3]] code and compare the output state fidelity based on how often syndrome measurements are applied and the error environment. In this way we demonstrate the tradeoff between accuracy and resource consumption.
Thus, we conclude that the ancilla-assisted gate synthesis is the best for a fault-tolerant QFT so far. To the initial expectation, the total resource required to perform specific single-qubit rotations required for the QFT exactly. It is unknown, however, which approach is better for the QFT. We estimated the resource requirements for a fault-tolerant quantum Fourier transform (QFT) to perform specific single-qubit rotations required for the QFT exactly. It is known, however, which approach is better for the QFT. We estimated the resource requirements for a QFT in each case, where the resource is measured by the total number of the \( \pi/8 \) gates denoted by \( T \), which is called the \( T \) count. Contrary to the initial expectation, the total \( T \) count for the state distillation is considerably larger than those for the ancilla-free and ancilla-assisted gate synthesis. Thus, we conclude that the ancilla-assisted gate synthesis is the best for a fault-tolerant QFT so far.
This work is supported by ARO, NSERC, FRQNT and CIFAR.
8:24AM F39.00003 Imaging non-Gaussian output fields produced by Josephson parametric amplifiers: experiments1, D.M. TOYLI, A.V. VENKATRAMANI, Quantum Nanoelectronics Laboratory, UC Berkeley, S. BOUTIN, Departement de Physique, Universite de Sherbrooke, A. EDDINS, Quantum Nanoelectronics Laboratory, UC Berkeley, N. DIDIER, Department of Physics, McGill University and Departement de Physique, Universite de Sherbrooke, A.A. CLERK, Department of Physics, McGill University, A. BLAIS, Departement de Physique, Universite de Sherbrooke, I. SIDDIQI, Quantum Nanoelectronics Laboratory, UC Berkeley — In recent years, squeezed microwave states have become the focus of intense research motivated by applications in continuous-variables quantum computation and precision qubit measurement. Despite numerous demonstrations of vacuum squeezing with superconducting parametric amplifiers such as the Josephson parametric amplifier (JPA), most experiments have also suggested that the squeezed output field becomes non-ideal at the large (>10dB) signal gains required for low-noise qubit measurement. Here we describe a systematic experimental study of JPA squeezing performance in this regime for varying lumped-element device designs and pumping methods. We reconstruct the JPA output fields through homodyne detection of the field moments and quantify the deviations from the ideal squeezed state using maximal entropy techniques. These methods provide a powerful diagnostic tool to understand how effects such as gain compression impact JPA squeezing. Our results highlight the importance of weak device nonlinearity for generating highly squeezed states.

1This work is supported by ARO and ONR.

8:36AM F39.00004 Theory of Dispersion Engineering in Traveling-Wave Kinetic Inductance Amplifiers1, ROBERT ERICKSON, MICHAEL VISSERS, DAVID PAPPAS, National Institute of Standards and Technology — Coplanar-waveguide parametric amplifiers of length extending to the order of a meter have been patterned from superconducting materials using long meandering geometries fabricated on cm2 chips [B. H. Eom, et al., Nat. Phys. 8, 623 (2012)]. These waveguides have highly reactive impedance and operate below the critical current by leveraging the low-temperature nonlinear kinetic inductance \( L(x,t) \) of the underlying superconductor, where \( L(x,t) = L_0(x) \left[ 1 + \left[ I(x,t) / I_c \right]^2 \right] \) at point \( x \) along the waveguide and time \( t \). Here, \( L_0(x) \) is the linear kinetic inductance at \( x \), \( I_c \) is a scaling constant, and \( I(x,t) \) is the total microwave current within the waveguide. As a consequence of the nonlinear kinetic inductance, degenerate four-wave mixing between a pump and signal can result in an idler product as well as significant signal gain as the pump transfers energy to these two side features. Frequency stops and other periodic loadings may be engineered to mitigate effects of higher pump harmonics as well as enhance signal gain, via alteration of phase mismatch. We describe here a simple band theory applicable to the waveguide frequency spectrum that allows us to optimize stop gaps and nonlinear signal gain.

1Work supported by DARPA and the NIST Quantum Information initiative. RPE acknowledges grant 60NANB14D002, US Dept. of Commerce, NIST.

8:48AM F39.00005 Frequency Comb Generation in Superconducting Resonators1, DAVID PAPPAS, ROBERT ERICKSON, MICHAEL VISSERS, HSIANG-SHENG KU, NIST — We have generated frequency combs spanning 0.5 to 20 GHz in superconducting λ/2 resonators at \( T = 3 \) K. Thin films of niobium-titanium nitride enabled this development due to their low loss, high nonlinearity, low frequency dispersion, and high critical temperature. The combs nucleate as sidebands around multiples of the pump frequency. Selection rules for the allowed frequency emission are calculated using perturbation theory, and the measured spectrum is shown to agree with the theory. Sideband spacing is measured to be accurate to 1 part in 109. The sidebands coalesce into a continuous comb structure observed to cover at least several frequency octaves. Generation of combs in this frequency range allows for unprecedented analysis of this non-linear phenomena in the time domain.

1We acknowledge DARPA and the NIST Quantum Information program.

9:00AM F39.00006 Phase-matched Josephson traveling-wave parametric amplifier for superconducting qubit readout - theory, KEVIN O’BRIEN, NSF Nano-scale Science and Engineering Center (NSEC), University of California, Berkeley, CHRIS MACKLIN, IRFAN SIDDIQI, QNL, University of California, Berkeley, XIANG ZHANG, NSF Nano-scale Science and Engineering Center (NSEC), University of California, Berkeley — Josephson parametric amplifiers approach quantum-noise-limited performance and are used in experiments requiring high-fidelity detection of single-photon-level microwave signals. Current Josephson parametric amplifiers couple the Josephson junction (a nonlinear inductor) to a resonant cavity, achieving high gain at the expense of limited instantaneous bandwidth. In contrast, Josephson traveling wave parametric amplifiers (JTWPAs) avoid this gain-bandwidth trade-off by employing long propagation lengths rather than a resonant cavity. A major challenge in JTWPa design is that optimum parametric gain is only achieved when the four-wave mixing process is phase matched. We show that by adding a series of resonant elements to the transmission line, phase matching and exponential gain can be achieved. Generation of higher harmonics is automatically suppressed due to the junction plasma resonance. We present the theory and selected results, including the gain, bandwidth, and dynamic range of the amplifier. The simultaneous achievement of high gain (greater than 20 dB), large instantaneous bandwidth (greater than 2 GHz), and high dynamic range make the JTWPa a promising device for the simultaneous readout of frequency-multiplexed superconducting qubits.

9:12AM F39.00007 Phase-matched Josephson traveling-wave parametric amplifier for superconducting qubit readout - experiment1, CHRIS MACKLIN, QNL, University of California, Berkeley, K. O’BRIEN, NSF Nano-scale Science and Engineering Center (NSEC), University of California, Berkeley, B. H. EOM, QNL, University of California, Berkeley, M. E. SCHWARTZ, QNL, University of California, Berkeley, D. HOVER, V. BOLKHOVSKY, S. TOLPYGO, G. FITCH, T. WEIR, MIT Lincoln Laboratory, W.D. OLIVER, MIT Lincoln Laboratory and Research Laboratory of Electronics, Massachusetts Institute of Technology, X. ZHANG, NSF Nano-scale Science and Engineering Center (NSEC), University of California, Berkeley, I. SIDDIQI, QNL, University of California, Berkeley — We have developed a new generation of Josephson traveling wave parametric amplifiers (JTWPAs) utilizing the technique of resonant phase matching. Due to its transmission line geometry, the JTWPa is not limited by the gain-bandwidth tradeoffs inherent in resonator-based parametric amplifiers. We present experimental results on the amplifier performance of the JTWPa, demonstrating gain in excess of 20 dB over an instantaneous bandwidth of more than 2 GHz with a 1 dB compression power of -100 dBm. The system noise temperature with the JTWPa is less than a factor of 3 above the quantum limit as measured using a 3D transmon in the weak measurement regime to provide a precise power calibration at the relevant experimental reference plane. We also utilize quantum weak measurement to provide an independent measure of the quantum measurement efficiency, in good agreement with the noise power measurement. We demonstrate projective qubit readout with a raw measurement fidelity exceeding 98% in an 80 ns integration window, and extrapolate this performance to a multi-qubit system.

1Work supported by IARPA.
9:24AM F39.00008 High-Fidelity Measurements of Long-Lived Flux Qubits. DAVID HOVER, MIT Lincoln Laboratory, CHRIS MACKLIN, KEVIN O’BRIEN, University California Berkeley, ADAM SEARS, JONILYN YODER, TEO GUDMUNSDEN, JAMIE KERMAN, VLADIMIR BOLKHOVSKY, SERGEY TOLPYGO, GEORGE FITCH, TERRY WEIR, MIT Lincoln Laboratory, ARCHANA KAMAL, SIMON GUSTAVSSON, FEI YAN, Research Laboratory of Electronics, MIT, JEFF BIRENBAUM, IRFAN SIDDIQI, University California Berkeley, TERRY ORLANDO, Research Laboratory of Electronics, MIT, JOHN CLARKE, University California Berkeley, WILL OLIVER, MIT Lincoln Laboratory;Research Laboratory of Electronics, MIT — We report on high-fidelity dispersive measurements of a long-lived flux qubit using a Josephson superconducting traveling wave parametric amplifier (JTWA). A capacitively shunted flux qubit that incorporates high-Q MBE aluminum will have longer relaxation and dephasing times when compared to a conventional flux qubit, while also maintaining the large anharmonicity necessary for complex gate operations. The JTWA relies on a Josephson junction embedded transmission line to deliver broadband, nonreciprocal gain with large dynamic range. This research was funded in part by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), and by the Assistant Secretary of Defense for Research & Engineering under Air Force Contract number FA8722-05-C-0001. All statements of fact, opinion or conclusions contained herein are those of the authors and should not be construed as representing the official views or policies of the Army Research Office.

9:36AM F39.00009 Quantum-limited Amplification via Dissipation in Superconducting Circuits. A. METELMANN, A.A. CLERK, McGill University, Department of Physics — The development of parametric amplifiers based on superconducting circuits has led to an impressive improvement in the precision and sensitivity of measurements in the quantum regime. However, standard cavity-based parametric amplifiers suffer from a fixed gain-bandwidth product. Moreover they are reciprocal devices, i.e., they amplify in both directions, leading to the requirement of additional noisy elements as circulators in the measurement chain. In our recent work we discussed a phase-insensitive quantum amplifier which utilizes dissipative interactions in a parametrically-coupled three-mode bosonic system [PRL 112, 133904 (2014)]. The use of dissipative interactions provides a fundamental advantage over standard cavity-based parametric amplifiers: large photon number gains are possible with quantum-limited added noise, with no limitation on the gain-bandwidth product. In this talk we present how this can be extended to phase-sensitive amplifiers and discuss the possibilities of making the amplifier directional.

9:48AM F39.00010 Dispersive qubit measurement using an on-chip parametric amplifier: theory. BENJAMIN LEVITAN, SAEED KHAN, McGill University, ANDREW EDDINS, DAVID TOYLI, IRFAN SIDDIQI, University of California, Berkeley, AASHISH CLERK, McGill University — Superconducting circuits directly integrating qubits and parametric amplifiers are a promising avenue for scalable measurement in circuit QED architectures. In such devices, the qubit is not protected against the amplified fluctuations of the paramp; understanding the backaction characteristics is thus crucial. We discuss recent theory work examining measurement-induced dephasing in a system where a flux-pumped paramp is directly coupled to a qubit, both in the limit of weak and strong dispersive coupling. We show that by careful design choices, the measurement-induced dephasing can be near quantum-limited despite the lack of circulators or explicitly directional amplifiers to protect the qubit. This work is supported by ARO.

10:00AM F39.00011 Dispersive qubit measurement using an integrated on-chip parametric amplifier1, A. EDDINS, D.M. TOYLI, E.M. LEVENVSON-FALK, QNL, University of California, Berkeley, B.A. LEVITAN, S. KHAN, A.A. CLERK, Department of Physics, McGill University, I. SIDDIQI, QNL, University of California, Berkeley — Superconducting parametric amplifiers (paramps) enable readout of superconducting qubits with unparalleled speed and efficiency. A variety of amplifier designs have been successfully used for readout; however, the most widely used devices require additional microwave components between qubit and paramp, limiting measurement efficiency and scalability. Our work aims to integrate qubit and amplifier on-chip, exploiting two-mode operation of the paramp to minimize measurement backaction on the qubit. To this end, we have developed a flux-pumped, high dynamic range amplifier compatible with qubit integration, and characterized the combined qubit-paramp circuit. We will discuss device design considerations and fabrication, studies of measurement-induced qubit dephasing in the presence of amplification, and prospects for enhanced weak, continuous measurements as well as strong, projective readout.

1This work was supported by funding from the Army Research Office.

10:12AM F39.00012 Broadband Kinetic Inductance Based Traveling Wave Amplifier for Qubit Readout. , MICHAEL VISSERS, ROBERT ERICKSON, HSJANG-SHENG KU, JIANSONG GAO, DAVID PAPPAS, NIST - Boulder — A broadband quantum-limited amplifier is desirable for multiplexed readout of superconducting qubits and detectors. The kinetic inductance traveling-wave parametric amplifier (KIT) is a new type of amplifier that utilizes the intrinsic dissipationlessness nonlinearity of kinetic inductance of superconductors like NbTiN and TiN for parametric amplification. The amplifier consists of a several meter long CPW transmission line fabricated from a 20nM NbTiN film on an intrinsic Si wafer. The transmission line is dispersion engineered with impedance loadings to achieve the ideal phase matching which leads to broadband gain. We measure over 20dB of gain across several GHz of bandwidth with a high gain-saturation power and dynamic range.

10:24AM F39.00013 A dispersion-engineered Josephson junction-based travelling wave parametric amplifier with low loss dielectric. , J. MUTUS, Google Santa Barbara, T. WHITE, I.-C. HOI, UC Santa Barbara, R. BARENDRES, Google, Santa Barbara, B. CAMPBELL, UC Santa Barbara, Y. CHEN, Google, Santa Barbara, Z. CHEN, B. CHIARO, UC Santa Barbara, A. FOWLER, Google, Santa Barbara, A. DUNSWORTH, UC Santa Barbara, E. JEFFREY, Google, Santa Barbara, J. KELLY, UC, Santa Barbara, A. MEGRANT, C. NEILL, P.J.J. O’MALLEY, UC Santa Barbara, P. ROUSHAN, Google, Santa Barbara, C. QUINTANA, UC Santa Barbara, D. SANK, Google, Santa Barbara, A. VAINSENCHER, J. WENNER, UC Santa Barbara, J. GAO, NIST, S. CHAUDHURI, Stanford, A.N. CLELAND, UC Santa Barbara, J.M. MARTINIS, University of California and Google, Santa Barbara — Travelling wave parametric amplifiers (TWPA) promise wide-band performance with high saturation power for amplifying microwave frequency signals. Designing a TWPA requires a careful balance of many parameters in order to approach quantum-limited noise performance with sufficient gain and saturation power. We present a design based on an LC-ladder transmission line of Josephson junctions and parallel plate capacitors using low-loss amorphous silicon dielectric. Crucially, we have inserted λ/4 resonators at regular intervals along the transmission line in order maintain the phase matching condition between pump, signal and idler in order to increase gain. The design and performance of the device will be presented, demonstrating high-gain, wide bandwidth and high dynamic range.

10:36AM F39.00014 Enhancing bandwidth of Josephson parametric amplifiers with impedance engineering. TANAY ROY, VADIRAJ A M, SUMAN KUNDU, MEGHAN PATANKAR, RAJAMANI VIJAYARGHAVAN, Tata Institute of Fundamental Research, Mumbai, India — Josephson parametric amplifiers (JPAs) are a crucial component of superconducting quantum information processing systems since they enable fast, high-fidelity measurement of qubits. However, JPAs based on a single SQUID oscillator suffer from two major drawbacks — narrow bandwidth and gain saturation at low signal powers, and are typically suited to single qubit experiments only. With the rapid development of multi-qubit systems, there is a practical need to develop an amplifier with larger bandwidth and signal handling capacity, while maintaining gain and noise performance. We will describe a new method to enhance the bandwidth by introducing a frequency dependent shunting impedance for the JPA. To prevent gain saturation, we also replace the single SQUID with a SQUID array. With an appropriate choice of device parameters, numerical calculations indicate the possibility of obtaining 20 dB gain with 700 MHz of bandwidth and near quantum limited noise performance. We will present experimental results demonstrating bandwidth enhancement and discuss strategies for optimizing overall amplifier performance.
semiflexible polymers. For many semiflexible chains, crystallization or thermal degradation can preclude the IN transition, so that $T_N$, BRANDON SMITH, Penn State University, Department of Chemical

Section F41 DPOLY: Focus Session: Organic Electronics and Photonics, Design of Semiconducting Materials 214A - Alejandro Briseno, University of Massachusetts, Amherst

8:00AM F41.00001 BREAK –

8:36AM F41.00002 Addition of ferrocene controls polymorphism and enhances charge mobilities in poly(3-hexylthiophene) thin-film transistors . BRANDON SMITH, Penn State University, Department of Chemical Engineering, MICHAEL CLARK, The Dow Chemical Company, CHRISTOPHER GIOCECCO, ALEC LARSEN, JOHN ASBURY, Penn State University, Department of Chemistry, ENRIQUE GOMEZ, Penn State University, Department of Chemical Engineering. — Crystalline organic molecules often exhibit the ability to form multiple crystal structures depending on the processing conditions. Exploiting this polymorphism to optimize molecular interaction between adjacent molecules within the unit lattice of conjugated polymers is an approach to enhance charge transport within the material. We have demonstrated the formation of different π-π stacking poly(3-hexylthiophene-2,5-diyl) polymers in films spin coated from ferrocene-containing solutions using varying incident X-ray diffraction. As a result, we found that the addition of ferrocene to casting solutions yields thin-film transistors which exhibit significantly higher source-drain current and charge mobilities than neat polymer devices. Insights gleaned from ferrocene/poly(3-hexylthiophene) mixtures can serve as a template for selection and optimization of next generation small molecule/polymer systems possessing greater baseline charge mobilities. Ultimately, the development of such techniques to enhance the characteristics of organic transistors without imparting high costs or loss of advantageous properties will be a critical factor determining the future of organic components within the electronics market.

8:48AM F41.00003 Predicting nematic coupling constants of semiflexible polymers from MD simulations , WENLIN ZHANG, ENRIQUE GOMEZ, SCOTT MILNER, Pennsylvania State University — The nematic phase is important for many semiflexible polymers. For example, semiflexible polymers with nematic phase can be directly used in many applications, including displays and high strength fibers. The existence of nematic phases also enables better processing of functional semiflexible polymers including conducting conjugated polymers. The nematic coupling constant $\alpha$, together with the chain stiffness $\kappa$, governs chain alignment and the isotropic-to-nematic (IN) transition temperature $T_{IN}$ for semiflexible polymers. For many semiflexible chains, crystallization or thermal degradation can preclude the IN transition, so that $T_{IN}$ cannot be used to estimate $\alpha$. We combine self-consistent field theory (SCFT) with atomistic molecular dynamics (MD) simulations of semiflexible chains under external tension in the isotropic phase to estimate the nematic coupling constant $\alpha$. Using our mean-field model, we can obtain the variational free energy of a given polymer, from which the IN transition temperature $T_{IN}$ can be determined. We apply our method to estimate $\alpha$ and $T_{IN}$ of a commonly studied conjugated polymer, poly(3-hexylthiophene) (P3HT). Using the estimated $T_{IN}$, we predict P3HT is nematic after melting from crystal.

9:00AM F41.00004 Heteroatom-Containing Contorted Molecular Semiconductors . NICHOLAS DAVY, Department of Chemical and Biological Engineering, Princeton University, GABRIEL MAN, Department of Electrical Engineering, Princeton University, SEAN PARKIN, Department of Chemistry, University of Kentucky, ANTOINE KAHN, Department of Electrical Engineering, Princeton University, YUEH-LIN LOO, Department of Chemical and Biological Engineering, Princeton University — Contorted polyaromatic hydrocarbons (c-PAHs), such as contorted hexabenzocoronene (c-HBC), are promising active ingredients for organic photovoltaic (OPV) devices due to their inherent stability, tunable frontier energy levels, and synthetic accessibility. The utility of c-HBC derivatives in OPV devices, however, has been limited by the large band gaps of these materials and, as a consequence, their reduced ability to absorb a broad range of the solar spectrum. Here, we report on the synthesis and photophysical characterization of tetrazabenzo[4,5-f]coronene (c-TBFDBC) and tetrabenzothienodibenzocoronene (c-TBTDBC) — a pair of heteroatom-containing c-PAHs that show broader absorption of the solar spectrum compared to c-HBC, with maximum absorptivities above 10^5 cm^-1 M^-1 in both the near-UV and in the visible. Bilayer OPV devices comprising c-TBFDBC or c-TBTDBC and C70 outperform those having c-HBC in photocurrent production and power conversion efficiency. External quantum efficiency spectra indicate improved light harvesting by both donor and acceptor molecules on annealing. Grazing incidence X-ray diffraction experiments reveal increases in the crystallinity of donor and acceptor layers on annealing and a preference for edge-on orientation in c-HBC and c-TBFDBC.

9:12AM F41.00005 Manipulating the backbone structure of semiconducting polymers . CHRISTINE LUSCOMBE, University of Washington, Seattle — π-Conjugated polymers are being used in the fabrication of a wide variety of organic electronic devices such as organic field-effect transistors (OFETs), organic photovoltaic (OPV) devices, and organic light-emitting diodes (OLEDs). The advances made in organic electronics have been driven by the syntheses of π-conjugated polymers with increasingly complex structures but have only relied on an Edisionian approach. Despite these advances, there are many contradictory reports in the literature about our understanding of the performance of π-conjugated polymers in many applications. Our group has been studying and developing techniques to grow semiconducting polymers using a living polymerization method. This has allowed us to synthesize polymers with control over the backbone structure of semiconducting polymers, star-shaped P3HT, as well as hyperbranched P3HT. It also allows us to accurately control the molecular weights of P3HT and produce materials with a narrow molecular weight distribution. In this presentation, our work towards creating brush polymers will be presented where a series of fully conjugated graft copolymers containing poly(3-hexylthiophene) (P3HT) side chains and a p-type carbazole-diketopyrrolopyrrole donor-acceptor backbone were synthesized via a graft through Suzuki polymerization.

9:48AM F41.00006 Synthesis and Self-Assembly of Rod-Coil Mitkaoarm Star Copolymers of Poly(3-dodecythiophene) and Poly(methyl methacrylate) with high rod fractions . JICHEOL PARK, Pohang Univ of Sci & Tech, HONG CHUL MOON, University of Minnesota, CHUNG-ROYNG CHOI, JIN KON KIM, Pohang Univ of Sci & Tech — Poly(3-dodecylthiophene)-b-poly(methyl methacrylate) diblock copolymer (P3DDT-b-PMMA) can self-assemble into various microdomains such as spheres, cylinders, and lamellae depending on weight fraction of P3DDT. However, only fibril morphology was formed when weight fraction of P3DDT was major ($w_{P3DDT}$ ~ 0.76). Here, we introduce a new approach to obtain microdomain structures even at high $w_{P3DDT}$ by using well-defined A$_2$B mitkaoarm star copolymer composed of P3DDT and PMMA ([(P3DDT)$_2$PMMA]. We found via small angle X-ray scattering and transmission electron microscopy that (P3DDT)$_2$PMMA showed PMMA cylinder packed hexagonally in the matrix of P3DDT and body-centered-cubic spheres of PMMA for $w_{P3DDT}$ of 0.66 and 0.75, respectively. This because of much reduction of the rod-rod interaction in (P3DDT)$_2$PMMA compared with (P3DDT-b-PMMA) diblock copolymers.
10:00AM F41.00007 A Quantum Chemical Study of Structural and Electronic Properties of DTBT and DTBT:C70 Complexes. Organic photovoltaic (OPV) devices containing the diethyl benzothiadiazole (DTBT) based conjugated polymers are promising candidates for solar energy harvesting. Practical realization of OPV devices requires further improving their performance, which relies on the fundamental understanding of the morphology and electronic properties of DTBT-based polymers. Nevertheless, even the conformational properties of DTBT have not been fully revealed yet. Here, we present the quantum chemical calculations of the structural and electronic properties of DTBT as well as DTBT:C70 complexes at the molecular level. These first principles principles include the two-dimensional potential energy surface, the band gap, DTBT:C70 equilibrium distance as well as the energy level offset at the interface compared to the energy levels of the individual material. The computed results are compared to the available experimental data.

1Work supported by the National Science Foundation (Grant No. DMR0847580)

10:12AM F41.00008 Theoretical modelling of high-dielectric constant donors for high-conversion organic film solar cells. KENJI MISHIMA, KOICHI YAMASHITA, The University of Tokyo, JST-CREST. In this contribution, we report our theoretical design of high dielectric-constant donors based on the DFT and TD-DFT quantum chemistry calculations. The motivation of our study lies in the importance of high-dielectric constant donors and acceptors for purposes of separating photo-generated excitons efficiently and preventing them from recombining, thus leading to high photo-conversion efficiency in the organic solar cells. Our theoretical design guideline is to bind the conventional thiophene-related one-dimensional donor molecules via benzene rings two-dimensionally, which leads to extended pi-conjugation and their high dielectric constants. Our numerical results indicate that the dielectric constant increases monotonically with the size of the molecule. The dielectric constant of the two-dimensionally extended thiophene donor amounts to 13.6, which is more than three times as much as that of the conventional P3HT donor molecule (~4). By using PCBM molecule as an acceptor, the total amount of photo-induced transferred charge transfer from the donor to the acceptor is comparable to that of the P3HT/PCBM system.

10:24AM F41.00009 ABSTRACT WITHDRAWN

10:36AM F41.00010 ABSTRACT WITHDRAWN

10:48AM F41.00011 High-throughput organic semiconductor discovery combining tight-binding and first-principles calculations, ANDRE LEITAO BOTELHO, TIM MUELLER, Johns Hopkins University. We present the combination of a tight-binding model and first-principles calculations as a two-step screening for the accelerated discovery of organic semiconductors. For the tight-binding model, we select the adapted Su-Schrieffer-Heeger Hamiltonian for its ability to provide both the electronic structure and optimized geometry based solely on the structural formula. We produce two sets of parameters, one to match the optical gaps to exciton energies from TDDFT, and another set to match the transport gaps to HOMO/LUMO energies from DFT with an experimental correction factor. Although the fittings use fewer than one thousand oligomers, the predictive results for the remaining one million oligomers agree with DFT (coefficient of determination of up to 0.8) and can be used as a pre-screening step. With the same set of parameters, we also calculate the charged states to predict the Marcus theory reorganizational energies as an estimate the conductivities of holes and electrons. Based on the calculated properties, we discuss materials selection for photovoltaics and transistors.

Tuesday, March 3, 2015 8:00AM - 11:00AM
Session F42 DPOLY: Wetting, Adhesion and Dynamics of Polymer Films and Interfaces 214B -
Ryan Hayward, University of Massachusetts, Amherst

8:00AM F42.00001 BREAK

8:36AM F42.00002 Molecular Velcro constructed from polymer loop brushes showing enhanced adhesion force, TIAN ZHOU, BIAO HAN, LIN HAN, CHRISTOPHER LI, Drexel University, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING TEAM, SCHOOL OF BIOMEDICAL ENGINEERING, SCIENCE AND HEALTH SYSTEMS TEAM. Molecular Velcro is commonly seen in biological systems as the formation of strong physical entanglement at molecular scale could induce strong adhesion, which is crucial to many biological processes. To mimic this structure, we designed, and fabricated polymer loop brushes using polymer single crystals with desired surface functionality and controlled chain folding. Compared with reported loop brushes fabricated using triblock copolymers, the present loop brushes have precise loop sizes, loop grafting density, and well controlled tethering locations on the solid surface. Atomic force microscopy-based force spectroscopy measurements using a polymer chain coated probe reveal that the adhesion force are significantly enhanced on the loop brush surface as compared with its single-strand counterpart. This study directly shows the effect of polymer brush conformation on their properties, and suggests a promising strategy for advanced polymer surface design.

8:48AM F42.00003 Probing the adhesion of particles to responsive polymer coatings with hydrodynamic shear stresses, RYAN TOOMEY, GULNUR EFE. University of South Florida. Lower critical solution temperature (LCST) polymers in confined geometries have found success in applications that benefit from reversible modulation of surface properties, including drug delivery, separations, tissue cultures, and chromatography. In this talk, we present the adhesion of polystyrene microspheres to cross-linked poly(N-isopropylacrylamide), or poly(NIPAAm) coatings, as studied with a spinning disk method. This method applies a linear range of hydrodynamic shear forces to physically adsorbed microspheres along the radius of a coated disk. Quantification of detachment is accomplished by optical microscopy to evaluate the minimum shear stress to remove adherent particles. Experiments were performed to assess the relationship between the surface chemistry of the microsphere, the thickness and cross-link density of the poly(NIPAAm) coating, the adsorption (or incubation) time, and the temperature on the detachment profiles of the microspheres. Results show that both the shear modulus and slow dynamic processes in the poly(NIPAAm) films strongly influence the detachment shear stresses. Moreover, whether an adsorbed microsphere can be released (through a modulation in the swelling of the poly(NIPAAm) coating by temperature) depends on both the surface chemistry of the microsphere and the extent of the adsorption time. Finally, the results show that the structure of the poly(NIPAAm) coating can significantly affect performance, which may explain several of the conflicting findings that have been reported in the literature.
mechanisms during solvent-based fabrication of polymer blends

1. The nanoscale dynamics of solvated systems. Forces and hydrodynamic interactions; the latter are extremely long ranged in 2D fluids. This study positively demonstrates a new method to visualize in situ unexpected particle pairing, both dynamic and static, was observed in films thin compared to particle diameter, suggesting a complicated interplay of capillary forces. Selecting appropriate viewing conditions to avoid charging and beam damage artifacts (neither trivial concerns), individual particles could be followed in competition with the relaxation of the contact angle at the three-phase contact line. Here, we study the dynamics of stepped interfaces of thin polystyrene films on hydrophilic substrates. Annealing the polymeric film above its glass transition temperature induces flow which is precisely monitored using ex- and in-situ atomic force microscopy. Both pinned and receding contact line regimes are observed, corresponding to capillary levelling and dewetting of the liquid film. Rescaling with regard to the viscosity, surface tension and film thickness collapses the data on a master curve, providing a universal time for the transition between both regimes. In addition, we prove that the pinned interface exhibits self-similar height profiles which are captured by a thin film model in lubrication approximation.

2. In one or more external stimuli as well as photocatalytic activity. For this we are inspired from nature to produce surfaces with a dual-scale hierarchical roughness morphology control with the ultimate goal of precise, yet affordable, morphology manipulation for a large spectrum of applications. When and where phases are formed, and how they evolve to form the final structure. We utilize a linear stability analysis to identify which mechanism of phase-separation is chosen for a given processing condition. Finally, we construct a mode diagram that maps processing conditions with individual modes. The films. Hence, it is of paramount importance to understand morphology evolution during fabrication. However, it is challenging to experimentally visualize morphology evolution during processing (processes involved are highly dynamic at low scale and typical components do not show high contrast). Consequently, details of morphology evolution during solvent-based thinning deposition are still under debate. Here, we identify four modes of phase formation and subsequent propagation within the thinning film during solvent-based fabrication. We unravel the origin of this behavior. Specifically, we focus on fundamental questions, when and where phases are formed, and how they evolve to form the final structure. We utilize a linear stability analysis to identify which mechanism of phase-separation is chosen for a given processing condition. Finally, we construct a mode diagram that maps processing conditions with individual modes. The idea introduced here enables choosing processing conditions to tailor film morphology characteristics and paves the ground for a deeper understanding of morphology control with the ultimate goal of precise, yet affordable, morphology manipulation for a large spectrum of applications.

3. Support from the UMass MRSEC is acknowledged.

10:12AM F42.00010 How do evaporating thin films evolve? Unravelling phase-separation mechanisms during solvent-based fabrication of polymer blends. OLGA WODO, State Univ of NY - Buffalo, BASKAR GANAPATHYSUBRAMANIAN, Iowa State University — Solvent-based fabrication is a flexible and affordable approach to manufacture organic thin films made from any combination of polymer, copolymers and/or small molecules. The properties of products made from such films can be tailored by the morphology of the films. Hence, it is of paramount importance to understand and control morphology evolution during fabrication. However, it is challenging to experimentally visualize morphology evolution during processing. Processes involved are highly dynamic at low scale and typical components do not show high contrast. Consequently, details of morphology evolution during solvent-based thinning deposition are still under debate. Here, we identify four modes of phase formation and subsequent propagation within the thinning film during solvent-based fabrication. We unravel the origin of this behavior. Specifically, we focus on fundamental questions, when and where phases are formed, and how they evolve to form the final structure. We utilize a linear stability analysis to identify which mechanism of phase-separation is chosen for a given processing condition. Finally, we construct a mode diagram that maps processing conditions with individual modes. The idea introduced here enables choosing processing conditions to tailor film morphology characteristics and paves the ground for a deeper understanding of morphology control with the ultimate goal of precise, yet affordable, morphology manipulation for a large spectrum of applications.

10:24AM F42.00011 Polymeric surfaces exhibiting photocatalytic activity and controlled anisotropic wettability. SPIROS H. ANASTASIADIS, MELANI A. FRYSALI, LAMPROS PAPOUTSAKIS, GEORGE KENANAKIS, EMMANUEL STRATAKIS, MARIA VAMVAKIKA, Foundation for Research and Technology - Hellas and Univ. of Crete, Greece, GRIGORIS MOUNTRICHAS, STERGIOS PISPAS, National Hellenic Research Foundation, Greece — In this work we focus on surfaces, which exhibit controlled, switchable wettability in response to one or more external stimuli as well as photocatalytic activity. For this we are inspired from nature to produce surfaces with a dual-scale hierarchical roughness and combines them with the appropriate inorganic and/or polymer coating. The combination of the hierarchical surface with a ZnO coating and a pH- or temperature-responsive polymer results in efficient photo-active properties as well as reversible superhydrophobic / superhydrophilic surfaces. Furthermore, we fabricate surfaces with unidirectional wettability variation. Overall, such surfaces require advanced design, combining hierarchically structured surfaces with suitable polymeric materials. Acknowledgment: This research was partially supported by the European Union (European Social Fund, ESF) and Greek national funds through the “ARISTEIA II” Action (SMART-SURF) of the Operational Programme “Education and Lifelong Learning,” NSRF 2007-2013, via the General Secretariat for Research & Technology, Ministry of Education and Religious Affairs, Greece.
10:36AM F42.00012 The Role of Contact Angle on the Depletion Layer when at the Interface Between Water and a Hydrophobic Surface, ADELE POYNOR, SHANNON PETERSEN, BROOKE OLLANDER, Allegheny College — By definition hydrophobic substances hate water. Water placed on a hydrophobic surface will form a drop in order to minimize its contact area. What happens when water is forced into contact with a hydrophobic surface? One theory is that an ultra-thin low-density depletion layer forms near the surface. We investigate the role of contact angle on depletion layer using the surface sensitive technique of Surface Plasmon Resonance.

10:48AM F42.00013 Wetting Properties of Chemically Modified Surfaces: The role of hydrogen bonding, SELEMON BEKELE, MESFIN TSIGE, The University of Akron, Department of Polymer Science, Akron, Ohio — Many industrial processing operations involve the spreading of a liquid on a solid material. Controlling the wetting of one material by another is of crucial importance in such applications as adhesion, coating, and oil recovery. A strategy often employed to control the wettability of solid surfaces is a combination of surface patterning and chemical surface modification. In order to understand the effect of surface chemistry on the wetting process, we have carried out all-atom molecular dynamics (MD) simulations of a water droplet spreading on pure and oxidized polystyrene surfaces. Our previous results show that the contact angle generally decreases with increasing oxygen concentration and there is a correlation between the spreading and hydrogen bonding. In this talk, we will present results on the structure and dynamics of the hydrogen bonds in the interfacial region between water and the polystyrene substrate. We will discuss our findings on hydrogen bond lifetimes, time correlations functions and number of hydrogen bonds per water molecule for the hydrogen bonds around the water/polystyrene interface which are found to play a role in the spreading process.

This work was supported by NSF Grant DMR0847580.

2Langmuir 2013 29, 13230-13238

Tuesday, March 3, 2015 8:00AM - 11:00AM
Session F43 DPOLY: Blends and Block Copolymers 214C - Ron Jones, National Institute of Standards and Technology

8:00AM F43.00001 BREAK

8:36AM F43.00002 Controlling Phase Separation of Interpenetrating Polymer Networks by Addition of Block Copolymers, BRIAN ROHDE, RAMANAN KRISHNAMOORTI, MEGAN ROBERTSON, University of Houston, Department of Chemical and Biomolecular Engineering — Interpenetrating polymer networks (IPNs) offer a unique way to produce mechanically superior thermostets blends relative to the neat components. In this study, IPNs were prepared consisting of polycyclopentadienentane (polyDCPD), contributing high fracture toughness, and an epoxy resin (the diglycidyl ether of bisphenol A cured with nadic methyl anhydride), contributing high tensile strength and modulus. In the absence of compatibilization, the simultaneous curing of the networks leads to a macroscopically phase separated blend that exhibits poor mechanical behavior. To control phase separation and drive the system towards more mechanically robust nanostructured IPNs, block copolymers were designed to compatibilize this system, where one block possesses affinity to polyDCPD (polyisoprene in this study) and the other block possesses affinity to NOCA (poly(c-caprolactone) in this study). The influence of the block copolymer composition on the degree of phase separation and interfacial adhesion in the IPN was studied using a combination of small-angle scattering and imaging techniques. The resultant mechanical properties were explored and structure-property relationships were developed in this blend system.

8:48AM F43.00003 Melt-Miscibility in Block Copolymers Containing Polyethylene and Substituted Polynorbornene Blocks, WILLIAM MULHEARN, RICHARD REGISTER, Princeton Univ — Block copolymers containing a crystallizable block, such as polyethylene (PE), and a high-*T_g* amorphous block are potentially interesting materials since the rigid glassy block can mitigate the poor yield strength of the PE crystals. However, chemical incompatibility between blocks, quantified by the Flory interaction parameter *q* or the interaction energy density *X*, drives microphase separation at low temperatures or high chain lengths. To prepare a high molecular weight PE-containing block copolymer that is easy to process (i.e. with a desired low-viscosity melt) it is necessary to select amorphous blocks that have low mixing energies with PE. The only suitable polymers currently known are chemically similar to PE and therefore have similarly low glass transition temperatures. We investigate a series of both low- and high-*T_g* polymers based on substituted norbornene monomers, polymerized via ring-opening metathesis polymerization (ROMP). Several ROMP polymers of this type exhibit high *T_g* and low interaction energy against PE. For example, hydrogenated poly(cyclohexyl norbornene) has *T_g* = 88 °C and has interaction energy density *X_{1p,CyN,PE} ≈ 0.8 MPa*, comparable to the interaction energy density between PE and hydrogenated polysoprene. The miscibility of an amorphous block can be further tuned by statistical copolymerization of norbornene units with aromatic side-groups (high Hildebrand solubility parameter) and norbornene units with aliphatic side-groups (low Hildebrand solubility parameter).

9:00AM F43.00004 Fluctuation Effects in AB/A/B Diblock Copolymer-Homopolymer Ternary Mixtures near the Lamellar-Disorder Transition, TIMOTHY GILLARD, ROBERT HICKEY, BRIAN HABERSBERGER, TIMOTHY LODGE, FRANK BATES, University of Minnesota — By definition hydrophobic substances hate water. Water placed on a hydrophobic surface will form a drop in order to minimize its contact area. What happens when water is forced into contact with a hydrophobic surface? One theory is that an ultra-thin low-density depletion layer forms near the surface. We investigate the role of contact angle on depletion layer using the surface sensitive technique of Surface Plasmon Resonance.

9:12AM F43.00005 How to Place Block Copolymer Molecules at the Interface of a Binary Blend, ZHONG-REN CHEN, YICI XU, SHUO ZHONG, Ningbo University — Block copolymers have been used to reduce the domain size of immiscible polymer blends and thus improve the mechanical and other properties. The effectiveness of this method, however, depends on the percentage of these polymeric surfactants residing at the interface of the blend. In fact, theoretical as well as experimental work indicate that a large percentage of block copolymers form micelles in the bulk of one or both of the component polymers. These micelles may serve as weak spots initiating crack propagation. Previous work have been focused on the design of molecular architecture and synthesis of new block copolymers to address this problem. In this presentation, a simple mixing strategy is applied to make each block copolymer molecule stay at the interface. As one example, when this strategy is used to mix natural rubber (NR) with butadiene rubber (BR), a small amount of low molecular weight block copolymer (LIR) improves both processing characteristics such as melt viscosity and mechanical properties of cured samples, such as crack resistance. AFM micrographs show the much smaller domain size; and an original real-time monitoring system reveals the lowest crack growth rate. Using a model A/B/A/B binary blend, we have witnessed by microscopy that all block copolymer molecules form micelles at the first mixing step, and all of these micelles are disappeared and all block copolymer molecules stay at the interface after the second mixing step.
9:24AM F43.00006 Pressure dependence of various phase transitions for the miscible block copolymer blends, DU YEOL RYU, YONGHOON LEE, HOYEON LEE, YEONGSIK KIM, Yonsei University, YONSEI UNIVERSITY TEAM — The phase behavior of block copolymer (BCP) blends composed of the weakly interacting (with no specific interaction) polystyrene-b-poly-(n-butyl methacrylate) (PS-b-PnBMA) and deuterated polystyrene-b-poly-(n-hexyl methacrylate) (dPS-b-PnHMA) were investigated by Small-Angle Neutron Scattering (SANS) and Depolarized Light Scattering (DPLS) measurements. The various composition-dependent phase behaviors were generated due to a miscible phase between the PnBMA and PnHMA blocks in the BCP blends. To elucidate the origin and difference in baroelasticity of weakly interacting BCP blends, the pressure dependence of transition temperatures was evaluated using enthalpic and volumetric changes at phase transitions. We also demonstrate that the entropic compressibility for the miscible BCP blends is a baroelastic indicator, which was characterized by the negative volume change on mixing (Vmix) at transitions.

9:36AM F43.00007 Crystallization of a bimodally distributed copolymer system and a blend containing propylene-ethylene moieties, ONYENKACHI WAMUO, YING WU, SHAW HSU, University of Massachusetts, Amherst, CHARLES(CHUCK) PAUL, ANDREA EODICE, Henkel Corporation — The competitive crystallization behavior of a multicomponent system is fundamentally interesting and has significant practical implications. The relative molecular weight and molecular architecture of the polymers involved needs to be considered carefully in the characterization of the entire crystallization process; nucleation and the crystal growth phase. We have considered two types of propylene-ethylene copolymers with virtually the same chemical composition but different block sequences. A comparison is being made between a bimodally distributed copolymer and a random copolymer. The unique feature of the bimodal system is the presence of a two-step crystallization process, where the longer sequences nucleated first and additional shorter segments are transported onto the crystal growth front. This system is compared to a copolymer of virtually identical random copolymer that is nucleated differently. Calorimetric, diffraction and spectroscopic measurements have been employed in order to understand the dynamics and mechanism of crystallization and the size and perfection of the crystals formed. The relative efficiency of crystallization by controlling the polymer configuration can then be compared to the traditional approach using a nucleation agent to affect the crystallization behavior. This new approach not only provides extremely fast crystallization but also overcomes practical considerations such as dispersion of the nucleation agents.

9:48AM F43.00008 Understanding How the Presence of Uniform Electric Fields Can Shift the Miscibility of Polystyrene / Poly(vinyl methyl ether) Blends, ANNIKA KRISA, CONNIE B. ROTH, Department of Physics, Emory University — Techniques which can externally control and manipulate the phase behavior of polymer systems, without altering chemistry on a molecular level, have great practical benefits. One such possible mechanism is the use of electric fields, shown to cause interfacial instabilities, orientation of morphologies, and phase transitions in polymer blends and block copolymers. We have recently demonstrated that the presence of uniform electric fields can also strongly enhance the miscibility of polystyrene (PS) / poly(vinyl methyl ether) (PVME) blends [J. Chem. Phys. 2014, 141, 134908]. Using fluorescence to measure the phase separation temperature $T_s$ of PS/PVME blends with and without electric fields, we show that $T_s$ can be reproducibly and reversibly increased by 13.5 +/- 1.4 K for electric fields of 17 kV/mm for this lower critical solution temperature (LCST) blend. This increase in blend miscibility with electric fields represents one of the largest absolute shifts in $T_s$ ever recorded, well outside of experimental error. The best theoretical prediction for the expected shift in $T_s$ with electric field for this system is still two orders of magnitude smaller than that observed experimentally. We discuss the limitations of this theoretical prediction and consider possible factors affecting miscibility that may need to be also included.

10:00AM F43.00009 Magnetic Field Alignment of PS-P4VP: a Non-Liquid Crystalline Coil-Block Copolymer, YEKATERINA ROKHLENKO, KAI ZHANG, Yale University, STEVEN LARSON, PADMA GOPALAN, University of Wisconsin-Madison, COREY O’HERN, CHINEDUM OSUJI, Yale University — Magnetic fields provide the ability to control alignment of self-assembled soft materials such as block copolymers. Most prior work in this area has relied on the presence of ordered assemblies of anisotropic liquid crystalline species to ensure sufficient magnetic anisotropy to drive alignment. Recent experiments with poly(styrene-b-4-vinylpyridine), a non-liquid crystalline BCP, however, show field-induced alignment of a lamellar microstructure during cooling across the order-disorder transition. Using in situ x-ray scattering, we examine the roles of field strength and cooling rate on the alignment response of this low MW coil-block BCP. Alignment is first observed at field strengths as low as 1 Tesla and improves markedly with both increasing field strength and slower cooling. We present a geometric argument to illustrate the origin of a finite, non-trivial magnetic susceptibility anisotropy for highly stretched surface-tethered polymer chains and corroborate this using coarse-grained molecular dynamics simulations. We rationalize the magnetic field response of the system in terms of the mobility afforded by the absence of entanglements, the intrinsic anisotropy resulting from the stretched polymer chains and sterically constrained conjugated rings, and the large grain size in these low molecular weight materials.

10:12AM F43.00010 Phase Behavior of Binary Blend Consisting of Asymmetric Polystyrene-block-poly(2-vinylpyridine) Copolymer and Asymmetric Deuterated Polystyrene-block-poly(4-hydroxystyrene) Copolymer Having Hydrogen Bonding, JONGHEON KWAK, SANG HYUN HAN, HONG CHUL MOON, Pohang Univ of Sci & Tech, VICTOR PRYAMITSYN, VENKAT GANESAN, University of Texas, JIN KON KIM1, Pohang Univ of Sci & Tech — We investigated the phase behavior of a binary blend of asymmetric polystyrene-block-poly(2-vinylpyridine) copolymer (PS-b-P2VP) and deuterated polystyrene-block-polyhydroxystyrene copolymer (dPS-b-PH5) blends. The blend showed highly asymmetric lamellar microdomains. To explain the unexpected results, we study, via small angle X-ray scattering (SAXS) and neutron reflectivity (NR), the exact location of shorter dPS block in the mixture near the interface of the microdomains.

1 Corresponding Author

10:24AM F43.00011 Quenching Phase Separation by Vapor Deposition Polymerization, RAN TAO, MITCHELL ANTHAMATTEN, University of Rochester — Initiated chemical vapor deposition (CVD) is a solventless, free radical technique predominately used to deposit homogeneous films of linear and crosslinked polymers directly from gas phase feeds. We report a template-free method to fabricate continuous-phase porous polymer films by simultaneous phase separation during iCVD. Phase separation during film growth is achieved by condensing an inert porogen, along with initiator, monomer, and crosslinker. When the vapor mixture transports to the cooled substrate, phase separation occurs along with polymerization and crosslinking, which quench the state of phase separation. The kinetics of spontaneously phase separation can be quantitatively understood on the basis of Cahn-Hilliard theory. A series of films were grown by varying monomer and porogen’s degree of saturation. Deposited films were studied by electron microscopy and spectroscopic techniques.
10:36AM F43.00012 Understanding Segregation Processes in Blends of Bottlebrush-Linear Polymer Thin Films, INDRANIL MITRA, University of Houston, XIANYU LI, Envia Systems, STACY L. PESEK, Rice University, BORIS MAKARENKO, University of Houston, BRAD S. LOKITZ, DAVID UHRIG, JOHN F. ANKNER, Oak Ridge National Laboratory, RAFAEL VERDÚZCO, Rice University, GILA E. STEIN, University of Houston — Bottlebrush polymer thin films have potential to generate surface coatings for a variety of applications ranging from tailored surface wettability and adhesion, anti fouling surface coatings and self-assembled photonics. In this study, we examined the phase behavior for athermal blends of bottlebrush polystyrene (PS) and linear deuterated polystyrene (dPS) in thin films. The bottlebrush loading was 10% by volume, and the ratio of linear dPS chain length to bottlebrush PS side chain length was systematically varied in the range of $\alpha = 0.3 - 4.1$. The depth-dependent concentration of inter-modulation products was measured using dynamic secondary ion mass spectroscopy. When $\alpha < 2$, the bottlebrushes are dispersed throughout the film thickness with a slight excess at the free surface and substrate interface. When $\alpha > 8$, the bottlebrushes are depleted from the interior of the film and segregated at the interfaces. This behavior is consistent with wetting and dewetting transitions at a melt/brush interface and entropic attraction of highly branched polymers to surfaces. This work demonstrates that brushlike surfaces and interfaces can be generated in a linear polymer film through spontaneous, entropy driven segregation of properly designed bottlebrush additives.

10:48AM F43.00013 Using $\beta$-NMR to Measure Surface Segregation of Short Chains in Binary Blends of Polystyrene, JAIN MCKENZIE, TRIUMF, DAVID L. CORTIE, University of British Columbia, CHAD R. DALEY, PENDAR MAHMOUDI, NASSER M. ABUKHDEIR, MARK W. MATSEN, University of Waterloo, ROBERT F. KIEFL, University of British Columbia, C. D. PHILIP LEVY, TRIUMF, W. ANDREW MACFARLANE, University of British Columbia, GERALD D. MORRIS, MATTHEW R. PEARSON, TRIUMF, JAMES A. FORREST, University of Waterloo — A problem of significant interest in the studies of polymers at interfaces is the segregation of short chain polymers to the interface in a system with both long and short chains. It is difficult to study the segregation as methods used to introduce contrast between short and long chains often have an effect rather than just simple to the different chain lengths. We have shown that $\beta$-detected nuclear spin relaxation of $^3\text{Li}^+$ can distinguish the two chains sizes without the need for any label. This, combined with the depth profiling ability of the technique, means we can determine the effective concentration of short and the chain blend without the need to introduce another pendent factor. We have performed experiments on a 50/50 blend of 627 kg/mol and 0.980 kg/mol polystyrene-d8 and at depths ranging from 2.5 to 79 nm from the free surface. The results show definite surface segregation of short chains to the free surface. We theoretically examine the segregation of short chains to the surface of the binary blend using self-consistent field theory (SCFT). The model used in the calculation assumes an incompressible melt consisting of the freely-jointed polymer chains with either $N_0$ or $N_1$ monomers.

Tuesday, March 3, 2015 8:00AM - 11:00AM –
Session F44 GSNP GSOFT: Focus Session: Extreme Mechanics: Snapping, Jumping and Popping 214D - Doug Holmes, Boston University

8:00AM F44.00001 Yanking a chain: Lift-off and snapping, PIERRE-THOMAS BRUN, MIT, BASILE AUDOLY, UPMC / CNRS, ALAIN GORIELY, DOMINIC VELLA, University of Oxford — We revisit the first mechanics problem that everyone meets in high school: a chain on a frictionless pulley. Rather than considering the problem of a mass on each end of the string, however, we suppose that one end is subject to a constant acceleration. This simple change has some dramatic consequences for the ensuing motion: the chain ‘lifts off’ from the pulley, the free end accelerates faster than the end that is being pulled and finally the chain undergoes a dramatic reversal of curvilinear reminiscent of the crack or snap of a whip. We present simple experiments, numerical simulations and theoretical arguments that explain some but not all of these phenomena.

8:12AM F44.00002 Unraveling the chain fountain, JOHN BIGGINS, MARK WARNER, University of Cambridge — If a chain is initially at rest in a beaker at a height $h_1$ above the ground, and the end of the chain is pulled over the rim of the beaker and down towards the ground and then released, the chain will spontaneously “flow” out of the beaker under gravity. Furthermore, the beads do not simply drag over the edge of the beaker but form a fountain reaching a height $h_2$ above it. I will show that the formation of a fountain requires that the beads come into motion not only by being pulled upwards by the part of the chain immediately above the pile, but also by being pushed upwards by an unexpected reaction force from the pile of stationary chain. I will propose possible origins for this force, argue that its magnitude will be proportional to the square of the chain velocity, and predict and verify experimentally that $h_2 \propto h_1^2$. I will also discuss the case where the pot is tilted, and show, experimentally and theoretically, that the chain rises and falls in an inverted catenary, and discuss the appropriate boundary conditions at the ends of the chain.

8:24AM F44.00003 Jumping, snapping and popping at nanometer scale, DAVID HAVILAND, Royal Institute of Technology — The ‘jump-to-contact’ instability is well known in Atomic Force Microscopy. When a tip attached to a soft cantilever approaches a surface, the large attractive force gradient disrupts the quasi-static force balance and the tip snaps into contact with the surface. Less appreciated is the converse instability, where a soft liquid-like polymer surface jumps to meet the tip. This nano-scale pop is inaudible, but it does leave a distinctive signature if one carefully monitors the cantilever’s steady state dynamics when driven at frequencies close to the cantilever resonance the spectrum can be transformed to reveal the in-phase quadrature forces acting on the tip, as a function of oscillation amplitude. We present experimental measurements and theoretical modelling that reveals the drive tones. When many intermodulation products are measured close to the cantilever resonance the spectrum can be transformed to reveal the in-phase and quadrature forces acting on the tip, as a function of oscillation amplitude. We present experimental measurements and theoretical modelling that reveals the drive tones.

8:36AM F44.00004 TBD, KEITH SEFFEN, Cambridge University, UK — No abstract available.

9:12AM F44.00005 The chocolate-egg problem: Fabrication of thin elastic shells through coating, ANNA LEE, JOEL MARTHELOT, PIERRE-THOMAS BRUN, PEDRO M. REIS, Massachusetts Institute of Technology — We study the fabrication of thin polymeric shells based on the coating of a curved surface by a viscous fluid. Upon polymerization of the resulting thin film, a slender solid structure is delivered after demolding. This technique is extensively used, empirically, in manufacturing, where it is known as rotational molding, as well as in the food industry, e.g. for chocolate eggs. This problem is analogous to the Landau-Levich-Derjaguin coating of plates and fibers and Bretherton’s problem of film deposition in cylindrical channels, albeit now on a double-curved geometry. Here, the balance between gravity, viscosity, surface tension and polymerization rate can yield a constant thickness film. We seek to identify the physical ingredients that govern the final film thickness and its profile. In our experiments using organosilicon, we systematically vary the properties of the fluid, as well as the curvature of the substrate onto which the film is coated, and characterize the final thickness profile of the shells. A reduced model is developed to rationalize the process.
9:24AM F44.00006 Folding of non-Euclidean curved shells, NAKUL BENDA, ARTHUR EVANS, University of Massachusetts Amherst, SARAH INNES-GOLD, Tufts University, LUIS MARIN, University of Massachusetts Amherst, ITAI COHEN, Cornell University, CHRISTIAN SANTANGELO, RYAN HAYWARD, University of Massachusetts Amherst — Origami-based folding of 2D sheets has been of recent interest for a variety of applications ranging from deployable structures to self-folding robots. Though folding of planar sheets follows well-established principles, folding of curved shells involves an added level of complexity due to the inherent influence of curvature on mechanics. In this study, we use principles from differential geometry and thin shell mechanics to establish fundamental rules that govern folding of prototypical curved sheets. In particular, we show how the normal curvature of a crease line controls whether the deformation is smooth or discontinuous, and investigate the influence of shell thickness and boundary conditions. We show that snap-folding of shells provides a route to rapid actuation on time-scales dictated by the speed of sound. The simple geometric design principles developed can be applied at any length-scale, offering potential for bio-inspired soft actuators for tunable optics, microfluidics, and robotics.

9:36AM F44.00007 Curvature-induced symmetry breaking selects elastic wrinkling patterns, NORBERT STOOP, ROMAIN LAGRANGE, DENIS TERVERGAN, PEDRO REIS, JOERN DUNKEL, Massachusetts Institute of Technology — Wrinkling in curved bilayer surfaces is a ubiquitous phenomenon, including embryogenesis, biological tissue differentiation or structure formation in heterogeneous thin films. Due to curved substrate and the strong nonlinearity in the elastic strains, predictions for the wrinkling morphology are notoriously difficult to obtain using classical analysis. Here, we derive a generalized Swift-Hohenberg theory to describe these morphologies and their pattern selection. Testing the theory against experiments on spherically shaped surfaces, we find quantitative agreement with analytical predictions for the phase transition curves separating labyrinth, hybrid and hexagonal wrinkling phases. Our approach builds on general differential-geometric principles and can be extended to arbitrarily shaped surfaces.

9:48AM F44.00008 Bi-stable characteristics of thick-walled domes with applications to soft material snapping, AMIT MADHUCHAR, UIUC — Bi-stable structures can exhibit interesting mechanical properties which makes them the focus of research in the field of extreme mechanics. Fast transitions can occur between equilibrium states with very little actuation force. One such bi-stable structure is the thick-walled dome. In this work, we apply finite element techniques to examine the stability of such spherical, thick-walled domes undergoing large deformation. We apply the following methods to two structures: a single-layered system as well as bi-layered colloidal microparticles which actuate through pH driven mismatched swelling. The presence of a metastable state is identified by the energy characteristics alone. Monotonically increasing energy represents a mono-stable structure. Bi-stability occurs when we achieve a local energy minimum at some non-zero displacement. Of more interest is the region near the transition of these states where we find a so called pseudo-bi-stable state where small perturbations results in fast transition from the elevated energy state, or snapping. We use our simulations to map out the critical geometric parameters that govern this behavior in order to design a dome to snap. Experimental results are used to validate the simulation results.

10:00AM F44.00009 Morphing and Snapping of Plates and Shells via Swelling, DOUGLAS HOLMES, Boston University, MATTEO PEZZULLA, PAOLA NARDINOCCHI, Università degli Studi di Roma “La Sapienza”, STEVEN SHILLIG, Virginia Tech — Non-homogenous swelling will induce curvature within thin structures - beams will bend and plates will morph into shells. In this work, we examine the dynamics of swelling plates by attaching with either positive or negative Gaussian curvature. The swelling process is driven by a concentration gradient between two partially swollen structures, and the curvature of the final shell is dictated by the geometric arrangement of the swelling materials. The dynamics of this process are driven by diffusion and the geometry of the contact line. We demonstrate that these dynamic deformations can occur over a much faster timescale if the structure is confined. Beginning with a beam bent into an arch, we show how this swelling leads to a snap-through instability with dynamics similar to an arch compressed by a point load. The swelling-induced morphing presented in this talk provides a very simple and controllable way to achieve complex shell structures from simple building blocks.

10:12AM F44.00010 Interface adhesion between 2D materials and elastomers measured by buckle delamination, CHRISTOPHER BRENNAN, NANSHU LU, Univ of Texas, Austin — A major application for 2D materials is creating electronic devices, including flexible and wearable devices. These applications require complicated fabrication processes where 2D materials are either mechanically exfoliated or grown via chemical vapor deposition and then transferred to a host substrate. Both processes require intimate knowledge of the interactions between the 2D material and the substrate to allow for a controllable transfer. Although adhesion between 2D materials and stiff substrates such as silicon and copper have been measured by bulge or peeling tests, adhesion between 2D materials and soft polymer substrates are hard to measure by conventional methods. Here we propose a new method of measuring adhesion between two materials by using mature cantilever beam techniques. In this work, we present buckle delamination in 2D atomic layers and measuring the buckle profile using an atomic force microscope, we can readily extract 2D-elastomer adhesion energy. Here we look at the adhesion of MoS2 and graphene to PDMS. The measured adhesion values are found insensitive to the applied strains in the substrate and are one order smaller than 2D-silicon oxide adhesion which is mainly attributed substrate surface roughness differences.

10:24AM F44.00011 Harnessing snap-through instability for shape-recoverable energy-absorbing structure, SUNG KANG, SICONG SHAN, JORDAN RANNEY, PAI WANG, FRANCISCO CANDIDO, JENNIFER LEWIS, KATIA BERTOLDI, Harvard Univ — Energy absorbing materials and structures are used in numerous areas for maintaining structural integrity, protection and comfort. To absorb/dissipate energy from shock/vibration, one generally relies on processes such as plastic deformation and damping as the case of metal foams and suspensions. Because plastic deformation and damping induce irreversible change in the energy-absorbing systems such as shape changes and degradation of damping elements by heat dissipation, it would be desirable to develop a new energy-absorption mechanism with reversibility. Furthermore, it would be desirable to implement energy-absorption mechanisms whose behavior is not affected by the rate of loading. Here, we report a shape-recoverable system that absorbs energy without degradation by harnessing multistability in elastic structures. Using numerical simulations, we investigate geometrical parameters that determine the onset of the snap-through and multi-stability. We subsequently manufacture structures with different geometrical parameters and sizes using a scalable direct-write 3D printing approach. We experimentally demonstrate reversible energy- absorption in these structures at strain rates over three orders of magnitude, with reduced peak acceleration under impact by up to one order of magnitude compared with control samples. Our findings can open new opportunities for scalable design and manufacturing of energy-absorbing materials and structures.

10:36AM F44.00012 Non-porous Elastic Sheets with Negative Poisson’s Ratio, FARHAD JAVID, School of Engineering and Applied Science, Harvard University, EVELYN SMITH-ROBERGE, Department of Mathematics and Statistics, McGill University, MATTHEW INNES, ALI SHANIAN, Rolls-Royce Energy, KATIA BERTOLDI, School of Engineering and Applied Science, Houston University, HARVARD UNIVERSITY COLLABORATION, ROLLS-ROYCE ENERGY COLLABORATION — Negative Poisson’s ratio (NPR) materials—materials that contract (expand) in transverse directions when compressed (stretched) uniably—have attracted significant interest both because of their unusual properties and their many potential applications. However, complex fabrication processes, high porosity, and low structural stiffness of most of the proposed NPR materials have significantly limited their practical applications. In this work, a novel NPR material is designed by coupling the in- and out-of-plane (popping) deformations in an elastic sheet with a periodic distribution of dimples. As a result, such NPR material has zero porosity, relatively high structural stiffness, and can be made from both hard and soft materials using industrial fabrication techniques.
steady states. As in the equilibrium scenario, the components of the metric are given by the time-integrals of correlation functions in nonequilibrium steady states, after a suitable renormalization of heat. With a novel expansion formula for the governing master equation, we propose an exact expression for Physical Science and Technology, University of Maryland, College Park — Within the linear response regime, minimally dissipative transitions between equilibrium states are given by the geodesics of a thermodynamic metric in parameter space. We derive an analogous geometric structure for transitions between nonequilibrium steady states, after a suitable renormalization of heat. With a novel expansion formula for the governing master equation, we propose an exact expression for the metric. As in the equilibrium scenario, the components of the metric are given by the time-integrals of correlation functions in nonequilibrium steady states.
9:36AM F45.00007 Work fluctuations for a colloidal particle in a time-varying optical trap in analogy with gas in expansion and compression\textsuperscript{1}. HYUK KYU PAK, UNIST, DONGYUN LEE, Pusan National University, CHULAN KWON, Myeongji University — The fluctuation theorem provides a rigorous statistical rule for thermally fluctuating quantities such as work, heat, and entropy production in nonequilibrium thermodynamic processes. However, testing the theorem needs small systems where the fluctuations are more observable. Therefore, there are great difficulties in the experimental measurements. In this work, we investigate the motion of a colloidal particle trapped in a harmonic potential with time-varying stiffness. Here, we estimate the work done on the particle during compression and expansion by measuring its particle position in the first time. The resultant probability distributions of the work in both processes satisfy very well the Jarzynski equality and the Crooks fluctuation theorem. Because this isoenthalpic expansion and compression process in a soft wall qualitatively mimics that in a rigid wall, it offers valuable tool for extracting work from micromechanical heat engines.

\textsuperscript{1}This research is supported by the U. S. Army Research Office under contract number W911NF-13-1-0390.

9:48AM F45.00008 Engineering Maxwell’s Demon\textsuperscript{1}. ZHIYUE LU, University of Maryland at College Park, DIBYENDU MANDAL, UC Berkeley, CHRISTOPHER JARZYNSKI, University of Maryland at College Park — We describe a hypothetical machine, with moving, mechanical components, that acts as an autonomous Maxwell’s demon. The machine operates in two useful modes. It can act as an information engine by rectifying the thermal motions of surrounding gas particles to lift a mass against gravity, while writing information to a stream of bits. Alternatively, it can act as an eraser, harnessing the energy of a falling mass to erase information from a stream of bits. We solve for the phase diagram and compute the efficiency of our model, both analytically and numerically. Our model provides a simple example of a mechanical machine that is driven by the information entropy of a stream of bits, rather than a difference in temperatures or chemical potentials.

10:00AM F45.00009 Work Relations from Doi-Peliti Field Theory. ANDREW BAISH, BENJAMIN VOLLMAYR-LEE, Bucknell University — We develop a field-theoretic description of non-equilibrium work relations, using Doi-Peliti field theory. We consider classical particles on a lattice, with pair interactions and a local potential, coupled to a thermal bath. Work protocols are imposed by varying the local potential, which drives the system out of equilibrium. In this framework, work relations appear simply as the result of a gauge-like transformation.

10:12AM F45.00010 Experimental test of Generalized Fluctuation Dissipation Theorems during a transient\textsuperscript{1}. SERGIO CILIBERTO, ISAAC THEURKAUFF, ARTYOM PETROSYAN, ENSL-CNRS — In recent years the study of the Fluctuation Dissipation Theorem (FDT) in out of equilibrium system have received a lot of attention both theoretically and experimentally. Several Generalized FDT (GFDT) have been proposed but many theoretical results concern the steady state regimes and only a few the transient regimes. We report here an experiment in which two formulations of GFDT have been tested during the relaxation dynamics of a liquid crystal quenched near the critical point of Fredericksz transition, which is similar to a second order phase transition and it presents a critical slowing down. Thus the relaxation dynamics after the quench is sufficiently slow to perform several measurements. During the relaxation, the equilibrium FDT is strongly violated and this allows us to test the two GFDT. One is based on a transient fluctuation theorem and the time dependent distribution function. The other is a generalization of the Hatano-Sasa relations for transient state and has the very clear interpretation that the violation of the equilibrium FDT is related to the heat fluxes. The advantages and draw back of the two GFDT are discussed from an experimental point of view.

\textsuperscript{1}ERC-Outeflucop

10:24AM F45.00011 Nonequilibrium equalities in absolutely irreversible processes. YUTO MURASHITA, KEN FUNO, MASAHIITO UEDA, University of Tokyo — Nonequilibrium equalities have attracted considerable attention in the context of statistical mechanics and information thermodynamics. Integral nonequilibrium equalities reveal an ensemble property of the entropy production $\sigma$ as $\langle e^{-\sigma} \rangle = 1$. Although nonequilibrium equalities apply to rather general nonequilibrium situations, they break down in absolutely irreversible processes, where the forward-path probability vanishes and the entropy production diverges. We identify the mathematical origins of this inapplicability as the singularity of probability measure. As a result, we generalize conventional integral nonequilibrium equalities to absolutely irreversible processes as $\langle e^{-\sigma} \rangle = 1 - \lambda_S$, where $\lambda_S$ is the probability of the singular part defined based on Lebesgue’s decomposition theorem. The acquired equality contains two physical quantities related to irreversibility: $\sigma$ characterizing ordinary irreversibility and $\lambda_S$ describing absolute irreversibility. An inequality derived from the obtained equality demonstrates the absolute irreversibility leads to the fundamental lower bound on the entropy production. We demonstrate the validity of the obtained equality for a simple model.

10:36AM F45.00012 Work Relations Connecting Nonequilibrium Steady States Without Detailed Balance. YING TANG, RUOISHI YUAN, PING AO, Shanghai Jiao Tong Univ — Bridging equilibrium and nonequilibrium statistical physics attracts sustained interest. Hallmarks of nonequilibrium systems include a breakdown of detailed balance, and an absence of a priori potential function corresponding to the Boltzmann-Gibbs distribution, without which classical equilibrium thermodynamical quantities could not be defined. Here, we construct dynamically the potential function through decomposing the system into a dissipative part and a conservative part. We then develop a nonequilibrium theory by defining thermodynamical quantities based on the potential function. We elucidate this procedure explicitly in a class of time-dependent linear diffusive systems without mathematical ambiguity. We also obtain the exact work distribution, and generalized work relations for the calculation of free energy difference between nonequilibrium steady states. Our results demonstrate that concepts for equilibrium can be naturally extended to nonequilibrium steady state, which provides a platform to study thermodynamics of systems without detailed balance.

Tuesday, March 3, 2015 8:00AM - 11:00AM — Session F46 DBIO: Invited Session: DBIO Award Symposium 217A - Wolfgang Losert, University of Maryland

8:00AM F46.00001 Max Delbruck Prize in Biological Physics Award Lecture. STANISLAS LEIBLER, Rockefeller University and Institute for Advanced Study — .
Using evolutionary sequence variation to make inferences about protein structure and function, LUCY COLWELL, Cambridge University — The evolutionary trajectory of a protein through sequence space is constrained by its function. Collections of sequence homologs record the outcomes of millions of evolutionary experiments in which the protein evolves according to these constraints. The explosive growth in the number of available protein sequences raises the possibility of using the natural variation present in homologous protein sequences to infer these constraints and thus identify residues that control different protein phenotypes. Because in many cases phenotypic changes are controlled by more than one amino acid, the mutations that separate one phenotype from another may not be independent, requiring us to understand the correlation structure of the data. To address this, we build a maximum entropy probability model for the protein sequence. The parameters of the inferred model are constrained by the statistics of a large sequence alignment. Pairs of sequence positions with the strongest interactions accurately predict contacts in protein tertiary structure, enabling all atom structural models to be constructed. We describe development of a theoretical inference framework that enables the relationship between the amount of available input data and the reliability of structural predictions to be better understood.

Dynamics of living matter: can we “see” collective motions in proteins? , DOEKE HEKSTRA, Green Center for Systems Biology, UT Southwestern Medical Center — Proteins are ideal model systems for quantitative study of the interplay of physical and evolutionary forces. Collective, anharmonic motions of amino acid residues within proteins are thought to be central to their function, and to explain, in large part, the complex dependence of protein function on its constituent parts. Currently, the experimental characterization of such motions poses a major stumbling block on the way to a physical understanding of protein function and evolution. We are addressing this problem in two ways. First, alternate conformations of protein residues can often be distinguished in the electron density estimated from room-temperature X-ray crystallography. The dense packing of residues in the folded protein requires that such conformational variations must propagate through networks of amino acids to preclude local steric clashes. Fraser and colleagues showed that such steric conflicts can be used to extract contact networks of residues collectively switching conformation. We ask if these networks are conserved over homologous sequences and connected to the functional reaction coordinate, both of which would demonstrate their fundamental importance. I will describe recent results for the family of PDZ domains: small ligand-binding proteins for which a network of energetically and conformationally coupled residues controlling ligand affinity has been demonstrated previously by a range of methods. Second, the analysis of collective motions in proteins, by nearly any means, is indirect: nothing is seen moving. To directly induce and “see” motions on a range of time scales, we developed a new approach based on (a) electric field pulses to induce motions within a protein crystal and (b) time-resolved crystallography to observe these motions. Since proteins generically have a heterogeneous, modifiable charge distribution, this method could provide a powerful, general way of probing the collective motions, and excited states, of proteins in kinetic and atomic detail. I will present initial experiments showing the method is feasible. Taken together, these experiments begin to provide a basis for the development of a physical theory of proteins consistent with their function and adaptation — the source of their survival throughout the evolutionary process.


Heredity in Evolution & Evolution of Heredity. OLIVIER RIVOIRE, CNRS & Université Grenoble Alpes — The inheritance of characteristics induced by the environment has often been opposed to the theory of evolution by natural selection. However, although evolution by natural selection requires new heritable traits to be produced and transmitted, it does not prescribe, per se, the mechanisms by which this is operated. The mechanisms of inheritance are not, however, unconstrained, because they are themselves subject to natural selection. We introduce a schematic, analytically soluble mathematical model to compare the adaptive value of different schemes of inheritance. Our model allows for variations to be inherited, randomly produced, or environmentally induced, and, irrespectively, to be either transmitted or not during reproduction. The adaptation of the different schemes for processing variations is quantified for a range of fluctuating environments, following an approach that links quantitative genetics with stochastic control theory.

Associative memory through self-assembly. ZORANA ZERAVIC, Rockefeller University — Self-assembly has recently emerged as a powerful technique for synthesizing structures on the nano- and micro-scale. The basis of this development is the use of biopolymers, like DNA, to design specific interactions between multiple species of components, allowing the spontaneous assembly of complex structures. Here we address a fundamental limitation of the existing approaches to self-assembly: Namely, every target structure must have its own dedicated set of components, which are programmed to assemble only that very structure. In contrast, in biological systems, the same set of components can assemble many different complexes. Inspired by this, we extend the self-assembly framework to mixtures of shared components capable of assembling distinct structures at will.

Docking Prediction of a Water Soluble Porphyrin and Tubulin Assisted with Resonance Raman and Vibrational Mode Analysis. BRADY MCMICKEN, Univ of Texas, San Antonio; 711th Human Performance Wing, Optical Radiation Bioeffects Branch, LORENZO BRANCADON, Univ of Texas, San Antonio, ROBERT THOMAS, 711th Human Performance Wing, Optical Radiation Bioeffects Branch, JAMES PARKER, Univ of Texas, San Antonio; 711th Human Performance Wing, Optical Radiation Bioeffects Branch — The ability to modify protein conformation by controlling its partial unfolding may have practical applications such as diminishing its function or blocking its activity. One method used to induce partial unfolding of a protein involves the use of a photosensitizer non-covalently bound to a protein that triggers photochemical reactions upon irradiation leading to protein conformational changes. We are investigating the photoinduced conformational changes of tubulin mediated by a bound water-soluble porphyrin that acts as a photosensitizer. Analysis of how tubulin conformational changes affect its biological function or blocking its activity.

8:36AM F46.00002 Using resonance Raman and vibrational mode analysis, BRADY MCMICKEN, Univ of Texas, San Antonio; 711th Human Performance Wing, Optical Radiation Bioeffects Branch, LORENZO BRANCADON, Univ of Texas, San Antonio, ROBERT THOMAS, 711th Human Performance Wing, Optical Radiation Bioeffects Branch — The ability to modify protein conformation by controlling its partial unfolding may have practical applications such as diminishing its function or blocking its activity. One method used to induce partial unfolding of a protein involves the use of a photosensitizer non-covalently bound to a protein that triggers photochemical reactions upon irradiation leading to protein conformational changes. We are investigating the photoinduced conformational changes of tubulin mediated by a bound water-soluble porphyrin that acts as a photosensitizer. Analysis of how tubulin conformational changes affect its biological function or blocking its activity.

8:12AM F47.00002 Broad-band opsin for effective stimulation of cells by white light. SUBRATA BATABYAL, GREGORY CERVENKA, YOUNG-TAE KIM, SAMARENDRA MOHANTY, University of Texas System — Currently, use of optogenetic sensitization of retinal cells combined with activation/inhibition has potential as alternative to retinal implants that would have required electrodes inside every single neuron for high visual resolution. However, clinical translation of optogenetic activation for restoration of vision suffers from the drawback that narrow spectral sensitivity of opsin requires active stimulation by blue laser or LED having intensity much higher than ambient light. In order to allow ambient-light based stimulation paradigm, here we report development of broad-band opsin that has broad spectral excitability in the entire visible spectrum. The cells sensitized with the broad-band opsin showed order of magnitude higher excitability with white light as compared to that using only the narrow-band light components. The use of broad-band opsin construct will allow higher sensitivity of the opsin-sensitized neurons in degenerated retina to ambient white light, and therefore, significantly lower activation-threshold in contrast to conventional approach of intense, narrow-band light based active-stimulation.
8:24AM F47.00003 Photoconductivity in DNA-Porphyrin Complexes¹, PEI MYINT, EMMA OXFORD, COLLENCE NYAZENGA, WALTER SMITH, Haverford College, ZHENQING QI, A.T. JOHNSON, University of Pennsylvania — We have measured the photoconductivity of λ-DNA that is modified by intercalating a porphyrin compound, meso-tetrakis(N-methyl-4-pyridinium)porphyrin (TMPyP), into its base stacks. Intercalation was verified by a red shift and hypochromism of the Soret absorption peak. The DNA/porphyrin strands were then deposited onto oxidized silicon substrates which had been patterned with interdigitated electrodes, and blown dry. Electrical measurements were carried out under nitrogen, using illumination from a 445 nm laser; this wavelength falls within the absorption peak of the DNA/porphyrin complexes. When initially measured under dry nitrogen, the resulting device showed no photoconductivity or dark conductivity. However, at relative humidities of 30% and above we do observe dark conductivity, and also photoconductivity that grows with time. Photoconductivity gets larger at higher relative humidity. Remarkably, when the humidity is lowered again, some photoconductivity is now observed, indicating a change that persists for more than 24 hours. It may be that the humidity alters the structure of the DNA, perhaps allowing for better alignment of the bases.

¹This work was supported by NSF grant BMAT-1306170.

8:36AM F47.00004 Optimization of a Quantum Biomimetic Photocell, NATHANIEL GABOR¹, VIVEK AJI, YAFIS BARLAS, University of California Riverside — We propose and describe the structure, function, and optimization of a biologically inspired two-channel quantum photocell. The photocell, which operates as a dual quantum heat engine, simultaneously performs the critical tasks of absorption, power conversion, and energy release. Graphene has been suggested as the stochastic solar photon irradiance, we determine the spectrum of optimal absorption characteristics and charge transfer probabilities necessary for the input supply to exactly meet the output demand. Strikingly, the regulation optimization spectrum peaks in the red and blue portions of the terrestrial solar irradiance, and exhibits close correspondence to the action spectrum of chlorophyll-based photosynthetic organelle. Moreover, a comparison of structure and function of the proposed two-color photocell to photosynthetic chlorophyll complexes in green plants may answer the question: why on Earth are terrestrial plants green?

8:48AM F47.00005 A Classical Theory of Multichromophoric Resonance Energy Transfer, SEBASTIAN DUQUE, Grupo de Física Atómica y Molecular, Instituto de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Antioquia UdeA. Medellín, Colombia, Paul BRUMLER, Chemical Physics Theory Group, Department of Chemistry and Center for Quantum Information and Quantum Control, University of Toronto, Toronto, Canada, LEONARDO A. PACHON, Grupo de Física Atómica y Molecular, Instituto de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Antioquia UdeA. Medellín, Colombia — Based on classical electrodynamics, a classical theory of multichromophoric resonance energy transfer is formulated. In the maximum coupling configuration between N₂ acceptors and N₃ donors, the present theory predicts a first-order-in-the-interactions enhancement of the energy transfer rate by a factor N₃ and additional second-order-in-the-interactions enhancement arising from the interaction between donors. The theory is applied to predict the transfer rate of the LH II and results are found to be in good agreement with experimental results.

9:00AM F47.00006 ABSTRACT WITHDRAWN —

9:12AM F47.00007 Coherent dimer dynamics in a dissipative environment maintained by an off-resonant single mode, ELLIOTT LEVI, BRENDON LOVETT, University of St Andrews — The role of quantum coherence in efficient energy harvesting has recently been the subject of intense research. In this paper, we explore the extent to which quantum coherence can be induced in a previously incoherent two level system (TLS) by strongly coupling to a single, off-resonant, bosonic mode. The rest of the environment is assumed to comprise a Markovian bath of bosonic modes. The TLS could, for example, represent the position of the exciton in an energy transfer dimer system. The TLS-single mode coupling strength is varied for several different forms of bath spectral density in order to assess whether the coherent dynamics of the TLS are modified. We find a clear renormalisation of the site population oscillation frequency, which also causes an altered interaction with the bath. This new interaction can cause enhanced or reduced coherent behaviour of the TLS depending on the parameters. We will discuss the usefulness and pitfalls of exploiting such a dynamics-altering tool in a quantum device.

9:24AM F47.00008 Identification of nucleobases using variable currents through graphene nanopores: A first principles study, J.T. HARALDSEN, Department of Physics and Astronomy, James Madison University, H. MCFARLAND, Department of Biology, James Madison University, T. AHMED, Theoretical Division, Los Alamos National Laboratory, J.-X. ZHU, Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, A.V. BALATSKY, Institute for Materials Science, Los Alamos National Laboratory — Nanopore-based technology has the potential to be an efficient method for DNA/RNA base sequencing, as well as an identifier of other biomolecules. However, the thickness of the nanopore substrate is critical for the identification of individual nucleobases due to resulting noise and resolution problems. Recent work has been suggested as the possibility of nanopore substrates due to its atomic thickness and high strength. In this study, we examine a possible device mechanism for the voltage dependence of nucleobases passing through a graphene nanopore. We utilize density functional theory with a generalization gradient approach on a graphene ribbon with a nucleobase in order to calculate the transmission spectra for each base. Transmission spectra for each base allows for the calculation of the ballistic current and differential current as a function of voltage. We show that applying various bias voltages across a graphene ribbon for the general, energy-minimized position of the translocated nucleobase, it is possible to distinguish individual bases using the resulting current. Overall, our goal is to improve nanopore device design by helping to further DNA/RNA nucleobase identification and sequencing.

9:36AM F47.00009 Physical limits to biomechanical sensing, FARZAN BEROZ, CHASE P. BROEDERSZ, NED S. WINGREEN, Princeton University — Experiments have shown that eukaryotic cells such as fibroblasts and mesenchymal stem cells are able to accurately probe and respond to the elastic properties of their microenvironment. These cells navigate across gradients in stiffness, a phenomenon that has been called “ durotaxis.” Spatial heterogeneity in the cell’s elastic environment produces sampling noise in local probing of stiffness, which places fundamental limits on the accuracy with which a cell can sense stiffness gradients. To determine the biophysical limits of durotaxis, we develop a quantitative model of a cell as a stiffening-measuring device in a disordered fiber network with two dimensions. We find that local stiffness measurements follow a broad distribution spanning several orders of magnitude.

9:48AM F47.00010 Graphene Nanonet for Biological Sensor, NARAE SHIN, TAEKYEONG KIM, Seoul Natl Univ, JAESUNG PARK, Pohang University of Science and Technology, HYE JIN JIN, HYUNGWOO LEE, KYUNG-EUN BYUN, Seoul Natl Univ, CHANG-SEUK LEE, Soonchunhyang Univ, KWANG S. KIM, Pohang University of Science and Technology, BYUNG HEE HONG, Seoul Natl Univ, TAE HYUN KIM, Soonchunhyang Univ, SEUNGHUN HONG, Seoul Natl Univ — Graphene nanoribbons (GNRs) have been drawing attentions because they exhibited improved transconductances compared with graphene, and their edges could be functionalized with various chemicals or biological molecules. Herein, we developed a facile method to fabricate graphene nanonet (GNN) patterns over a large surface area for biological applications. In this method, the networks of V₂O₅ nanowires were adsorbed selectively in the desired regions on a graphene layer, and they were utilized as a shadow mask during the reactive ion etching on the graphene layer. This fabrication process allowed us to prepare large scale patterns of GNN structures which were comprised the continuous networks of GNRs with chemical functional groups on their edges. The chemical functional groups in the GNN could be functionalized with biological molecules such as DNAs for biological applications. Using the GNN-based biochip devices, we have successfully achieved the fluorescence imaging of the GNN channels and the electrical detection of the DNAs at InN concentrations. Our method could be a powerful strategy to mass-produce GNR-based devices and should enable various practical bio-applications.
10:00AM F47.00011 Optical detection of cellular activation by optical stimulation, SARMISHTHA SATPATHY, University of Texas at Arlington, SUBRATA BATBHYAL, University of Texas System, YOUNG-TAE KIM, SAMARENDRA MOHANTY, University of Texas at Arlington — Despite the many advantages of patch clamp recordings, there have been efforts to find alternative methods for measuring action potentials in neurons as electrode methodologies have limited spatial resolution, rely on mechanical stability, and are hence cumbersome to use. Here, we report use of optical methods that allow detection of cells with increased spatial information. We demonstrate use of calcium dyes or genetic voltage/ion indicators for optical detection of influx of Ca\(^{2+}\) ions as a measure of optical stimulation. We also show that phase information of light transmitted or reflected from the activated cell can be used to non-invasively measure changes in optical path length of the cells during optical activation. Further, we report use of polarized light for wide-field detection of optogenetically-stimulated activity in cells, requiring no exogenous labeling, making it possible to detect cellular activity with high spatial and temporal resolution by wide-field polarimetric/phase imaging. With optical detection of neural activities, the whole process of identification, activation and detection can be made non-invasive added with the advantages of high throughput and least requirement of mechanical stability and contamination.

10:12AM F47.00012 Ultra-low field T1 vs. T1rho at 3T and 7T: study of rotationally immobilized protein gels and animal brain tissues, HUI DONG, Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, BEN INGLIS, Henry H. Wheeler Jr. Brain Imaging Center, University of California, Berkeley, IAN BARR, College of Chemistry, University of California, Berkeley, JOHN CLARKE, Department of Physics, University of California, Berkeley — Clinical magnetic resonance imaging (MRI) machines operating in static fields of typically 1.5 T or 3 T can capture information on slow molecular dynamics utilizing the so-called T1rho technique. This technique, along with frozen-density DFT to achieve efficient quantum-mechanical description of explicit solvent. Calculations have so far investigated copper ion attachment to CXXC motifs present in Atox1. The addition of the platinum ion and the competition between the two metals is currently being studied. These calculations could contribute towards accurate simulation of MR images/signals and extraction of parameters of clinical importance through comparison of the measured and the simulated images/signals.

10:24AM F47.00013 New formulation of Magnetization Equation for Flows Under NMR/MRI Excitation (I), DILIP DE, MOSES EMETERE, VICTOR OMOTOSHO, Covenant University — We have obtained for the first time from the Bloch NMR equations the correct dependence of the single component of magnetization, \(M_y\), and \(M_z\) at resonance (NMR/MRI) on relaxation times, if \(B_1\) field (pulsed or continuous), blood(nuclear spin) flow velocity, etc. in the rotating frame of reference. The equations are applicable for both CW and pulsed NMR experiments with or without flow of spins. Our approaches can be extended easily to include gradient fields and diffusion of spins, if needed in NMR/MRI experiments. We also discuss the application of our equations to a specific case of low excitation scheme: Free induction decay (FID). The first time new equations of single component of MR magnetization and further equations that can be derived with the methodologies used here, can be applied towards accurate simulation of MR images/signals and extraction of parameters of clinical importance through comparison of the measured and the simulated images/signals.

10:36AM F47.00014 The reference-probe model in avian magnetoreception, MARIA PROCOPIO, THORSTEN RITZ, University of California, Irvine — The sensory mechanism that allows magneto-sensitive organisms to detect the direction of the geomagnetic field for navigation purposes is still largely unclear. One of the two leading hypothesis stipulates that photoinduced radical-pair reactions in photoreceptor proteins act as the primary magnetic sensor in migratory birds. In recent years the radical-pair mechanism has been receiving considerable support, qualifying the avian compass as a plausible emergent property of photochemical reactions. However, the relevance of the reference character has not been studied yet. Here we introduce a method to investigate the contribution of the reference character to optimality and robustness. By analytical and computational studies, we find that the probe character is crucial for optimality, while the reference character captures robust features. Our results suggest the reference-probe model to contain both optimal and robust design features.

Tuesday, March 5, 2013 8:00AM - 10:48AM
Session F48 DBIO: Focus Session: Physics of Proteins I

10:00AM F48.00001 Reversible cluster formation in concentrated monoclonal antibody solutions, P. DOUGLAS GODFRIN, University of Delaware, LIONEL PORCAR, PETER FALUS, Institut Laue-Langevin, ISIDRO ZARRAGA, Genentech Inc., NORM WAGNER, University of Delaware, YUN LIU, University of Delaware/NIST — Protein cluster formation in solution is of fundamental interest for both academic research and industrial applications. Recently, industrial scientists are also exploring the effect of reversible cluster formation on biopharmaceutical processing and delivery. However, despite of its importance, the understanding of protein clusters at concentrated solutions remains scientifically very challenging. Using the neutron spin echo technique to study the short time dynamics of proteins in solutions, we have recently systematically studied cluster formation in a few monoclonal antibody (mAb) solutions and their relation with solution viscosity. We show that the existence of anisotropic attraction can cause the formation of finite-sized clusters, which increases the solution viscosity. Interestingly, once clusters form at relatively low concentrations, the average size of clusters in solutions remains almost constant over a wide range of concentrations similar to that of micelle formation. For a different mAb we have also investigated, the attraction is mostly induced by hydrophobic patches. As a result, these mAbs form large clusters with loosely linked proteins. In both cases, the formation of clusters all increases the solution viscosity substantially. However, due to different physics origins of cluster formation, solutions viscosities for these two different types of mAbs need to be controlled by different ways.

8:12AM F48.00002 Simultaneous Platinum and Copper Ion Attachment to a Human Copper Chaperone Protein, MIROSLAV HODAK, North Carolina State University, JOHN CVITKOVIĆ, Worcester Polytechnic Institute, COREY YU, OLEG DMITRIEV, University of Saskatchewan, GEORGE KAMINSKI, Worcester Polytechnic Institute, JERRY BERNHOLC, North Carolina State University — Cisplatin is a potent anti-cancer drug based on a platinum ion. However, its effectiveness is decreased by cellular resistance, which involves cisplatin attaching to copper transport proteins. One of such proteins is Atox1, where cisplatin attaches to the copper binding site. Surprisingly, it was shown that both cisplatin and copper can attach to Atox1 at the same time. To study this dual metal ion attachment, we use the KS/FD DFT method, which combines Kohn-Sham DFT with frozen-density DFT to achieve efficient quantum-mechanical description of explicit solvent. Calculations have so far investigated copper ion attachment to CXXC motifs present in Atox1. The addition of the platinum ion and the competition between the two metals is currently being studied. These calculations start from a molecular mechanics (MM) structural model, in which glutathione groups provide additional ligands to the Pt ion. Our goals are to identify possible Cu-Pt structures and to determine whether copper/platinum attachment is competitive, independent, or cooperative. Results will be compared to the 1H, 13C, and 31P NMR experiments, in which binding of copper and cisplatin to Atox1 produces distinct secondary chemical shift signatures, allowing for kinetic studies of simultaneous metal binding.

1H, 13C, and 31P NMR experiments, in which binding of copper and cisplatin to Atox1 produces distinct secondary chemical shift signatures, allowing for kinetic studies of simultaneous metal binding.

10:48AM F48.00003 Testing magnetic field changes inside the brain using ULF MRI, JOHN CLARKE, Department of Physics, University of California, Berkeley — The use of magnetic resonance imaging (MRI) for clinical applications has led to the development of high-field magnets and advanced MR pulse sequences. However, the use of magnetic resonance imaging (MRI) machines operating in static fields of typically 1.5 T or 3 T can capture information on slow molecular dynamics utilizing the so-called T1rho technique. This technique, along with frozen-density DFT to achieve efficient quantum-mechanical description of explicit solvent. Calculations have so far investigated copper ion attachment to CXXC motifs present in Atox1. The addition of the platinum ion and the competition between the two metals is currently being studied. These calculations start from a molecular mechanics (MM) structural model, in which glutathione groups provide additional ligands to the Pt ion. Our goals are to identify possible Cu-Pt structures and to determine whether copper/platinum attachment is competitive, independent, or cooperative. Results will be compared to the 1H, 13C, and 31P NMR experiments, in which binding of copper and cisplatin to Atox1 produces distinct secondary chemical shift signatures, allowing for kinetic studies of simultaneous metal binding.
8:24AM F48.00003 Native dynamics from diversity in NMR structures. HEIKO LAMMERT, JOSE ONUCHIC, Rice Univ — Protein function relies on the characteristic dynamics that arise in the protein’s unique native structure, controlled by the smooth, funneled energy landscape evolved to enable fast and reliable folding. Structure-based models draw on energy landscape theory to build an ideally funneled energy landscape only from a protein’s native structure. Simplified interactions of homogeneous strength are used to eliminate energetic frustration. The dynamics of the model are controlled by geometric constraints imposed by the native fold. The energy landscapes of many actual proteins are smooth enough to let such unfrustrated models describe their folding mechanisms. But conflicting functional demands upon the sequence may introduce sufficient frustration into the energetics to affect the dynamics. For such cases heterogeneous interactions can be optimized based on additional data. We use the diversity among the conformations deposited in a set of NMR structures to estimate the extent of fluctuations in the native state to build an improved model of protein S6. Qualitative modifications bring the observed mechanism into agreement with experiment, and matching of the entire fluctuation profile leads to similar contact maps as optimization based on either phi-values of sequence data.

8:36AM F48.00004 Redox-controlled proton gating in bovine cytochrome c oxidase I. JOSE ONUCHIC, Rice University — Cytochrome c oxidase is the terminal enzyme in the electron transfer chain of essentially all organisms that utilize oxygen to generate energy. It reduces oxygen to water and harnesses the energy to pump protons across the mitochondrial membrane in eukaryotes and the plasma membrane in prokaryotes. The mechanism by which proton pumping is coupled to the oxygen reduction reaction remains unresolved, owing to the difficulty of visualizing proton movement within the massive membrane-associated protein matrix. Here, with a novel hydrogen/deuterium exchange resonance Raman spectroscopy method, we have identified two critical elements of the proton pump: a proton loading site near the propionate groups of heme a, which is capable of transiently storing protons uploaded from the negative-side of the membrane prior to their release into the positive-side of the membrane and a conformational gate that controls proton translocation in response to the change in the redox state of hemeo. These findings form the basis for a postulated molecular model describing a detailed mechanism by which unidirectional proton translocation is coupled to electron transfer from heme a to heme a3, associated with oxygen chemistry occurring in the heme a1 site, during enzymatic turnover. Each time heme a undergoes an oxidation-reduction transition a proton is translocated across the membrane accounting for the observation that two protons are translocated during the oxidative phase of the enzyme cycle and two more are translocated during the reductive phase. This work was done in collaboration with Drs. Tsuyoshi Egawa and Syun-Ru Yeh.

1This work was supported the National Institutes of Health grant GM098799 to D.L.R and National Science Foundation Grant NSF0956358 to S.-R.Y.

9:12AM F48.00005 Dissecting the relationship between protein structure and sequence variation I, AMIR SHAHMORADI, CLAUS WILKE, Univ of Texas, Austin, WILKE LAB TEAM — Over the past decade several independent works have shown that some of the structural properties of proteins are capable of predicting protein evolution. The strength and significance of these structure-sequence relations, however, appear to vary widely among different proteins, with absolute correlation strengths ranging from 0.1 to 0.8. Here we present the results from a comprehensive search for the potential biophysical and structural determinants of protein evolution by studying more than 200 structural and evolutionary properties in a dataset of 209 monomeric enzymes. We discuss the main protein characteristics responsible for the general patterns of protein evolution, and identify sequence divergence as the main determinant of the strengths of virtually all structure-evolution relationships, explaining ~ 10 – 30% of observed variation in sequence-structure relations. In addition to sequence divergence, we identify several protein structural properties that are moderately but significantly coupled with the strength of sequence-structure relations. In particular, proteins with more homogeneous back-bone hydrogen bond energies, large fractions of helical secondary structures and low fraction of beta sheets tend to have the strongest sequence-structure relation.

1BEACON-NSF center for the study of evolution in action.

9:24AM F48.00006 Develop Infrared Structural Biology for Probing Structural Dynamics of Protein Functions I, AIHUA XIE, ZHOUYANG KANG, OLIVER CAUSEY, CHARLES LIU, Oklahoma State University — Protein functions are carried out through a series of structural transitions. Lack of knowledge on functionally important structural motions of proteins impedes our understanding of protein functions. Infrared structural biology is an emerging technology with powerful applications for protein structural dynamics. One key element of infrared structural biology is the development of vibrational structural marker (VSM) database library that translates infrared spectroscopic signals into specific structural information. We report the development of VSM for probing the type, geometry and strength of hydrogen bonding interactions of buried COO− side chains of Asp and Glu in proteins. Quantum theory based first principle computational studies combined with bioinformatic hydrogen bond analysis are employed in this study. We will discuss the applications of VSM in mechanistic studies of protein functions. Infrared structural biology is expected to emerge as a powerful technique for elucidating the functional mechanism of a broad range of proteins, including water soluble and membrane proteins.

1This work is supported by OCAST HR10-078 and NSF DBI1338097.

9:36AM F48.00007 ABSTRACT WITHDRAWN —

9:48AM F48.00008 ABSTRACT WITHDRAWN —

10:00AM F48.00009 Building toy models of proteins using coevolutionary information I, RYAN CHENG, MOHIT RAGHUNATHAN, JOSE ONUCHIC, Rice University — Recent developments in global statistical methodologies have advanced the analysis of large collections of protein sequences for coevolutionary information. Coevolution between amino acids in a protein arises from compensatory mutations that are needed to maintain the stability or function of a protein over the course of evolution. This gives rise to quantifiable correlations between amino acid positions within the multiple sequence alignment of a protein family. Here, we use Direct Coupling Analysis (DCA) to infer a Potts model Hamiltonian governing the coevolutionary information. We report the development of VSM for probing the type, geometry and strength of hydrogen bonding interactions of buried COO− side chains of Asp and Glu in proteins. Quantum theory based first principle computational studies combined with bioinformatic hydrogen bond analysis are employed in this study. We will discuss the applications of VSM in mechanistic studies of protein functions. Infrared structural biology is expected to emerge as a powerful technique for elucidating the functional mechanism of a broad range of proteins, including water soluble and membrane proteins.

1This research has been supported by the NSF INSPIRE award MCB-1241332 and by the CTBP sponsored by the NSF (Grant PHY-1427654).
If the temperature decreases under 0 °C during a cycle, the water situated between the grains experiences a strong dilatation during the freezing step and a contraction during the ice melting step. In this case, we show how the freeze-thaw transition affects the packing fraction of the pile.

We present experimental results concerning the effect of thermal cycling on the packing fraction of equal spheres with the presence of water. First, we minimize the effect of avalanching and shear localization. We observe that the resistance against deformation of the wet (partially saturated) sand is much smaller than that of the dry sand, and that the latter dissipates more energy under flow. Second we show experimentally that the sliding friction on sand is greatly reduced by the addition of some— but not too much—water. The formation of capillary water bridges increases the shear modulus of the sand, which is smaller than that of the dry sand, and that the latter dissipates more energy under flow. Second we show experimentally that the sliding friction on sand is greatly reduced by the addition of some— but not too much—water. The formation of capillary water bridges increases the shear modulus of the sand, which facilitates the sliding.

In the present study, we perform analogous simulations for wet particles. We account for capillary and viscous interaction forces between particles, which result from the liquid bridges, and allow for liquid transfer between the particles and the liquid bridge. It is found that the bifurcation of the inertial regime observed with van der Waals force has been shown to lead to bifurcation of the inertial regime into two regimes: (a) a cohesive rate-independent regime and (b) an inertial regime. In the present study, we perform analogous simulations for wet particles. We account for capillary and viscous interaction forces between particles, which result from the liquid bridges, and allow for liquid transfer between the particles and the liquid bridge. It is found that the bifurcation of the inertial regime observed with van der Waals interaction persists for capillary cohesion and that the span of the cohesive rate-independent regime increases with liquid loading in the pendular regime. A simple model for steady shear rheology is obtained by blending the results in various regimes. The presentation will also discuss the effect liquid viscosity on the flow behavior.
9:24AM F49.00006 Flow and clogging of submerged hoppers. JUHA KOIVISTO, DOUGLAS DURIAN, University of Pennsylvania. The discharge rate for granular hoppers was recently found to depend on the filling height when the hopper is submerged in water. This effect is further studied with an automated experimental setup consisting of cylindrical flat bottomed hoppers with various diameters and orifices. The grains are spherical glass beads of diameter 1.1 ± 0.1 mm. The flow rate is measured with an electric scale connected to a computer. With this, we confirm the counterintuitive surge in the flow rate as the filling height decreases toward zero. We also find a similar surge for dry gains, but the size of the effect is much smaller and the knowledge is previously unseen. In both cases we notice that the flow of grains near the wall changes from creep like behavior to mass flow as the hopper diameter decreases. The hypothesis for the surge effect is changes in compaction stresses and force chains. To alter such behavior, on-going work includes changing the fluid pressure and flow rate near the orifice as well as changing the roughness of the walls. Work has also begun on clogging for small orifices in submerged hoppers, where preliminary observations show an exponential distribution of flow durations.

Supported by NSF Grant Number CBET 1335928

9:36AM F49.00007 Armoring, stability, and transport driven by fluid flow over a granular bed. BENJAMIN ALLEN, ARSHAD KUDROLLI, Department of Physics, Clark University. We discuss experiments investigating the evolution of a granular bed by a fluid flow as a function of shear rate at the fluid-bed interface. This is a model system to investigate a variety of physical examples including wind blowing over sand, sediment transport in rivers, tidal flows interacting with beaches, flows in slurry pipelines, and sand proppants in hydraulic fracturing. In order to examine the onset and entrainment of the granular bed under steady state conditions, we have constructed a novel conical rheometer system which allows a variable amount of shear to be applied to the granular bed. The grain-fluid system is index matched so that we can visualize the grains away from the sides as well as visualize the fluid flow above and below the interface by using fluorescent tracer particles. We demonstrate that the onset of erosion arises as particles rotate out of their stable position highlighting the importance of torque balance to onset. We find significant armoring of the bed, as the bed is sheared by the fluid flow. Above onset, at least three distinct regions of bed mobility can be found. We will discuss the measured integrated granular flux as a function of shear rate and compare them with empirical laws found in the geophysical literature.

9:48AM F49.00008 Creep and Dynamical Heterogeneities of Fluid-Driven Granular Flows. CARLOS ORTIZ, MORGANE HOUSSAIS, DOUGLAS DURIAN, DOUGLAS JEROLMACK, Univ of Pennsylvania. Earth’s surface is a fluid-sediment interface evolving through fluid-driven granular flow. To probe long-time dynamics, we construct an annular chamber that mimics an infinitely-long river channel. We use non-Brownian, spherical plastic grains, fully submerged in a less dense index-matching fluid. We drive the packs with a laminar flow and record dynamics by laser scanned particle tracking. “Bed load” grains near the surface exhibit relatively fast shear. By long-time averaging grain trajectories, we find that grains deep in the pack, which appear frozen by eye, exhibit a slow creep dynamics. The transition between bed load and creep occurs at a critical value of the local relaxation time, characterized by a critical dimensionless shear rate, the viscous number. We also characterize the important length and time scales for dynamical heterogeneities as a function of depth and find that grain dynamics are spatially and temporally heterogeneous at all depths. The dynamics slow down monotonically as a function of depth, but the domain size is largest at the transition to creeping. We propose a new phase diagram for fluid-sheared granular transport, where “bed load” sediment transport is defined as a dense granular flow driven by fluid shear from above and granulic creep from below.

10:00AM F49.00009 Onset and cessation of grain motion in riverbed erosion experiments. JULIA SALEVAN, ABRAM CLARK, Yale University, MARK SHATTUCK, City College of New York, COREY O’HERN, NICHOLAS OUELLETTE, Yale University. Erosion due to fluid flow plays a principal role in shaping landscapes. However, the complexity of the coupling between hydrodynamic shear, sediment transport, and internal granular bed rearrangements limits our understanding of the particle-scale physics that governs erosion. In particular, it is unclear whether particle rearrangements as a function of depth and find that grain dynamics are spatially and temporally heterogeneous at all depths. The dynamics slow down monotonically as a function of depth, but the domain size is largest at the transition to creeping. We propose a new phase diagram for fluid-sheared granular transport, where “bed load” sediment transport is defined as a dense granular flow driven by fluid shear from above and granulic creep from below.

10:12AM F49.00010 Jamming and unjamming in model riverbeds. ABE CLARK, JULIA SALEVAN, Yale University, MARK SHATTUCK, City College of New York, NICHOLAS OUELLETTE, COREY O’HERN, Yale University. When fluid flows laterally over a granular bed, it exerts shear stress on the particles. The ratio of this stress to the gravitational stress is known as the Shields number, and bulk sediment transport is thought to occur once the Shields number has passed a critical threshold. However, the particle-scale mechanisms that control this transition are not well understood. Here, we perform molecular dynamics simulations of a model riverbed to understand the particle-scale origins of jamming and unjamming in these systems. The particles interact via purely repulsive harmonic forces and are coupled to the flow using a Stokes-like drag model. The interstitial fluid velocity is determined from the local packing density using a relation similar to Darcy’s law. Near the transition to sediment transport, we observe hysteresis and avalanches, and connect their statistical properties to the packing geometry at the particle scale.

Funding: ARO W911NF-14-1-0005

10:24AM F49.00011 Erosion and flow of hydrophobic granular materials. BRIAN UTTER, THOMAS BENNS, BENJAMIN FOLTZ, JOSEPH MAHLER, James Madison University. We experimentally investigate submerged granular flows of hydrophobic and hydrophilic grains both in a rotating drum geometry and under erosion by a surface water flow. While slurry and suspension flows are common in nature and industry, effects of surface chemistry on flow behavior have received relatively little attention. In the rotating drum, we use varying concentrations of hydrophobic and hydrophilic grains of sand submerged in water rotated at a constant angular velocity. Sequential images of the resulting avalanches are taken and analyzed. High concentrations of hydrophobic grains result in an effectively cohesive interaction between the grains forming aggregates, with aggregate size and repose angle increasing with hydrophobic concentration. However, the formation and nature of the aggregates depends significantly on the presence of air in the system. We present results from a related experiment on erosion by a surface water flow designed to characterize the effects of heterogeneous granular surfaces on channelization and erosion.

10:36AM F49.00012 Fluid and particulate suspension flows at fracture junctions. TAK S. LO, JOEL KOPLIK, The Levich Institute and the Physics Department, City College of New York, CUNY. Suspended particles can be a serious problem in geological contexts such as fluid recovery from reservoirs because they alter the rheology of the flowing liquids and may obstruct transport by narrowing flow channels due to deposition or gravitational sedimentation. In particular, the irregular geometry of the fracture walls can trap particles, induce jamming and cause unwanted channeling effects. We have investigated particle suspension flows in tight geological fractures using lattice Boltzmann methods in the past. In this work we extend these studies to flows at a junction where two fractures intersect, an essential step towards a complete understanding of flows in fracture networks. The fracture walls are modeled as realistic self-affine fractal surfaces, and we focus on the case of tight fractures, where the wall roughness, the aperture and the particle size are all comparable. The simulations provide complete detail on the particle configurations and the fluid flow field, from which the stresses in the fluid and the forces acting on the bounding walls can be computed. With these information, phenomena such as particle mixing and dispersion, mechanical responses of the solid walls, possible jamming and release at junctions, and other situations of interest can be investigated.

Work supported by NERSC and DOE

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Tuesday, March 3, 2015 8:00AM - 11:00AM –
Session F50 GSOF D POLY: Soft Glasses 218 - Mark Shattuck, City College of New York

8:00AM F50.00001 Controlling disordered materials from the boundaries1. A. ALAN MIDDLETOWN, SEAN SWEENEY, Syracuse University — We study general models of materials with frozen disorder, such as spin glasses or solids with heterogeneities, and ask how domain walls or optical fracture surfaces can be controlled by selection of the boundary conditions on the surface of a given sample. We have developed and applied algorithms for optimal ground states that can explore all possible sets of boundary conditions (e.g., the boundary conditions for a disordered Ising model on a square lattice with sides \( L \), with sizes up to \( L = 2048 \)) and thereby rapidly determine all possible paths for domain walls for certain two-dimensional models. We apply this algorithm to uncorrelated and power-law correlated disorder. While this computation has implications for the uniqueness of the ground state in disordered magnetic materials, it fits within a broader set of questions on the sensitivity of the interior of disordered material, as might be seen in the force chains in a given granular packing, when one considers all possible boundary conditions. Interior regions that are shielded by disorder from boundary effects then act as rigid sets of degrees of freedom.

1Supported in part by NSF grant DMR-1410937

8:12AM F50.00002 Connecting glassy dynamics to micro-scale elasticity. WENHAI ZHENG, MATTIEU WYART, DAVID PINE, Center for Soft Matter Research, Department of Physics, New York University — We report a new experimental method for exploring the connection between the dynamics and structure in colloidal glasses. Using ellipsoids of controlled size and eccentricity as passive micro-probes, we explore the rheological properties of the local environment of the colloidal glass, in particular fluctuations in the local elasticity. We do this by measuring the random fluctuations in the rotational motion of the probe ellipsoids using depolarized light scattering. This is facilitated by index matching the spherical colloidal particles that form the glass to the background fluid: the only optical contrast is provided by the ellipsoids. Decoupling the optical anisotropy from the eccentricity of the probe particles further enhances the sensitivity of the probe to rotational motion.

8:24AM F50.00003 Jamming and free energy landscapes for three caged soft disks. XIN DU, Graduate student, ERIC WEEKS, Professor — We use a Monte Carlo simulation to study jamming in a model of three soft Brownian disks with harmonic repulsive potential confined in a circular corral. For large corrals, the disks can freely rearrange where one particle passes in between the other two, but for small corrals rearrangements become rare. Rearrangement events correspond to the system crossing over the energy barrier. With low temperature and/or small corral size, the energy barrier becomes larger and the system approaches a glass transition. We calculate the Helmholtz free energy from the distribution of configurations in the system and quantify both the entropic and potential components of the free energy barrier. In a hard disk model, the free energy barrier for rearrangements is entirely entropic. By comparing the entropic component of the soft model to a model of hard disks, we model the soft disks as hard disks with a temperature-dependent effective size. We find that our results are generalizable to other soft disk potentials as well.

8:36AM F50.00004 Microscopic Theory of Activated Penetrant Diffusion in Liquids and Glasses. RUI ZHANG, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — We formulate a force-level, self-consistent, nonlinear Langevin equation theory for the long-time diffusivity of a penetrant in molecular and polymeric supercooled liquids and glasses. The theory predicts that for a wide range of penetrant to matrix molecular unit size ratios (\( R \)), activated hopping is the dominant transport mechanism. The penetrant diffusivity (\( D \)) and jump distance exhibit different R-dependences in three dynamic regimes: \( R<0.5 \), \( 0.5<R<1 \), \( R>1 \), which are physically distinguished by the nature of the matrix motion required to facilitate hopping. The penetrant diffusion constant decreases the fastest with \( R \) in the first regime where the matrix behaves as a harmonic amorphous solid. The other two regimes involve larger scale, anharmonic matrix motions. Below and above the matrix glass transition temperature, \( D \) exhibits an Arrhenius and supra-Arrhenius temperature dependence, respectively. The reduction of \( D \) associated with penetrant-matrix attractive forces has also been studied. Our approach to theoretical calculations agrees reasonably well with experiments for both fast transport (e.g., gas permeation) and slow transport (e.g., barrier materials) systems, covering more than 10 orders of magnitude of variation of the diffusion constant.

8:48AM F50.00005 Antiferromagnetic Ising Model in Hierarchical Networks1. XIANG CHENG, STEFAN BOETTCHER, Department of Physics, Emory University — The Ising antiferromagnet is a convenient model of glassy dynamics. It can introduce geometric frustrations and may give rise to a spin glass phase and glassy relaxation at low temperatures [1]. We apply the antiferromagnetic Ising model to 3 hierarchical networks which share features of both small world networks and regular lattices. Their recursive and fixed structures make them suitable for exact renormalization group analysis as well as numerical simulations. We first explore the dynamical behaviors using simulated annealing and discover an extremely slow relaxation at low temperatures. Then we employ the Wang-Landau algorithm to investigate the energy landscape and the corresponding equilibrium behaviors for different system sizes. Besides the Monte Carlo methods, renormalization group [2] is used to study the equilibrium properties in the thermodynamic limit and to compare with the results from simulated annealing and Wang-Landau sampling.

1Supported through NSF grant DMR-1207431

9:00AM F50.00006 Protein crowding in solution, frozen, and freeze-dried states: small-angle neutron and X-ray scattering study of lysozyme/sorbitol/water systems. SUSAN KRUEGER, NIST, SHEILA KHODADADI, Delft Univ. of Tech., NICHOLAS CLARK, NIST and Amgen, ARNOLD MCAULEY, Amgen, VIVIANA CRISTIGLIO, ILL, NARAYANAN THIYENCHERI, ESF, JOSEPH CURTIS, NIST, EVGENIY SHALAEV, Allergan — For effective preservation, proteins are often stored as frozen solutions or in glassy states using a freeze-drying process. However, aggregation is often observed after freeze-thaw or reconstitution of freeze-dried powder and the stability of the protein is no longer assured. In this study, small-angle neutron and X-ray scattering (SANS and SAXS) have been used to investigate changes in protein-protein interaction distances of a model protein/cryoprotectant system of lysozyme/sorbitol/water, under representative pharmaceutical processing conditions. The results demonstrate the utility of SANS and SANS methods to monitor protein crowding at different stages of freezing and drying. The SANS measurements of solution samples showed at least one protein interaction peak corresponding to an interaction distance of \( \sim 90 \text{ Å} \). In the frozen state, two protein interaction peaks were observed by SANS with corresponding interaction distances at \( 40 \text{ Å} \) as well as \( 90 \text{ Å} \). On the other hand, both SANS and SAXS data for freeze-dried samples showed three peaks, suggesting interaction distances ranging from \( \sim 15 \text{ Å} \) to \( 170 \text{ Å} \). Possible interpretations of these interaction peaks will be discussed, as well as the role of sorbitol as a cryoprotectant during the freezing and drying process.
9:12AM F50.00007 Typical Value of Susceptibilities in the Three Dimensional Edwards-
Anderson Spin Glass Model in an External Field, SHENG FENG, KA-MING TAM,
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA, YE FANG, J. RAMANULIJA,
JE Division School of Electrical Engineering and Computer Science, Louisiana State University, Baton Rouge, LA 70803, USA, JUANA MORENO, MARK JARRELL,
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA. — We study the Edwards-Anderson model on a simple cubic lattice with a
finite constant external field using a Monte Carlo simulation code, which employs graphics processing units to dramatically speedup the simulation. Conventional indicators, such as the Binder ratio and correlation length, do not show any signs of a phase transition. We also studied R12, or the ratio of spin glass susceptibilities at finite wavenumbers, and show it is quite noisy that a systematic analysis cannot come to clear conclusion. This is largely due to the fact that the susceptibilities follow a broad, fat-tailed distribution, and the average is possibly dominated by rare events. Therefore we propose to study the typical value of these parameters by taking the geometric average over different disorder realizations, and compare it with the average linear measurements. We argue that the typical value should be also studied in additional to conventional linear average value, to provide another perspective for the study of phase transition in spin glasses.

9:24AM F50.00008 Dimensional dependence of mobility correlations and dynamic heterogeneity
in two-dimensional and three-dimensional glass forming fluids, ELIJAH FLENNER,
GRZEGORZ SZAMEL, Colorado State Univ — We examine mobility correlations and heterogeneous
dynamics in simulations of glass-forming two-dimensional and three-dimensional binary Lennard-Jones fluids. We compare the relationships between the dynamic correlation length $\xi_d$, the dynamics susceptibility $\chi_d$, and the alpha-relaxation time $\tau_\alpha$, by analyzing four-point structure factors $S_3(q,t)$ that are designed to investigate heterogeneous dynamics. We find that the relationships between $\xi_d$, $\chi_d$, and $\tau_\alpha$ depend strongly on dimension. Specifically, in two dimensions these relationships depend on whether the underlying dynamics is Newtonian or Brownian, but there is no dynamics dependence in three dimensions. Furthermore, in systems undergoing Newtonian dynamics $\xi_d$ grows much faster with $\tau_\alpha$ in two-dimensions than three-dimensions. Therefore, we demonstrate that dynamic heterogeneities have different properties in two and three dimensional glass forming fluids.

9:36AM F50.00009 Correlations of structure and dynamics in colloidal supercooled liquids.
MOYOSORE ODUNSI, ERIC WEEKS, Emory Univ — We are studying the correlations between measured quantities in colloidal samples that are in equilibrium. We track the movement of particles in systems using confocal microscopy. We see correlations between a particle’s displacement during short time scales and its long term displacement. In addition, we look at correlations between a particle’s displacement during different time scales and structural variables such as its vononoi volume or local volume fraction. We study how these correlations vary as the colloidal volume fraction approaches the glass transition volume fraction.

9:48AM F50.00010 Measurement of Stress Networks in 3D Colloidal Glasses, NEIL LIN,
MATTHEW BIERBAUM, JAMES SETHNA, ITAI COHEN, Department of Physics, Cornell University — We measure the inhomogeneous stress fields in a 3D colloidal glass by using a confocal microscope to image a binary suspension’s microstructure. Despite extensive studies of the contact forces in static systems (e.g., granular systems and emulsions), it has been difficult to measure these inhomogeneous stress fields in thermal systems. We determine these particle level Brownian stresses from all particle positions using the “Stress Assessment from Local Strucutural Anisotropy” (SALSA) method. First, we show that SALSA method accurately reports the stress field of a colloidal glass at particle-level resolution using molecular dynamics simulations. Furthermore, we quantify the measured pressure statistics and examine the q-model, Edwards ensemble and other theoretical predictions. Finally, the SALSA method enables us to investigate the underlying origin of the mechanical heterogeneities by comparing stress distribution with particle configuration.

10:00AM F50.00011 Physical Aging in a Colloidal Glass Subjected to Concentration Jump
Conditions, XIAOGUANG PENG, GREGORY B. MCKENNA, Department of Chemical Engineering, Texas Tech University, Lubbock, 79409, Texas, USA. — We have prepared a thermo-sensitive core-shell PS-PNIPAM/AA latex system and have investigated the aging dynamics of its colloidal dispersions subsequent to the temperature (or concentration)-jump perturbations using sequential creep experiments to probe the response of the system. The aging experiments were performed in the vicinity of the glass transition concentration, or temperature as evidenced by the strongly varying relaxation time with decreasing temperature (or increasing concentration). The aging results from the current colloidal glass study are compared with those expected in the Kovacs’ catalogue of experiments in structural recovery of glassy polymers, viz., intrinsic isotherms, asymmetry of approach and memory events [1]. We found that colloidal glass displays aging behavior and time-aging-time superposition is valid here. There are similarities in aging dynamics between colloidal glasses and molecular glasses, and differences also persist.


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10:12AM F50.00012 Structural signatures of dynamic heterogeneities in monolayers of colloidal
ellipsoids, ZHONGYU ZHENG, YUREN WANG, Institute of Mechanics, Chinese Academy of Sciences, YIOLONG HAN, Hong Kong University of Science and Technology — When a liquid is supercooled towards the glass transition, its dynamics drastically slows down, whereas its static structure remains relatively unchanged. Finding a structural signature of the dynamic slowing-down is a major challenge, yet it is often too subtle to be uncovered. Here we discover the structural signatures for both translational and rotational dynamics in monolayers of colloidal ellipsoids by video-microscopy experiments and computer simulations. The correlation lengths of the dynamic slowest-moving clusters, the static glassy clusters, the static local structural entropy and the dynamic heterogeneity follow the same power-law divergence, suggesting that the kinetic slowing down is caused by a decrease in the structural entropy and an increase in the size of the glassy cluster. Ellipsoids with different aspect ratios exhibit single- or double-step glass transitions with distinct dynamic heterogeneities. These findings demonstrate that the particle shape anisotropy has important effects on the structure and dynamics of the glass. The power-law divergence of the static correlation length with exponent -1 suggests that the glass transition is likely a two-dimensional Ising-type critical phenomenon.

This work was supported by grants GRF601613, PRC11SC04 and NSFC1137424, 11104286, 11372314, 51071166.

10:24AM F50.00013 Dynamics approaching the 2D colloidal glass transition, SKANDA VIVEK,
ERIC WEEKS, Emory University — We make 2D colloidal glasses by allowing bidisperse silica particles of diameters 2.53 and 3.38 $\mu$m to settle down under gravity in a monolayer at a coverslip interface. Controlling the area fraction gives us a wide range of behaviour, from liquid-like to supercooled and glassy. We use this model glass forming system to study the dynamics on approaching the glass transition, in 2D. We measure the increasing alpha relaxation times as the area fraction is increased toward the glass transition. We measure the growth of dynamical heterogeneity on approaching the glass transition. We quantify dynamical heterogeneity through the non-Gaussian parameter and the four point susceptibility $\chi_4$. Further, we measure the probability of local cage rearrangements as a function of waiting time (time since quench), for different area fractions, and relate this to other dynamical quantities such as diffusion coefficients, dynamical heterogeneity, etc. For glassy samples, we observe the slowing down of mean square displacements with waiting time, a sign of aging.
bubbles do not present a threat to humans, as their brains develop at the same speed as people’s, and begin their life as naive as an infant. I show that evolved brains that can learn can be transplanted onto physical robots, who then learn about our world by interacting with it. Such robots can learn to play games like chess. I will discuss what I believe is the central reason behind this failure, and how using the biological process of evolution can overcome that problem. For over fifty years, engineers have attempted to achieve machine intelligence that rivals human performance, but with only limited success in some specialized arenas such as chess. I will discuss what I believe is the central reason behind this failure, and how using the biological process of evolution can overcome that problem. I show that evolved brains that can learn can be transplanted onto physical robots, who then learn about our world by interacting with it. Such robots can learn to play games like chess. I will discuss what I believe is the central reason behind this failure, and how using the biological process of evolution can overcome that problem.  

Tuesday, March 3, 2015 8:00AM - 11:00AM
Session F51 DCMP GSOFT DPOLY: Invited Session: Smart Assemblies: Self-Replication, Computation and Error-Free Self-Assembled Systems  
Grand Ballroom C1 - Pablo Damasceno, University of Michigan

8:00AM F51.00001 Self-Replication of Colloidal Clusters , MICHAEL BRENNER, Harvard University — No abstract available.

8:36AM F51.00002 The Evolutionary Path Towards Sentient Robots , CHRIS ADAMI, Michigan State University — For over fifty years, engineers have attempted to achieve machine intelligence that rivals human performance, but with only limited success in some specialized arenas such as chess. I will discuss what I believe is the central reason behind this failure, and how using the biological process of evolution can overcome that problem. I show that evolved brains that can learn can be transplanted onto physical robots, who then learn about our world by interacting with it. Such robots do not present a threat to humans, as their brains develop at the same speed as people’s, and begin their life as naive as an infant.

9:12AM F51.00003 Simple self-replicators: growth via self-assembly and fissioning via bursting bubbles , DAMIEN WOODS, California Institute of Technology — We explore the principles of and experimentally demonstrate an autonomous and natural scheme for molecular self-replication. The talk will discuss a design for a simple DNA self-replicator that in principle exhibits exponential population growth, is limited by resource consumption, and has the potential to exhibit complicated population dynamics such as competition between species for a common food source. The replicating species are DNA nanotubes made from single-stranded tiles. Our proposed model for self-replication is designed around two basic principles that are ubiquitous on the Earth, and indeed on any oceanic world with crashing waves: growth via molecular self-assembly and fragmentation via violent hydrodynamic flows in bursting bubbles. The talk will focus on recent work to carefully characterise and understand both of these principles. In particular, on the nucleation and growth properties of various kinds, or species, of single-stranded tile nanotubes, and on the capability of bursting bubbles to break these micron-length structures. The proposed experimental system is conceptually very simple, completely autonomous, has the potential for information-based evolution, exploits energy from the environment to release replicated structures, and uses physically plausible mechanisms that could be implicated in the origin of life. The is joint work with collaborators Erik Winfree, Bernard Yurke, Joy Hui and Rizal Hariadi.

9:48AM F51.00004 Self-Replication, Exponential Growth, Selection and Competition in Artificial Systems , PAUL CHAIKIN, New York University — Self-replication and evolution under selective pressure are inherent phenomena in life, but few artificial systems exhibit these phenomena. We have designed a process and a system of DNA origami tiles that exponentially replicate a seed pattern, doubling the copies in each diurnal-like cycle of temperature and UV illumination, producing more than 7 million copies in 24 cycles. We use this system to demonstrate exponential selection: two similarly-growing sub-populations, one with a “red” dye incorporated, the other with a “green” dye, can be controlled by colored light. The light heats one species reducing its replication rate. The progeny of the non-absorbing species replicate preferentially and take over the system. The species selection is enhanced by competition for a resource, critical crosslinking strands required for replication. This addressable selectivity of different constituents in the same solution should be adaptable to the selection and evolution of multi-component nanoscopic-microscopic self-replicating materials. Materials that multiply exponentially and can be selected for specific properties may provide a new paradigm for design from the nanoscopic to the microscopic. Further such systems can provide insights into diverse problems ranging from the origin of life to information, computation and materials science.

1:04AM F51.00005 Self-assembly of multicomponent structures near and far from equilibrium , STEVE WHITELAM, Lawrence Berkeley National Laboratory —

Tuesday, March 3, 2015 8:00AM - 11:00AM
Session F52 DCMP: Invited Session: Tunable Topological States in Monolayer and Bilayer Graphene  
Grand Ballroom C2 - Allan MacDonald, University of Texas at Austin
8:00AM F52.00001 Direct capacitive probe of valley order in a bilayer graphene quantum Hall ferromagnet. ANDREA YOUNG, University of California, Santa Barbara — Bilayer graphene is a highly tunable quantum Hall system: both the spin and valley splitting can be manipulated independently of the electron density. Recent experiments have revealed a rich phase diagram of gapped ground states corresponding to diverse spin/valley isospin polarizations; however, all of these studies are indirect, relying on the dependence of features associated with gapped states on electric or magnetic field to infer the isospin ordering of these states. In this talk, I will describe a capacitive technique capable of directly detecting the valley component of the isospin order. By sensitively measuring the difference in capacitance between top and bottom gates of a dual-gated bilayer graphene device, we extract layer-charge response—the tendency of the layer polarization to change in response to a change in chemical potential of the entire bilayer. The asymmetric capacitance reflects the ground state layer polarization, and thus, in the zero Landau level (zLL), the valley polarization. In agreement with theoretical expectations, we find that the phase diagram of the octet zLL is, for the most part, characterized by the filling of pairs of degenerate sublevels with different orbital quantum numbers. Surprisingly, however, we also observe numerous additional states at intermediate electric fields, associated with an "odd" layer occupation. Finally, we find that phase transitions between states with different layer polarization are characterized by large anomalies in the asymmetric capacitance, which persist well into the compressible state of the Landau level.

8:36AM F52.00002 Topological phases in the zeroth Landau level of bilayer graphene. ZLATKO PAPIC, Perimeter Institute — Over the past years, a remarkable variety of novel correlated states was discovered in graphene and its bilayer in a magnetic field. These states exhibit previously unseen richness due to an interplay of electron spin, valley and orbital degrees of freedom. They are further enriched by their high degree of tunability, e.g. via the in-plane magnetic or the perpendicular electric field, which allows one to probe their properties in a more flexible and direct way than in GaAs semiconductor systems. In this talk I will present a theoretical overview of the phase diagram of the partially-filled zeroth Landau level of bilayer graphene. Using realistic large-scale numerical calculations[1] that incorporate strong mixing between orbitally degenerate sublevels, as well as the screening of the Coulomb interaction, we identify several robust quantum Hall states with odd denominators such as ν = −4/3, −5/3, −8/5. Although these states bear some relation to their more familiar analogs in GaAs, their collective excitations are expected to be different, as we illustrate on an example of the ν = −1 state that acquires a neutral gap in bilayer graphene. Furthermore, we find evidence for the existence of an incompressible, even-denominator ν = −1/2 state, and argue that this state is in the universality class of the non-Abelian Moore-Read state or its particle-hole conjugate, while other candidates such as the 331 state are unlikely to describe it. Finally, it will be shown that symmetry breaking, induced by an electric field applied perpendicular to the basal plane, is a useful experimental knob to tune the quantum phase transitions between integer or fractional states in bilayer graphene at a fixed filling factor[2]. These results illustrate the potential of bilayer graphene as a model platform to study the emergent topologically ordered phases and transitions between them via symmetry breaking.[1] Z. Papic and D. Abanin, Phys. Rev. Lett. 112, 046602 (2014). [2] Patrick Maher, Lei Wang, Yuanda Gao, Carlos Forsythe, Takashi Taniguchi, Kenji Watanabe, Dmitry Abanin, Zlatko Papic, Paul Cadden-Zimansky, James Hone, Philip Kim, and Cory R. Dean, Science 345, 61-64 (2014).

9:12AM F52.00003 Even-denominator fractional quantum Hall effect in multi-terminal suspended bilayer graphene. ALBERTO MORPURGO, University of Geneva — I will discuss magneto-transport experiments through multi-terminal suspended bilayer graphene devices of very high quality (mean-free path larger than the device size; density of charge inhomogeneity 10⁻⁷ cm⁻²). The multi-terminal geometry enables independent measurements of the longitudinal and transverse magneto resistance, which are essential to properly measure quantum Hall states. At high magnetic field, different fractional states emerge on the hole side, including states at ν = −4/3 and ν = −1/2 that are fully developed (plateau in Rₓᵧ quantized with an accuracy better than 0.5%, and a concomitant minimum in Rₘᵧ) and other states (e.g., at −5/2, −2/3, −8/5), which manifest themselves through a small change in a clear minimum in Rₓᵧ. These results are consistent with predictions of recent theory by Papic and Abanin, that describes the mixing of the degenerate, zero-energy N=0 and N=1 Landau levels of graphene bilayers due to e-e interactions, and which indicates that the even denominator ν = −1/2 state is of the Moore-Read type. If time allows, I will also discuss our recent experiments of suspended multi-terminal 4-layer graphene, on which we made different interesting observations. One is an integer quantum Hall effect consistent with an even larger degeneracy of the E=0 Landau levels, for which it may be interesting to start exploring theoretically possible new physics in the fractional regime. The second is the occurrence of an unexpected gapped insulating state at zero magnetic field. Together with previous experiments on suspended monolayer, bi, and trilayers, this observation points to an even-odd effect of e-e interaction (at zero magnetic field) in graphene multilayers: even layers are gapped by e-e interactions while odd layers stay conducting, due to the presence of a Dirac-like band in their electronic structure. A comparison of the gapped state in bilayers and four-layers show that the magnitude of the effect of e-e interaction is not becoming smaller with increasing layer thickness, suggesting that interactions remain important even in even thicker layers.

I am grateful to my collaborators, D.K. Ki, A. Grushina, D. Abanin, V. Falko, M. Koshino, E. McCann, M. Potemski, C. Fagueras, A. Nicolet.

9:48AM F52.00004 Electron-hole asymmetry in the integer and fractional quantum Hall effect in bilayer graphene. ANGELA KOU, Yale University — The nature of fractional quantum Hall (FQH) states is determined by the interplay between the Coulomb interaction and the symmetries of the system. The unique combination of spin, valley, and orbital degeneracies in bilayer graphene is predicted to produce an unusual and tunable sequence of FQH states. In this talk, I will present local electronic compressibility measurements of the lowest Landau level in bilayer graphene performed using a scanning single-electron transistor. In the integer quantum Hall regime, we find that the background compressibility between filling factors breaks particle-hole symmetry and instead obeys a ν → ν+ 2 symmetry. We also find the above-mentioned ν → ν+ 2 symmetry in the FQH regime; we observe incompressible FQH states at filling factors ν = 2p + 2/3 with hints of additional states appearing at ν = 2p+ 3/5, where p = −2, −1, 0 and 1. These observations highlight the importance of the orbital degeneracy for many-body states in bilayer graphene.

10:24AM F52.00005 Chemical potential and tunneling in bilayer graphene using double bilayer graphene heterostructures.1 EMANUEl TUTUC, The University of Texas at Austin — Vertical heterostructures consisting of atomic layers separated by insulators can open a window to explore the role of electron interaction in these materials, otherwise not accessible in single layer devices. We describe here one such heterostructure, consisting of two bilayer graphene flakes separated by a hexagonal boron-nitride dielectric. Using the top layer as a resistively detected Kelvin probe we map the chemical potential of the bottom bilayer graphene as a function of electron density, perpendicular magnetic field, and transverse electric field. At zero magnetic field the chemical potential reveals a strongly non-linear dependence on density, with an electric field induced energy gap at charge neutrality. The data allow a direct measurement of the electric field-induced bandgap at zero magnetic field, the orbital Landau level energies, and the broken symmetry quantum Hall state gaps in high magnetic fields[1]. In samples where the two layers are rotationally aligned the interlayer tunneling current measured as a function of interlayer bias reveals a gate-tunable negative differential resistance thanks to momentum conserving tunneling[2]. Remarkably, the resonance width has a weak temperature dependence in the range 1.5 K to 200 K.


1This work supported by the Office of Naval Research, the Nanoelectronics Research Initiative SWAN center, and Intel Corp.
Tuesday, March 3, 2015 8:00AM - 11:00AM —
Session F53 GMAG DCMP: Invited Session: Physics at Magnetic Interfaces, Both Engineered and Unexpected  Grand Ballroom C3 - Barry Zink, University of Denver

8:00AM F53.00001 Kondo Physics at Interfaces in Metallic Non-Local Spin Transport Devices

Chris Leighton, University of Minnesota — Despite the maturity of metallic spintronics there remain large gaps in our understanding of spin transport in metals, particularly with injection of spins across ferromagnetic/non-magnetic (FM/NM) interfaces, and their subsequent diffusion and relaxation. Unresolved issues include the limits of applicability of Elliott-Yafet spin relaxation, quantification of the influence of defects, surfaces, and interfaces on spin relaxation at nanoscopic dimensions, and the importance of magnetic and spin-orbit scattering. The non-local spin-valve is an enabling device in this context as, in addition to offering potentially disruptive applications, it allows for the separation of charge and spin currents. One particularly perplexing issue in metallic non-local spin valves is the widely observed non-monotonicity in the T-dependent spin accumulation, where the spin signal actually decreases at low T; in contrast to simple expectations. In this work, by studying an expanded range of FM/NM combinations (encompassing NiO, Fe2O3, Ni, Fe, Co, Cu, and Al), we demonstrate that this effect is not a property of a given FM or NM, but rather of the FM/NM pair. The non-monotonicity is in fact strongly correlated with the ability of the FM to form a dilute local magnetic moment in the NM. We show that local moments, resulting in this case from the ppm-level tail of the FM/NM interdiffusion profile, suppress the injected spin polarization and diffusion length via a novel manifestation of the Kondo effect, explaining all observations associated with the low T downturn in spin accumulation [1]. We further show: (a) that this effect can be promoted by thermal annealing, at which point the conventional charge transport Kondo effect is simultaneously detected in the NM, and (b) that this suppression in spin accumulation can be quenched, even at interfaces that are highly susceptible to the effect, by insertion of a thin non-moment-supporting interlayer. Important implications for room temperature devices will be discussed.

Work supported by: Seagate Technology, NSF MRSEC (DMR-0819885), Marie Curie International Outgoing Fellowship, 7th European Community Framework Programme (No. 299376). Work at SNS, ORNL, supported by DOE.


8:36AM F53.00002 Spin-orbit torques in magnetic bilayers

Paul Haney, National Institute for Standards and Technology — Spintronics aims to utilize the coupling between charge transport and magnetic dynamics to develop improved and novel memory and logic devices. Future progress in spintronics may be enabled by exploiting the spin-orbit coupling present at the interface between thin film ferromagnets and heavy metals. In these systems, applying an in-plane electrical current can induce magnetic dynamics in single domain ferromagnets, or can induce rapid motion of domain wall magnetic textures. There are multiple effects responsible for these dynamics. They include spin-orbit torques and a chiral exchange interaction (the Dzyaloshinskii-Moriya interaction) in the ferromagnet. Both effects arise from the combination of ferromagnetism and spin-orbit coupling present at the interface. There is additionally a torque from the spin current flux impinging on the ferromagnet, arising from the spin hall effect in the heavy metal. Using a combination of approaches, from drift-diffusion to Boltzmann transport to first principles methods, we explore the relative contributions to the dynamics from these different effects. We additionally propose that the transverse spin current is locally enhanced over its bulk value in the vicinity of an interface which is oriented normal to the charge current direction.

9:12AM F53.00003 Anomalous net magnetization in collinear antiferromagnets with uncompensated surfaces

Frances Hellman, UC Berkeley Physics and Materials Sciences and Engineering Departments, and Materials Sciences Division, LBNL — Like ferromagnets (FM), antiferromagnets (AFM) exhibit spontaneous long-range spin order below a transition temperature. The traditional FM order parameter is the spontaneous magnetization, while that of a simple AFM is the staggered magnetization, sometimes called the Neel vector N. The net magnetization M of a perfect AFM is (seemingly) zero at all temperatures T; however, defects such as vacancies, grain boundaries, and even surfaces create an M(T) which has a non-trivial relationship to the staggered magnetization N(T), even in ideal systems. As a specific example, we consider AFM CoO, which consists of AFM-coupled FM (111) planes; (111)-oriented epitaxial films with an odd number of planes will exhibit non-zero M due to uncompensated surfaces. These uncompensated surfaces were used to produce an artificially-structured FM semiconductor using epitaxial layers of AFM CoO with a doped semiconductor Al:ZnO (AZO). Both M(T) and the anomalous Hall effect show oscillatory behavior with thickness of either CoO (odd vs even numbers of planes) or AZO (~1 nm RKKY-like oscillations related to the AZO Fermi wavevector due to electron-induced coupling between Co moments at its two CoO surfaces). Mean field theory and Monte Carlo simulations show that M(T) of collinear AFM such as CoO with uncompensated surfaces exhibits T-dependence unlike that of N(T), of the absolute value of its individual layers, or m(T) of any single atomic plane including the uncompensated surface, due to incomplete cancellations of different planes. This phenomenon is valid even in the limit of semi-infinite systems; it is a topological state due to the presence of a free surface. Modifications of surface exchange coupling (leading to ordinary or extraordinary transitions), due to electron correlations in these Mott insulators, changes in crystal fields, spin-orbit coupling, or an incomplete (rough) surface, result in compensation points and highly non-Brillouin-like M(T).

1Work supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division

9:48AM F53.00004 Interface-induced magnetism and strong correlation in oxide heterostructures

Susanne Stember, University of California, Santa Barbara — Two-dimensional electron gases (2DEGs) at interfaces between two insulating oxides have attracted significant attention because they can exhibit unique properties, such as strong electron correlations, superconductivity and magnetism. In this presentation, we will discuss the emergent properties of 2DEGs in SrTiO3 quantum wells that are interfaced with Mott insulating rare earth titanates (RTIO3). We show that the magnetic properties of the 2DEG can be tuned to be either (incipient) ferromagnetic or (incipient) antiferromagnetic, depending on the specific RTIO3 that interfaces it. The thickness of the quantum well is a critical tuning parameter and determines the onset of magnetism, the proximity to a quantum critical point, and the onset of non-Fermi liquid behavior for those quantum wells that are in proximity to an antiferromagnetic transition. We will also discuss the role of symmetry-lowering structural transitions in the quantum well.
growth of bilayers. We detail our CVD synthesis of the monolayer TMDs (MoS\textsubscript{2}, WSe\textsubscript{2}) that are produced in quantities exceeding a million tons a year annum are a good example. In recent years, techniques honed to cater for the high-\texttau; superconductor boom have been applied to produce a range of oxide thin films and nanoparticles, which exhibit magnetic properties that are quite different to those of the bulk material. Oxide-oxide interfaces are full of surprises, especially when one of them is polar, inducing electronic reconstruction to avoid a polar catastrophe. The formation, location and magnetism of the resulting two-dimensional electron gas will be discussed. The data give lie to the common assumption of additivity of the magnetism of a thin film and its substrate. More puzzling is the elusive temperature-independent, anhysteretic magnetism of some thin films and nanoparticles, which cannot be accommodated in the current paradigm of magnetism in solids. Classical micromagnetic analysis would suggest that only a tiny fraction of the sample volume is involved (\approx 10^{-3} for thin films, \approx 10^{-6} for nanoparticles), yet there are no signs of collective magnetic order such as increasing coercivity at low temperatures or a Curie point at high temperature. The anhysteretic magnetisation curve is temperature-independent (unlike that of a superparamagnet). In CeO\textsubscript{2} nanoparticles there is a characteristic length scale of order 100 nm required for the appearance of the anomalous magnetic response. We propose that an analogy to terms of giant orbital paramagnetism due to coupling with zero-point fluctuations of the vacuum electromagnetic field, which predicts a magnetization curve of the form \textit{M} = M_{0}\left(1+x^{2}\right)^{1/2}, where \textit{x} = \textit{CB}; the constant \textit{C} corresponds to the characteristic wavelength and lengthscale, 330 nm in this case.

\textsuperscript{1}Work supported by Science Foundation Ireland.

Tuesday, March 3, 2015 11:15AM - 2:15PM
Session G1 DMP: Focus Session: Beyond Graphene - Growth I
001A - John Schaibley, University of Washington

11:15AM G1.00001 An In-Plane Epitaxial Heterostructure of Two-Dimensional Crystals. GONG GU, University of Tennessee, Knoxville — By adapting the concept of epitaxy to two-dimensional (2D) space, a single-atomic-layer, in-plane heterostructure of a prototypical material system, graphene and hexagonal boron nitride (h-BN), has been grown. It is shown by multiple complementary experimental techniques that monolayer crystalline h-BN grows from fresh edges of monolayer graphene with lattice coherence, forming an abrupt 1D interface. The challenges of obtaining truly 2D heterostructures with lattice coherence and sharp interface unassisted by templates in the third dimension will be discussed. Importantly, the h-BN lattice orientation is solely determined by the graphene, forging configurations favored by the supporting substrate, a polycrystalline Cu foil with an anisotropic (100) surface. To illustrate this important feature of heteropaxty in 2D, this talk will briefly discuss the graphene/Cu(100) and h-BN/Cu(100) orientational relations when the two materials are grown alone on Cu foils. For a counterintuitive reason, when grown alone, h-BN strictly aligns to Cu(100) exhibiting four and only four symmetrically equivalent orientations, while graphene shows a wide spread of rotations. The energetically favored h-BN/Cu(100) orientational alignment is overridden when h-BN is grown as an “epistrip” templated by a graphene edge. This talk will allude to the interesting physics of the 1D boundary states that has been theoretically predicted, such as spin polarization. As an intermediate step towards establishing the long-predicted planar magnetic properties of graphene, this work reports on the scanning tunneling microscopy and tunneling spectrum mapping, although the sought-after spin polarization is destroyed by the presence of the Cu substrate.

This work was partially supported by DARPA (approved for public release; distribution is unlimited) and NSF (ECCS-1231808). A portion of this research was conducted at the Center for Nanophase Materials Sciences (CNMS), sponsored at Oak Ridge National Laboratory through the Scientific User Facilities Division, by Office of Basic Energy Sciences, US Department of Energy (DOE), who also supported the work at Sandia under contract DE-AC04-94AL85000. Support received by contributors to the work also includes: Natural Science Foundation of China (Grants 11034006 and 11204286), National Key Basic Research Program of China (Grant 2014CB921103), and the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory. Computational resources at the National Energy Research Scientific Computing Center of the US DOE were used.

11:51AM G1.00002 Wafer-Scale Monolayer Films of Semiconducting Metal Dichalcogenides for High-Performance Electronics. SAIEN XIE, KIBUM KANG, LUIJIE HUANG, YIMO HAN, PINSHANE HUANG, KIN FAI MAK, CHEOL-JOO KIM, DAVID MULLER, JIWWONG PARK, Cornell University — Two-dimensional semiconducting transition metal dichalcogenides (TMDs) have shown their potential in electronic and photonic devices, with complete knowledge of the electronic properties, controlled synthesis of ultrathin films has enabled the demonstration of materials with limited structural and electrical uniformity, hindering further technological applications. Here we present a 4-inch scale growth of continuous monolayer molybdenum disulphide (MoS\textsubscript{2}) and tungsten disulphide (WS\textsubscript{2}) films that show excellent structural and electrical uniformity over the entire wafer using metal-organic chemical vapor deposition. The resulting monolayer films show high mobility of 30 cm\textpersecond;\textpervolt\textpercentimeter\textsuperscript{2} at room temperature, as well as the phonon-limited transport of MoS\textsubscript{2} regardless of the channel length and device location. They allow for the batch fabrication of monolayer MoS\textsubscript{2} field effect transistors with a 99% yield, which display spatially-uniform n-type transistor operation with a high on/off ratio. We further demonstrate the multi-level growth and fabrication of vertically-stacked monolayer MoS\textsubscript{2} films and devices, which could enable the development of novel three-dimensional circuitry and device integration.

12:03PM G1.00003 Synthesis and Investigation of van der Waals Heterostructures. KATHLEEN MCREARY, AUBREY HANBICKI, JAMES CULBERTSON, BEREND JONKER, Naval Research Laboratory — The recent isolation of single-nanometer MX\textsubscript{2} (M = Mo, W; X = S, Se, Te) TMDs has demonstrated that reducing dimensionality can alter the material properties. In particular, MoS\textsubscript{2}, MoSe\textsubscript{2}, WSe\textsubscript{2}, and WS\textsubscript{2} exhibit an abrupt transition from indirect to direct bandgap semiconductors at monolayer thickness. Monolayer TMDs are promising materials for electronic components due to their high mobility, high on/off ratio, and low standby power dissipation. Additionally, selective layer-by-layer stacking to form vertically-stacked monolayer MoS\textsubscript{2} films and devices, which could enable the development of novel three-dimensional circuitry and device integration.

12:15PM G1.00004 Large Area Growth and Characterization of Monolayer MoS\textsubscript{2}. PAYAM TAHERI, Physics Department, The State University of New York at Buffalo, JIEQIONG WANG, Department of Materials Science, Xin Jiaotong University, China, HUI SITNG, Physics Department, The State University of New York at Buffalo, JOEL DESTINO, Chemistry Department, The State University of New York at Buffalo, FRANK BRIGHT, Chemistry Department, The State University of New York at Buffalo, ATHOS PETROU, HAO ZENG, Physics Department, The State University of New York at Buffalo — Two-dimensional transition metal dichalcogenides have garnered extensive attention due to their direct band gap with great potential in semiconductor application complementing graphene. While most of the experiments were carried out on either exfoliated films or CVD grown crystals, sample size are restricted in hundreds of micrometers. Synthesis of large-area samples was less successful. Here, we report the growth of cm\textsuperscript{2}-scale molybdenum disulphide (MoS\textsubscript{2}) monolayer with a facile method by sulfurizing molybdenum trioxide film on sapphire substrates. Uniformity and quality of the monolayer films were verified by Raman, PL mapping and PL efficiency. A quasi- molten phase of the precursor in the initial stage of the reaction is found to be crucial for the monolayer growth.
12:27PM G1.00005 Direct growth of hexagonal boron nitride on epitaxial graphene1, PATRICK MENDE, JUN LI, RANDALL FEENSTRA, Carnegie Mellon University - Department of Physics — In this work, we demonstrate recent attempts at achieving the direct growth of hexagonal boron nitride (h-BN) on epitaxial graphene. By exposing our graphene samples (grown on Si-face SiC) to a low-pressure (~1 × 10⁻⁴ Torr) background of borazine at temperatures exceeding 1000°C, we obtain in-situ low-energy electron diffraction patterns consistent with the presence of many randomly oriented grains of h-BN. We find that increasing the growth temperature leads to the development of a preferential orientation, with the h-BN aligning with the underlying SiC substrate. Atomic-force microscopy and low-energy electron microscopy (LEEM) show triangular crystals exceeding 1 μm in extent. Additionally, using a first-principles method for examining low-energy electron reflectivity spectra, we are capable of determining the coverage of h-BN on our samples. We show that our method is sufficiently robust to discriminate between various combinations of numbers of h-BN monolayers (MLs) and graphene MLs based on unique features in their spectra. Prospects for improvement of the h-BN crystallinity, as well as the controlled growth of a specific number of MLs are discussed.

1This work was supported in part by the Center for Low Energy Systems Technology (LEAST), one of the six SRC STARnet Centers, sponsored by MARCO and DARPA.

12:39PM G1.00006 Chemically controlled dislocation migration in two-dimensional MoS₂, XIAOLONG ZOU, MINGJIE LIU, BORIS YAKOBSON, Department of Materials Science and NanoEngineering, Dept. of Chemistry, and Smalley Institute for Nanoscale Science and Technology, Rice University — As an additional Gibbs degree of freedom, chemical potential plays an important role in determining various properties of hetero-elemental two-dimensional (2D) materials, ranging from the equilibrium shape [1], to defect structures [2,3], electronic [3], and magnetic properties [4]. Here, by first-principles calculations, we demonstrate how the chemical potential control can be adopted as a feasible strategy to tune the dislocation dynamics in 2D MoS₂. Depending on the structures of the migrating dislocations, two different dynamic mechanisms are revealed, either through the direct bond-rebinding (BR) mechanism, where only single metal atom moves significantly, or concerted migration (CM), in which case several atoms rearrange concurrently. The migration barriers for CM mechanism could be 2 to 4 times larger as the BR ones. Our detailed analyses show that under certain range of chemical potential some dislocations with high mobility could nevertheless also have quite high stability, which opens up the possibility of enhanced plasticity and suggests intriguing future applications.


12:51PM G1.00007 Growth, transfer, structural, optical, and electrical properties of large-size transition-metal dichalcogenide monolayer single-crystals1, ZHENG YANG, BO HSU, JIAO XIAO, GEORGE POULOS, Univ of Illinois - Chicago, YANG RESEARCH GROUP TEAM — We report growth, transfer process, as well as structural, optical, and electrical properties of large-size and high-quality two-dimensional transition-metal dichalcogenide MX₂ (M=Mo, W; X=S, Se) single-crystalline triangular-shape nanosheets composed of one to a few monolayers. A vapor-trapping enhanced chemical vapor deposition approach was employed for the MX₂ monolayer single crystal growth. The number of layers, crystallinity, and uniformity of the as-grown MX₂ were characterized and confirmed by Raman and photoluminescence measurements. The MX₂ monolayer single-crystal triangles show comparable size and uniformity to the state-of-the-art results reported as of now. The optical properties of the MX₂ were studied based on the analysis of the photoluminescence results. The electrical properties including resistivity, mobility, carrier type and concentration, and contact resistance of the MX₂ were characterized by both three-terminal field-effect transistor and Hall effect transport measurements. The Hall bar devices were fabricated by lithography and dry-etching of the as-grown single-crystalline MX₂. The transfer process of the MX₂ from growth substrate (SiO₂-on-Si) to various substrates was successfully demonstrated.

1Acknowledgement to the funding support from Ignite Award.

1:03PM G1.00008 Vacancy-induced growth of inversion domains in transition-metal dichalcogenide monolayer: an atomic view of defect dynamics, JUNHAO LIN, Vanderbilt University/ORNL, WU ZHOU, ORNL, SOKRATES PANTELIDES, Vanderbilt University — In this work, we systematically study the nucleation and growth of inversion domains within a monolayer MoSe₂. We use a focused electron beam to generate and excite Se vacancies in the monolayer, and monitor their dynamics through sequential atomic-scale Z-contrast imaging. We find that Se vacancies are first randomly created and then preferentially agglomerate into line defects under the energy transferred from the electron beam. Successive evolution of these line defects induces nucleation of distinct triangular inversion domains within the MoSe₂ layer and generates conductive 60⁰ grain boundaries within the semiconducting matrix. Density functional theory shows that the nucleation of inversion domain lowers the system energy due to the release of vacancy-induced lattice shrinkage. Migration of the grain boundaries can be further activated by deformation of the peripheral lattice, giving rise to the growth of the inversion domain. The grain nucleation and growth process observed under energy transferred from the electron beam can provide new insights into the structural stability of TMDC monolayers under severe (e.g. high temperature) working conditions.

1:15PM G1.00009 Development of Novel Two-dimensional Layers, Alloys and Heterostructures, ZHENG LIU, School of Materials Science & Engineering, Nanyang Technological University, Singapore — The one-atom-think graphene has fantastic properties and attracted tremendous interests in these years, which opens a window towards various two-dimensional (2D) atomic layers. However, making large-size and high-quality 2D layers is still a great challenge. Using chemical vapor deposition (CVD) method, we have successfully synthesized a wide varieties of binary 2D materials. Ternary 2D alloys including BCN and MoS₂-Se₂(1−x) are also prepared and characterized. In addition, synthesis of 2D heterostructures such as vertical and lateral graphene/h-BN, vertical and lateral TMDs are also demonstrated. Complementary to CVD grown 2D layers, 2D single-crystal (bulk) such as Phosphorene (P), WTe₂, SnSe₂, PtS₂, PtSe₂, PdSe₂, WSe₂Te₂(1−x), Ta₃N₅Se, and T₄₄N₄Se₄ are also prepared by solid reactions. There work provide a better understanding of the atomic layered materials in terms of the synthesis, atomic structure, alloying and their physical properties. Potential applications of these 2D layers e.g. optoelectronic devices, energy device and smart coating have been explored.
1:27PM G1.00010 The kinetics of white graphene (h-BN) growth on the planarized Ni foil surfaces1, MYUNG JONG KIM, HYUNJIN CHO, SUNGCHAN PARK, KIST, DONG-IL WON, SANG OOK KANG, Korea University, SEONG-SOO PYO, DO-CHAN KIM, SOO-MIN KIM, KIST, HWAN CHUL KIM, Chonbuk National University, KIST COLLABORATION, KOREA UNIVERSITY COLLABORATION, CHONBUK NATIONAL UNIVERSITY COLLABORATION — Morphology of the surface and the grain orientation of the metal catalysts have been considered as two important factors for the growth of h-BN by a CVD method. We report correlation between growth rate of h-BN and orientation of nickel grains. The surface of the nickel foil was first planarized by electrochemical polishing and subsequently annealed in atmospheric pressure hydrogen to suppress the effect from the surface morphology. The atmospheric annealing with hydrogen reduced nucleation site of h-BN such that large crystal size mainly has grown from the grain boundary and has no nucleation sites in the nickel foil. Higher growth rate of h-BN was observed from the nickel grains that has (110) or (100) orientation due to higher surface energy.

1This work was supported by grants from the Korea Institute of Science and Technology (KIST) Institutional Program and the Converging Re-search Center Program funded by the Ministry of Science, ICT & Future Planning Technology (2014M3C1A8054009).

1:39PM G1.00011 Nanoscale topographical replication of graphene architecture by manufactured DNA nanostructures, YOUNGKWON MOON, Department of Physics, Sungkyunkwan University, JIHOON SHIN, Sungkyunkwan Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University, SOONBEOM SEO, Department of Physics, Sungkyunkwan University, SUNG HA PARK, Department of Physics, Sungkyunkwan Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University, JOUNG REAL AHN, Department of Physics, Sungkyunkwan University — Despite many studies on how geometry can be used to control the electronic properties of graphene, certain limitations to fabrication of designed graphene nanostructures exist. Here, we demonstrate controlled topographical replication of graphene by artificial deoxyribonucleic acid (DNA) nanostructures. Owing to the high degree of geometrical freedom of DNA nanostructures, we controlled the nanoscale topology of graphene. The topography of graphene replicated from DNA nanostructures showed enhanced thermal stability and revealed an interesting negative temperature coefficient of sheet resistivity when underlying DNA nanostructures were denatured at high temperatures.

1:51PM G1.00012 Seeded Growth of Highly Crystalline Molybdenum Disulphide Monolayers at Controlled Locations, CARL NAYLOR, GANGHEE HAN, NICHOLAS KLYBERT, JINGLIE PING, A.T. CHARLIE JOHNSON, Univ of Pennsylvania — Various approaches have been demonstrated for growth on insulating substrates of molybdenum disulphide (MoS₂), but to date growth of isolated crystalline flakes has been only at random locations. We have developed a method to obtain MoS₂ flakes in precisely defined locations. By patterning molybdenum source material that acted both as material feedstock and growth seed at predetermined areas across a wafer, we were able to grow isolated flakes of MoS₂ at these locations with micrometre-scale resolution. These MoS₂ flakes are predominantly of monolayer thickness and high material quality, as confirmed by atomic force microscopy, transmission electron microscopy, Raman and photoluminescence spectroscopy. Since the monolayer flakes are isolated and in predetermined locations, fabrication of transistor structures requires only a single lithographic step. Thus we are able to obtain multiple arrays of MoS₂ transistors, that are highly crystalline and monolayer, making this method ideal for large scale production. Device measurements showed a carrier mobility and on/off ratio that exceeded 10 cm²/V·s and 10⁶, respectively. This growth technique provides a path for in-depth physical analysis of monolayer MoS₂ as well as fabrication of MoS₂-based integrated circuits.

2:03PM G1.00013 Wafer-scale arrayed p-n junctions based on few-layer epitaxial GaTe, XIANG YUAN, LEI TANG, State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai 200433, China, WEIDAHU, National Laboratory for Infrared Physics, Shanghai Institute of Technical Physics, Chinese Academy of Sciences, Shanghai 200033, China, FAXIAN XIU, State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai 200433, China — Two dimensional (2D) materials have showed appealing applications in electronics and optoelectronics. Gapless graphene presents ultra-broadband and fast photosponse while the 2D semiconducting MoS₂ and GaTe exhibit highly sensitive and tunable responsivity to the visible light. However, the device yield and its repeatability call for a further improvement of 2D materials to render large-scale uniformity. Here we report 2D material growth of the wafer-scale GaTe by molecular beam epitaxy. To develop the arrayed p-n junctions, the few-layer GaTe was grew on three-inch Si wafers. The resultant diodes reveal good rectifying characteristics and photoresponse with maximum photodetection responsivity of 2.74 A/W and photovoltaic external quantum efficiency up to 62%. The photocurrent reaches saturation very fast within 22 μs and shows no sign of device degradation after 1.37 million cycles of operation. Most strikingly, such high performance has been achieved across the entire wafer, making the volume production of devices accessible. Finally, several photo-images was acquired by using these photodiodes with a reasonable contrast and resolution, demonstrating for the first time the potential for these 2D technology coming into the real life.


11:15AM G2.00001 k·p theory for two-dimensional transition metal dichalcogenide semiconductors, ANDOR KORMANYOS, GUIDO BURKARD, University of Konstanz — We present k·p Hamiltonians (for a review see [1]) parametrised by ab initio density functional theory calculations to describe the dispersion of the valence and conduction bands at their extrema (the K, Q, Γ, and M points of the hexagonal Brillouin zone) in atomic crystals of semiconducting monolayer transition metal dichalcogenides. We review the parametrisation of the essential parts of the k·p Hamiltonians for MoS₂, MoSe₂, WS₂, and WSe₂, including the spin-splitting and spin-polarisation of the bands We use k·p theory to analyse: i) optical transitions in two-dimensional transition metal dichalcogenides over a broad spectral range; ii) to discuss magnetotransport properties of the charge carriers in the K and −K valleys.


11:27AM G2.00002 Magneto-optics in WSe₂ and MoSe₂ monolayers1, BERNHARD URBASZEK, GANG WANG, LOUIS BOUET, ETIENNE PALLEAU, MAEL VIDAL, XAVIER MARIE, THIERRY AMAND, Toulouse University - CNRS — We perform photoluminescence (PL) experiments at T=4K on MoSe₂ and WSe₂ in magnetic fields up to 9T applied perpendicular to the monolayer (ML) plane. In both systems the neutral exciton is spectroscopically well separated from the charged exciton (trion). For both exciton complexes in both systems we observe a clear Zeeman splitting of the order of -2meV at 9T between the σ⁺ and σ⁻ polarized PL components, from the K⁺ and K⁻ valley, respectively. The extracted g-factors for both exciton complexes in both materials are of the order of g ≈ -4. This indicates a dominant contribution from the transition metal valence band d-orbitals to the exciton magnetic moment, contributions from the valley magnetic moments are discussed. In ML MoSe₂ the exciton valley polarization can be tuned with the magnetic field, independent of the excitation laser polarization. In the investigated ML WSe₂ sample the evolution of the valley polarization depends for the trion both on the applied magnetic field and the excitation laser helicity, for the neutral exciton only on the latter. In the absence of optical orientation, the trion polarization amplitude increases linearly with the applied magnetic field, albeit with opposite signs in MoSe₂ compared to WSe₂.

1We acknowledge partial funding from ERC Grant No. 306719.
11:39 AM G2.00003 Experimental evidence for dark excitons in monolayer transition metal dichalcogenide crystals, XIAOXIAO ZHANG, YUMENG YOU, Columbia University, FRANK ZHAO, Harvard University, TONY HEINZ, Columbia University — Transition metal dichalcogenides in the family of MoS$_2$, WSe$_2$, and WTe$_2$ have been identified as direct-gap semiconductors in the limit of monolayer thickness. In addition to the optically bright states associated with dipole-allowed excitonic transitions between these bands, it is predicted that excitonic states will form that are optically dark either because of momentum or spin selection rules. In this paper, we report studies of the temperature dependence of the bright exciton population using photoluminescence and time-resolved photoluminescence spectroscopy. The experimental results indicate the presence of dark states lying below the optically bright states in some members of this family of materials. These states, unlike the usual bright states, are not constrained by rapid radiative decay and offer new avenues for control of the valley and spin degrees of freedom.

11:51 AM G2.00004 Probing the valley Hall effect in MoS$_2$ transistors, KIN FAI MAK, Penn State University — Two-dimensional (2D) atomic layers of molybdenum disulfide (MoS$_2$) possess a new valley degree of freedom (DOF) that has finite Berry curvatures. As a result, not only optical control of the valley DOF is allowed, but each valley is also predicted to exhibit an anomalous Hall effect whose sign depends on the valley index. In this talk, we will discuss our recent observation of this new valley Hall effect (VHE) in monolayer MoS$_2$ transistors. This is manifested experimentally as a finite anomalous Hall effect when circularly polarized light is used to preferentially excite electrons into a specific valley. We will describe the dependence of the anomalous Hall conductivity on photon helicity, photon energy, doping levels and crystal symmetry, and will compare these observations with theoretical predictions. Possibilities of using the valley DOF as an information carrier in next-generation electronics and optoelectronics will also be discussed.

12:27 PM G2.00005 Magneto-optical Kerr effect in Transition Metal Dichalcogenides, RYUJI SUZUKI, Department of Applied Physics and Quantum Phase Electronics Center (QPEC), University of Tokyo, SANDOR BORDACS, Budapest university of technology and economics, YOSHINORI TOKURA, YOSHIIRO IWASA, RIKEN CENTER for Emergent Matter Science (CEMS); Department of Applied Physics and Quantum Phase Electronics Center (QPEC), University of Tokyo — Transition-metal dichalcogenides (TMDs) are attracting a great deal of interest beyond graphene materials because of their rich physical properties. The key of the monolayer TMDs in contrast to the bulk is the broken inversion symmetry, which results in novel valley properties, coupled with spins through their strong spin-orbit interaction. On the other hand, 3R-MoS$_2$ is known to keep the broken inversion symmetry and thus strong valley polarization in PL spectra even in multilayers, providing opportunities to investigate properties of monolayers with use of bulk materials and the stacking dependent properties between the 2H (centrosymmetric) and 3R-non-centrosymmetric) [R. Suzuki et al., Nat. Nano. 9, 611 (2014)]. In this presentation, we report comparative studies of 3R MoS$_2$ and 2H series of TMDs on magnetooptical properties, with a particular focus on magneto-optical Kerr effect (MOKE) spectroscopy. We found systematic evolution of MOKE spectra in the 2H series of TMDs, and more interestingly, that 3R polytypes displayed significant difference not only in exciton dimensionality and but also in the $g$ values estimated from the excitons peak splitting in the MOKE spectra. Discussion will be given based on the electronic structures and the spin-orbit interactions.

12:39 PM G2.00006 Valley entanglement of carriers in monolayers of transition-metal dichalcogenides, ALEXEY BELYANIN, Texas A&M University, MIKHAIL TOKMAN, Institute of Applied Physics, Russian Academy of Sciences — The entanglement of two quantum systems or ensembles is usually considered as a result of coupling between them. This coupling can be mediated by classical electromagnetic fields. At the same time, one can also entangle non-interacting quantum systems by a quantum field. Here we consider the optical excitation of electron-hole or exciton states near the band gap of a transition-metal dichalcogenide monolayer in two valleys K and K' with opposite valley indices. We show that a linearly polarized single-photon field in a cavity or a stationary stream of linearly polarized single photons gives rise to an efficient entanglement of non-interacting carriers in different valleys, i.e. the generation of electron states entangled with respect to the valley degree of freedom. An intuitive explanation of this effect is that the carriers "view" linearly polarized photons as entangled left- and right-circularly polarized photon states. Valley entanglement of carriers gives rise to peculiar properties of the reemitted optical field and photocurrent fluctuations.

12:51 PM G2.00007 Electrical Valley Excitation by Spin Injection in Monolayer Transition Metal Dichalcogenide Heterojunction, YU YE, XIAOBO YIN, University of California, Berkeley, HAILONG WANG, Institute of Semiconductors, Chinese Academy of Sciences, ZILIANG YE, HANYU ZHU, YUAN WANG, University of California, Berkeley, JIANHUA ZHAO, Institute of Semiconductors, Chinese Academy of Sciences, XIZANG ZHANG, University of California, Berkeley — Embracing the spin degree of freedom of charge carriers enables nonvolatile electronic with increased operation speed and reduced power consumption. Recently discovered atomic materials of monolayer transition metal dichalcogenides (TMDs) possess unbalanced carrier distribution in the momentum space and introduce a new independent valley of freedom. Here we demonstrate experimentally the unique spin and valley locking relationship in TMDs and report a new scheme of electronic devices taking advantages of both degrees of freedoms. A valley-polarized light-emitting device is achieved experimentally through spin injection using (Ga, Mn)As as a spin aligner. The electrical generation and the control of valley polarization in TMD semiconductors through spin manipulation opens the new dimension in utilizing both spin and valley degrees of freedom for next-generation electronics and computing.

1:03 PM G2.00008 Interplay of spin, valley and layer pseudospins in folded MoS$_2$ bilayers, TAO JIANG, HENGUI LIU, DI HUANG, SHUAI ZHANG, YINGGUO LI, XINGAO GONG, Fudan University, YUEN-RON SHEN, Fudan University and University of California at Berkeley, WEI-TAO LIU, SHIWEI WU, Fudan University — Two dimensional material such as graphene and transition metal dichalcogenide is beyond graphene materials because of their rich physical properties. The key of the monolayer TMDs in contrast to the bulk is the broken inversion symmetry, which results in novel valley properties, coupled with spins through their strong spin-orbit interaction. Different from sheet paper, each of two dimensional materials has its own crystal lattice. In two-dimensional materials one can also entangle non-interacting quantum systems by a quantum field. Here we consider the optical excitation of electron-hole or exciton states near the band gap of a transition-metal dichalcogenide monolayer in two valleys K and K' with opposite valley indices. In this talk, we will present our recent study of folded MoS$_2$ bilayers, which were obtained by folding exfoliated MoS$_2$ monolayers. As characterized by second harmonic generation and photoluminescence, folded bilayers can exhibit broken inversion symmetry and reduced interlayer coupling, evoking strong valley and/or spin polarization that results in valley-mixed states. We show that a linearly polarized single photon field in a cavity or a stationary stream of linearly polarized single photons gives rise to an efficient entanglement of non-interacting carriers in different valleys, i.e. the generation of electron states entangled with respect to the valley degree of freedom. An intuitive explanation of this effect is that the carriers "view" linearly polarized photons as entangled left- and right-circularly polarized photon states. Valley entanglement of carriers gives rise to peculiar properties of the reemitted optical field and photocurrent fluctuations.

1:15 PM G2.00009 Hofstadter spectrum in MoS$_2$, YEN-HUNG HO, Physics, National Tsing Hua University, Taiwan, WU-PEI SU, Physics and Texas Center for Superconductivity, University of Houston, TX, MING-FA LIN, Physics, National Cheng Kung University, Taiwan — In studying the Hofstadter problem of monolayer molybdenum disulfide (MoS$_2$), we systematically demonstrate the magnetic energy spectra due to various hoppings between $d$-orbital electrons. The magnetoelectronic spectrum shows a mirror symmetry as a result of the particle-hole symmetry in the Bloch bands. At small field, specific Landau fan diagrams can be ascribed to certain Bloch-band singularities. In the spectrum of real MoS$_2$, we further illustrate a breaking of spectral symmetry, the spin and valley polarization, and a flux-dependent energy gap. Our numerical results can facilitate the qualitative understanding of topological nature of $d$-bands and provide a basis for exploring the Landau levels in transition-metal dichalcogenides.

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1: Yen-Hung HO, Physics, National Tsing Hua University, Taiwan, WU-PEI SU, Physics and Texas Center for Superconductivity, University of Houston, TX, MING-FA LIN, Physics, National Cheng Kung University, Taiwan — In studying the Hofstadter problem of monolayer molybdenum disulfide (MoS$_2$), we systematically demonstrate the magnetic energy spectra due to various hoppings between $d$-orbital electrons. The magnetoelectronic spectrum shows a mirror symmetry as a result of the particle-hole symmetry in the Bloch bands. At small field, specific Landau fan diagrams can be ascribed to certain Bloch-band singularities. In the spectrum of real MoS$_2$, we further illustrate a breaking of spectral symmetry, the spin and valley polarization, and a flux-dependent energy gap. Our numerical results can facilitate the qualitative understanding of topological nature of $d$-bands and provide a basis for exploring the Landau levels in transition-metal dichalcogenides.

2: Robert A. Welch Foundation (E-1070); National Science Council of Taiwan (NSC 101-2112-M-003-005-MY3); NTHU Start-Up Grant (103H1114)
Spatially-resolved measurements of these Hall effects have recently been achieved in monolayer MoS$_2$. In monolayers of transition metal dichalcogenides (1L-TMDs), a valley degree of freedom emerges for charge carriers due to the absence of spatial inversion symmetry. Strong spin-orbit interaction couples spin and valley, resulting in correlated spin, valley, and charge transport such as transverse Hall effects. Spatially-resolved measurements of these Hall effects have recently been achieved in monolayer MoS$_2$ necessitating a detailed picture for understanding transport and relaxation mechanisms in 1L-TMDs that considers carrier, valley, and spin motion and generation processes. Here, we study spin and valley Hall effects in 1L-TMD devices by simulating the transport of spin- and valley-polarized carriers with a generalized drift diffusion model incorporating circularly polarized optical excitation. Spin and valley accumulation and the transverse voltage are analyzed in different device geometries. We compare the electron and hole contributions to the transverse voltage and discuss the potential for a measurement of the valley relaxation times of free carriers in 1L-TMDs.

1 This work was supported by the Institute for Sustainability and Energy at Northwestern and the U.S. Department of Energy (DE-SC0012130). N.P.S. acknowledges support as an Alfred P. Sloan Research Fellow.


Valley selective optical Stark effect in monolayer WS$_2$. EDBERT J. SIE, JAMES W. MCIVER, MIT, YI-HSIEN LEE, NTHU Taiwan, LIANG FU, JING KONG, NUH GEDIK, MIT — Monolayer semiconductors, such as WS$_2$, have a pair of valleys that, by time-reversal symmetry, are energetically degenerate. Lifting the valley degeneracy in these materials is of great interest because it would allow for valley specific band engineering and offer additional control in valleytronic applications. Here we show that circularly polarized light, which breaks time-reversal symmetry, can be used to lift the valley degeneracy by means of the optical Stark effect. We demonstrate that this effect is capable of raising the exciton level in monolayer WS$_2$ by as much as 18 meV in a controllable valley selective manner. The resulting energy shift is extremely large, comparable to the shift that would be obtained using a very high magnetic field (200 Tesla). These results offer a novel way to control valley degree of freedom, and may provide a means to realize new valley-selective Floquet topological state of matter.

Valley-Exciton Locked Optical Selection Rule in Monolayer WS$_2$. JUN XIAO, ZILIANG YE, YING WANG, YUAN WANG, XIANG ZHANG, UC Berkeley — Layered transition metal dichalcogenide (TMDC) with hexagonal lattice structure has six valleys at corners of the Brillouin zone. The nontrivial Berry curvature distribution renders the adjacent valleys with distinguishable valley angular momentum. Recent studies reported strong excitonic effect in monolayer WS$_2$ and each excitonic state is identified with a well-defined orbital angular momentum, however the anticipated selection rules involve nonlinear optical processes are not clear. Here we show valley angular momentum (VAM) together with exciton angular momentum (EAM) impose different valley-exciton locked selection rules for second harmonic generation (SHG) and two photon luminescence (TPL) in monolayer WS$_2$. Moreover, the two-photon induced valley populations yield net circular polarized photoluminescence after a sub-ps interexciton relaxation. The work demonstrates a new approach to control valley population at different excitonic states for next generation of optical circuits and quantum information computing.

Trion dynamics in Transition Metal Dichalcogenide Monolayers. AKSHAY SINGH, KHA TRAN, Uni of Texas, Austin, SANWENG WU, JASON ROSS, University of Washington, GALAN MOODY, National Institute of Standards and Technology, XIAODONG XU, University of Washington, ELAINE LI, Univ of Texas, Austin — Transition Metal Dichalcogenides (TMD’s) in the monolayer limit, exhibit interesting phenomena including increased photoluminescence, spin-valley coupling and many-body effects. Excitons (bound electron-hole pairs) and trions (charged excitons) in these materials have unusually large binding energy and dominate the optical response near the band gap. In particular, trions can drift under application of an electric field and have higher spin lifetimes increasing applications in quantum spin models. We study the temporal dynamics of excitons and trions including their formation and lifetimes using time resolved two-color pump-probe spectroscopy on a monolayer TMD (MoSe$_2$). Trions are observed to have vastly different temporal dynamics with much slower decay than excitons. We also observe rapid formation of trions when resonantly pumped while a slow rise (in temporal response) is seen for other excitation energies. We suggest that localization of trions needs to be taken into account to explain these observations.

Tuesday, March 3, 2015 11:15AM - 2:15PM –
Session G3 FEd: Invited Session: NSF-Funded Physics Education: Celebrating Accomplishments and Looking Forward

11:15AM G3.00001 NSF Support for Physics at the Undergraduate Level: A View from Inside. DUNCAN MCBRIDE, National Science Foundation (Retired) — NSF has supported a wide range of projects in physics that involve undergraduate students. These projects include NSF research grants in which undergraduates participate: Research Experiences for Undergraduates (REU) centers and supplements; and education grants that range from upper-division labs that may include research, to curriculum development for upper- and lower-level courses and labs, to courses for non-majors, to Physics Education Research (PER). The NSF Divisions of Physics, Materials Research, and Astronomy provide most of the disciplinary research support, with some from other parts of NSF. I recently retired as the permanent physicist in NSF’s Division of Undergraduate Education (DUE), which supports the education grants. I was responsible for a majority of DUE’s physics grants and was involved with others overseen by a series of physics rotators. There I worked in programs entitled Instrumentation and Laboratory Improvement (IIL); Course and Curriculum Development (CCD); Course, Curriculum, and Laboratory Improvement (CCLI); Transforming Undergraduate STEM Education (TUES); and Improving Undergraduate STEM Education (IUSE). NSF support has enabled physics Principal Investigators to change and improve substantially the way physics is taught and the way students learn physics. The most important changes are increased undergraduate participation in physics research; more teaching using interactive engagement methods in classes; and growth of PER as a legitimate field of physics research as well as outcomes from PER that guide physics teaching. In turn these have led, along with other factors, to students who are better-prepared for graduate school and work, and to increases in the number of undergraduate physics majors. In addition, students in disciplines that physics directly supports, notably engineering and chemistry, and increasingly biology, are better and more broadly prepared to use their physics education in these fields. I will describe NSF support for undergraduate physics with both statistics and examples. In addition I will talk about trends in support for undergraduate physics at NSF and speculate about directions such support might go.

1 Contents of this paper reflect the opinions of the author and do not necessarily reflect those of the National Science Foundation.
11:51 AM G3.00002 The Impact of NSF-funded Physics Education Research at the University of Washington, PAULA HERON, University of Washington — It is now well known that many students who complete introductory physics courses are unable to apply fundamental concepts in situations that involve qualitative reasoning. Systematic investigations have helped researchers understand why so many students fail to develop robust and coherent conceptual frameworks, and have led to the development of new teaching practices and materials that are far more effective than conventional ones. The Physics Education Group at the University of Washington has played a leading role in raising awareness of the need to improve instruction, and in supporting physics faculty in their efforts to do so. With support from the National Science Foundation, the group has helped build a research base that instructors can draw on, and has produced practical, flexible instructional materials that promote deeper learning in physics classrooms. Both “Tutorials in Introductory Physics” (Pearson, 2002) and “Physics by Inquiry” (Wiley, 1996) have been developed in an iterative process in which ongoing assessment of student learning plays an integral role. These materials have had a widespread and significant impact on physics teaching and on student learning from kindergarten through graduate school. In this talk I will describe the role of research in curriculum development, and speculate on the next generation of tools and resources to support physics teaching and learning.

12:27 PM G3.00003 The Maryland PERG: Two decades of learning how students learn1, EDWARD REDISH, University of Maryland — Over the past twenty years, the University of Maryland’s Physics Education Research Group (UMd-PERG) has carried out educational research and development using a variety of NSF funding opportunities, building from basic research in cognitive modeling, to instructional materials development, to basic research on professional development. The group has drawn on opportunities in teacher training, K-12 teaching and learning, and university level research and development. In this talk I will recap some of the key lessons we have learned and how it all fits together.

1 This work has been supported by many grants from the NSF over a 20 year period.

1:03 PM G3.00004 An NSF rotator’s perspective: view from inside the hamster wheel, GARY WHITE, AAPT and The George Washington University — Duncan McBride served as my unofficial mentor during my time at NSF as a “rotator” (or, in NSF-speak, an IPA, short for an Intergovernmental Personnel Act assignee), from fall 2012 through summer of 2013. A rotator’s main job is to help keep the wheels of the grant submission process turning, shepherding individual proposal jackets through the submission cycle. While most proposals are eventually “Declined” it is the few that are funded that evoke the most vivid memories of my time there. I hope to relay a little bit about what that was like on a daily basis, to give one hamster’s take on the machinations of the NSF machine, and testify to Duncan McBride’s critical role in establishing physics as the leader in disciplinary based educational research (DBER). It was a heady experience in many ways, despite the sheer girth of proposal jackets to be processed and the uncertain footing upon which federal employees tread these days.

1:39 PM G3.00005 The SCALE-UP Project1, ROBERT BEICHNER, North Carolina State University — The Student Centered Active Learning Environment with Upside-down Pedagogies (SCALE-UP) project was developed nearly 20 years ago as an economical way to provide collaborative, interactive instruction even for large enrollment classes. Nearly all research-based pedagogies have been designed with fairly high faculty-student ratios. The economics of introductory courses at large universities often precludes that situation, so SCALE-UP was created as a way to facilitate highly collaborative active learning with large numbers of students served by only a few faculty and assistants. It enables those students to learn and succeed not only in acquiring content, but also to practice important 21st century skills like problem solving, communication, and teamwork. The approach was initially targeted at undergraduate science and engineering students taking introductory physics courses in large enrollment sections. It has since expanded to multiple content areas, including chemistry, math, engineering, biology, business, nursing, and even the humanities. Class sizes range from 24 to over 600. Data collected from multiple sites around the world indicates highly successful implementation at more than 250 institutions. NSF support was critical for initial development and dissemination efforts.

1 Generously supported by NSF (9752313, 9981107) and FIPSE (P116B971905, P116B000659.)

Tuesday, March 3, 2015 11:15AM - 2:15PM –
Session G4 FGSA: Invited Session: Physics Beyond the Lab: Science and Communication Mayor Cockrell Room 004 - Valerie Gray, College of William and Mary

11:15 AM G4.00001 Communicating Science in the Capitol: The Graduate Student Voice, TYLER GLEMBO, APS — Fundamental scientific research, as a majority federally funded initiative, is becoming more deeply embedded in politics. Since the end of the Space Race, funding of basic physical sciences research as a percent GDP has continuously declined, indicating that policy makers see funding scientific research as less of a priority than they once did. A lack of understanding about both science and how science is done amongst members of Congress has led to both reduced prioritization and also to misguided attempts at regulation, such as making peer review a public process and considering Congressional oversight for specific grants. Here we will examine a few current issues in science policy, the effect on graduate students, and why the student voice is effective. We will also consider the positive or negative effects such public engagement may have on our scientific careers and ways in which you can get involved.


12:27 PM G4.00003 Science publishing: A day in the life of an APS editor, KATHERINE THOMAS, Physical Review Letters, American Physical Society — I will share my experience in working as an editor for a scholarly journal. The talk will include information on my career path, the skills and qualifications needed, and give insight into my day-to-day activities.

1:03 PM G4.00004 Panel Discussion –
Tuesday, March 3, 2015 11:15AM - 2:15PM –
Session G5 FIAP: Integer Quantum Hall Effects Juan Gorman Room 005 - Ramesh Mani, Georgia State University
11:15AM G5.00001 Mach-Zehnder interferometry with periodic voltage pulses¹. PATRICK HOFER, CHRISTIAN FLINDT, University of Geneva — We investigate theoretically a Mach-Zehnder interferometer driven by periodic voltage pulses. We illustrate how the electronic energy distribution of the driven contact influences the visibilities of the Aharonov-Bohm oscillations in the current and in the noise. For the current, the visibility factors in analogy to the static case and we find a universality at path-length differences equal to multiples of the spacing between the voltage pulses. In the noise oscillations, we find additional features which are characteristic to time-dependent transport. Finite electronic temperatures are found to have a qualitatively different influence on the current and the noise.

¹The work was funded by the Swiss NSF

11:27AM G5.00002 Evolution of the linear-polarization-angle-dependence of the radiation-induced magnetoresistance-oscillations with the microwave power². TIANYU YE, RAMESH MANI, Department of physics and Astronomy, Georgia State University, Atlanta, GA 30303, USA, WERNER WEGSCHREIDER, Laboratorium fur Festkorporphysik, ETH Zurich, 8093 Zurich, Switzerland — Microwave radiation-induced magnetoresistance oscillations (MRIMRO) are huge photo-excited oscillations in the resistance in a transverse magnetic field, which are sensitive to different aspects of the microwave radiation such as the microwave frequency, microwave power, and linear polarization angle. As a consequence, MRIMROs are potentially interesting for sensing applications. In order to better understand the role of the microwave power and the linear polarization angle in MRIMROs, the role of these variables have been more carefully examined in this experimental study. Thus, the diagonal resistance $R_{xx}$ was measured as a function of both the microwave power ($P$) and the linear polarization angle ($\theta$) at the MRIMRO extrema. Color contour plots reveal that $R_{xx}$ vs $\theta$ follows a cosine square function at relatively low microwave power with systematic lineshape distortions occurring with increasing microwave power. Here, we demonstrate that the non-linearity of $R_{xx}$ vs $P$ relation is the main factor that influences the lineshape distortion from the sinusoidal $R_{xx}$ vs $\theta$ relation observed at low $P$.

²Magnetotransport measurements by Ye at GSU were supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Material Sciences and Engineering Division under DE-SC0001762. Additional support was provided by the ARO under W911NF-07-01-015.

11:39AM G5.00003 Tunneling spectroscopic evidence of quasiparticle crystallization near $v = 1$ quantum Hall ferromagnet. JOONHO JANG, BENJAMIN HUNT, RAYMOND ASHOORI, Massachusetts Inst of Tech-MIT, LOREN PFEIFFER, KEN WEST, Princeton University — We have used Time Domain Capacitance Spectroscopy to measure the density of states of 2 dimensional holes in Carbon doped GaAs at temperature of 20 mK and high magnetic fields. Filling factor dependent anomalous features, which is antisymmetric in energy and density, were observed around the quantum Hall ferromagnet $v = 1$. The analysis of the quasiparticle dynamics around $v = 1$ is consistent with the picture that holes are dressed by interactions with bosonic degrees of freedom. We attribute this bosonic mode to the gapless Goldstone mode emergent due to the development of crystalline order of charged quasiparticles.

11:51AM G5.00004 Dynamics of Quantal Heating in Electron Systems with Discrete Spectra. WILLIAM MAYER, SCOTT DIETRICH, SERGEY VITKALOV, Physics Department, City College of the City University of New York, New York 10031, USA, ALEXEY BYKOV, Novosibirsk State University, Novosibirsk 630090, Russia; A.V.Rzhanov Institute of Semiconductor Physics, Novosibirsk 630090, Russia — The temporal evolution of quantal Joule heating of 2D electrons in GaAs quantum well placed in quantizing magnetic fields is studied using a difference frequency method. The method is based on measurements of the electron conductivity oscillating at the beat frequency $f_1 - f_2$ between two microwaves applied to 2D system at frequencies $f_1$ and $f_2$. The method provides direct access to the dynamical characteristics of the heating and yields the inelastic scattering time $\tau_{in}$ of 2D electrons. The obtained $\tau_{in}$ is strongly temperature dependent, varying from 0.13 ns at 5.5K to 1 ns at 2.4K in magnetic field $B = 0.33T$. When temperature $T$ exceeds the Landau level separation the relaxation rate $1/\tau_{in}$ is proportional to $T^2$, indicating the electron-electron interaction as the dominant mechanism limiting the quantal heating. At lower temperatures the rate tends to be proportional to $T^3$, indicating considerable contribution from electron-phonon scattering.

This work was supported by the National Science Foundation (DMR 1104503), the Russian Foundation for Basic Research (project no.14-02-01158) and the Ministry of Education and Science of the Russian Federation.

12:03PM G5.00005 The Quantum Hall Effect with electron-boson interaction is not exact. KARIN EVERSCHOR-SITTE, MATTHIAS SITTE, ALLAN MACDONALD, Univ of Texas, Austin — The quantum Hall effect (QHE) normally refers to quantized Hall conductivity due to Landau quantization, as observed in 2D electron systems. The precision of the QHE which occurs near integer Landau level filling factors has been verified to more than 8 figures. There are no known limitations to the accuracy of the QHE in the limit of zero temperature. Here, we show explicitly within a toy model that electron-boson interactions can sometimes lead to corrections to the exact quantization of the Hall conductivity.

This work was supported by the National Science Foundation (DMR 1104503), the Russian Foundation for Basic Research (project no.14-02-01158) and the Ministry of Education and Science of the Russian Federation.

12:15PM G5.00006 Intersubband Oscillations in GaAs Quantum Wells with Three Populated Subbands. JESSE KANTER, SCOTT DIETRICH, WILLIAM MAYER, Graduate Center, City University of New York, New York 10016, USA, SERGEY VITKALOV, CUNY-CCNY, ALEXEY BYKOV, Novosibirsk State University, Novosibirsk 630090, Russia; A.V.Rzhanov Institute of Semiconductor Physics, Novosibirsk 630090, Russia — The magnetotransport of highly mobile 2D electrons is studied in GaAs quantum wells with three occupied subbands. The lower two subbands have nearly the same energy while the third subband has a much higher energy ($E_1 \approx E_2 < < E_3$). Observed magneto-intersubband oscillations (MISO) obey the relation $\Delta_{ij} = (E_i - E_j) = \hbar \omega_c$ for oscillations between the $i^{th}$ and $j^{th}$ bands where $\omega_c$ is the cyclotron frequency and $k$ is an integer. The slight difference in the energies of the lower subbands produces noticeable interference effects in the magnetoresistance. By analyzing the amplitude of each component of the MISOs separately, the temperature dependence of the quantum lifetime $\tau_q^{(i)}$ of electrons in $i^{th}$ subband is extracted. The studies indicate that $\tau_q^{(1)} \approx \tau_q^{(2)} > \tau_q^{(3)}$ while it appears that $\tau_q^{(3)} < \tau_q^{(1,2)}$ which can be related to a reduced electron density in the third subband.

This work was supported by the National Science Foundation (DMR 1104503), the Russian Foundation for Basic Research (project no.14-02-01158) and the Ministry of Education and Science of the Russian Federation.
phenomena observed in 2DEG system. Bosonization DE-FG03-02ER45958 and Welch Foundation grant TBF1473. interlayer tunneling strength. at the inner and outer edges of Corbino rings. We propose a microscopic picture in which disorder is the main agent responsible for the reduction of the effective charge fractionalization is mathematically described by functional determinants with overlapping pulses. We develop a framework for the evaluation of such formalism of non-equilibrium bosonization, the above physics is reflected in the separation of initially overlapping square pulses in the effective scattering phase. to injection with a given source-drain voltage, a finite time is needed until the separation between the fractionalized pulses is larger than their width. In the materials and Graphene Centre — In quantum Hall edge states and in other one-dimensional interacting systems, charge fractionalization can occur due to the two-dimensional electron gas system in high magnetic fields. High magnetic field \( B \) is supported by the Pappalardo Fellowship in Physics. HC and AHM are supported by DOE Division of Materials Sciences and Engineering grant DE-FG03-02ER45958 and Welch Foundation grant TBF1473.

Enhancement of spin susceptibility of low-density two-dimensional electrons in a high quality Si/SiGe quantum well. TZU-MING LU, XIAOYAN SHI, WEI PAN, Sandia National Laboratories, SHI-HSIEN HUANG, CHEEWEE LIU, JIUN-YUN LI, National Taiwan University — We report magneto-transport measurement results of two-dimensional electrons in a high quality Si/SiGe quantum well under tilted magnetic fields. The electron peak mobility reaches \( 2 \times 10^{11} \) cm\(^2\)/Vs and the density is varied from 0.8 to 2.1 \( 10^{11} \) cm\(^{-2}\). Under tilted magnetic fields, two Landau levels with opposite spins are brought into energetic coincidence. From the coincidence angles we determine the effective spin susceptibility \( g \approx m^* \). At \( n = 2.1 \times 10^{11} \) cm\(^{-2}\) \( g \approx m^* \approx 4 \) (in units of \( m_e \)). Consistent with previous work \( \approx Lai et al, PRL 96, 076805 (2006) \). Our results further show that the spin susceptibility is enhanced by 20\% at \( 0.8 \times 10^{11} \) cm\(^{-2}\) from its high density value. Surprisingly, unlike previous results in modulation doped Si/SiGe quantum wells, a resistance peak is observed at \( n = 3 \) when Landau level coincidence occurs in our undoped Si/SiGe field-effect transistor sample. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

Experimental Study of Low Density Quantum Hall Fabry-Perot Interferometer. SIMAS GLINSKIS, SANGHUN AN, WOO WON KANG, Univ of Chicago, LEONIDAS OCOLA, Argonne National Lab, LOREN PFIEFFER, KEN WEST, KIRK BALDWIN, Princeton — In this talk we report on interference oscillations observed in Fabry-Perot 1.5\( \mu \)m diameter interferometers fabricated from low density, high mobility AlGaAs/GaAs heterostructures. The Fabry-Perot interferometers were fabricated using e-beam lithography and inductively coupled plasma etching to minimize sample damage. Optimization of the quantum point contacts were made by systematically varying the etching depth and monitoring the resistance of the device. So far we have been able to detect clear interference oscillations which are observed at integer quantum Hall states. The interference oscillations occur in the low magnetic field side of the Hall plateaus when there is substantial backscattering at the quantum point contacts. A linear relationship between filled Landau levels and oscillation frequencies establishes that our interferometers are in the Coulomb dominated regime described by the interacting model of quantum Hall Fabry-Perot interferometers. Study of interference oscillations in the fractional quantum Hall states are currently under progress and will be discussed.

Theory of Transport Phenomena in Coherent Quantum Hall Bilayers. ALLAN H. MACDONALD, HUA CHEN, University of Texas at Austin, INTI SODEMANN, Massachusetts Institute of Technology — We will describe a theory that allows to understand the anomalous transport properties of the excitonic condensate state occurring in quantum Hall bilayers in terms of a picture in which the condensate phase is nearly uniform across the sample, and the strength of condensate coupling to layer tunneling processes is substantially reduced compared to the predictions of disorder-free microscopic mean-field theory. These ingredients provide a natural explanation for recently established I-V characteristics which show conductance quantization. Experimentally, the conductance quantization is observed in the two-layer quantum Hall regime, at the inner and outer edges of Corbino rings. We propose a microscopic picture in which disorder is the main agent responsible for the reduction of the effective interlayer tunneling strength.

1:03PM G5.00010 Transient Features in Charge Fractionalization and Non-equilibrium Bosonization. BERND ROSENOW, ALEXANDER SCHNEIDER, University of Leipzig, MIRCO MILLETARI, NUS Centre for Advanced 2D Materials and Graphene Centre — In quantum Hall edge states and in other one-dimensional interacting systems, charge fractionalization can occur due to the fact that an injected charge pulse decomposes into eigenmodes propagating at different velocities. If the original charge pulse has some spatial width due to injection with a given source-drain voltage, a finite time is needed until the separation between the fractionalized pulses is larger than their width. In the formalism of non-equilibrium bosonization, the above physics is reflected in the separation of initially overlapping square pulses in the effective scattering phase. When expressing the single particle Green function as a functional determinant of counting operators containing the scattering phase, the time evolution of charge fractionalization is mathematically described by functional determinants with overlapping pulses. We develop a framework for the evaluation of such determinants, and compare our theoretical results with recent experimental findings.

1:15PM G5.00011 Transient Features in Charge Fractionalization and Non-equilibrium Bosonization. BERND ROSENOW, ALEXANDER SCHNEIDER, University of Leipzig, MIRCO MILLETARI, NUS Centre for Advanced 2D Materials and Graphene Centre — In quantum Hall edge states and in other one-dimensional interacting systems, charge fractionalization can occur due to the fact that an injected charge pulse decomposes into eigenmodes propagating at different velocities. If the original charge pulse has some spatial width due to injection with a given source-drain voltage, a finite time is needed until the separation between the fractionalized pulses is larger than their width. In the formalism of non-equilibrium bosonization, the above physics is reflected in the separation of initially overlapping square pulses in the effective scattering phase. When expressing the single particle Green function as a functional determinant of counting operators containing the scattering phase, the time evolution of charge fractionalization is mathematically described by functional determinants with overlapping pulses. We develop a framework for the evaluation of such determinants, and compare our theoretical results with recent experimental findings.

1:27PM G5.00012 ABSTRACT WITHDRAWN
1:51PM G5.00014 Hall Viscosity and Momentum Transport in Lattice and Continuum Models of the Integer Quantum Hall Effect in Strong Magnetic Fields, THOMAS TUEGEL, TAYLOR HUGHES, Univ of Illinois - Urbana — Hall viscosity describes non-dissipative transport in systems with broken time-reversal and parity symmetries. We develop a new method for computing the Hall viscosity of lattice systems in strong magnetic fields based on momentum transport, which we compare to the method of momentum polarization used by Tu et al. [Phys. Rev. B 88, 195412 (2013)] and Zalewski et al. [Phys. Rev. Lett. 110, 236801 (2013)] for noninteracting systems. We compare the Hall viscosity of square-lattice tight-binding models in magnetic field to the integer quantum Hall effect (IQHE) showing agreement when the magnetic length is much larger than the lattice constant, but deviation as the magnetic field strength increases. We also relate the Hall viscosity of relativistic electrons in magnetic field (the Dirac IQHE) to the conventional IQHE. The Hall viscosity of a lattice Chern insulator in magnetic field agrees with the Dirac Hall viscosity when the magnetic length is much larger than the lattice constant. We also show that the Hall viscosity of the lattice model deviates further from the continuum model if the C4 symmetry of the square lattice is broken, but the deviation is again minimized as the magnetic length increases.

2:03PM G5.00015 Relaxation of the electron wave packet in the quantum Hall edge1,2, ARTUR SLOBODENIUK, EDVIN IDRISOV, EUGENE SUKHORUKOV, Univ of Geneva — Recently, single-electron wave packets in the quantum Hall edge (QHE) become very important objects in the so called electron optics. The properties of these excitations are well known only in the case of free-fermion description of the QHE. The role of the Coulomb interaction in such systems have not received a clear theoretical description yet. We propose the method of calculation of characteristics of single-electron excitations of the QHE which takes into account this interaction. We realise it on the QHE with filling factor ν = 2. The difference of the obtained quantum state with the free-fermion answer is investigated. It is shown that role of the Coulomb interaction is crucial and it’s effects can be measured in the Hong-Ou-Mandel and Hanbury-Brown-Twiss experiments. As an example, the influence of Coulomb interaction for the case of electronic Mach-Zehnder interferometer is calculated.

1 Swiss NSF

Tuesday, March 3, 2015 11:15AM - 2:15PM
Session G6 DMP DCOMP: Focus Session: Ferroic Materials by Design
006A - Sang-Wook Cheong, Rutgers University

11:15AM G6.00001 Revealing and understanding the behavior of structural domain walls from first principles1,2, JORGE INIGUEZ, ICMAB-CSIC — Ferroelectric and ferroelastic domain walls (DWs) are becoming the focus of renewed excitement. Modern experimental techniques permit an unprecedented control on domain structures, and it is now possible to produce materials with a large volume fraction occupied by the DWs themselves. Also, recent experiments show that DWs can display distinct properties not present in the domains, which suggests the possibility of using the walls themselves as the functional material in nano-devices. In this talk I will review recent projects in which we have used theory and first-principles simulation to reveal and explain a variety of DW-related effects. The presentation will include the formation of novel two-dimensional crystals at the DWs of a ferroelastic material, the occurrence of ferroic orders (ferroelectric, ferromagnetic) confined at the DWs of various compounds, and cases in which peculiar (and useful) responses and switching properties rely on existence of a multi-domain state. I will also summarise experimental evidence for most of these incredible findings, which clearly ratify domain and domain-wall engineering as a powerful strategy to obtain novel functional nano-materials. / Work done in collaboration with many researchers, the main ones being: J.C. Wójcik (ICMAB-CSIC), C. Magén (INA at U. Zaragoza), M. Mostovoy (U. Groningen), P. Zubko (U. College London), as well as the groups of Beatriz Noheda (U. Groningen), R. Ramesh (UC Berkeley) and J.-M. Triscone (U. Geneva).

1Supported by MINECO-Spain.
2Current affiliation: Luxembourg Institute of Science and Technology (LIST)

11:51AM G6.00002 Magnetic charge and magnetoelectricity in hexagonal manganites and ferrites1,2, MENG YE, DAVID VANDERBILT, Rutgers Univ — Magnetoelectric (ME) materials are of fundamental interest and are investigated for their broad potential for technological applications. Commonly the dominant contribution to the ME response is the lattice-mediated one, which is proportional to both the Born effective charge Zm and its analogue, the dynamical magnetic charge Zmu. A previous study has shown that exchange striction acting on noncollinear spins induces much larger magnetic charges than when Zmu is driven by spin-orbit coupling. The hexagonal manganites RMnO3 and ferrites RFeO3 (R = Sc, Y, In, Ho-Lu) exhibit strong couplings between electric, magnetic and structural degrees of freedom, with the transition-metal ions in the basal plane are antiferromagnetically coupled through super-exchange so as to form a 120° spin arrangement. Here we present a theoretical study of the magnetic charges, and of the spin-lattice and spin-electronic ME constants, in these hexagonal manganites and ferrites, clarifying the conditions under which exchange striction leads to enhanced Zm’s and anomalously large in-plane spin-lattice ME effects.

1Supported by ONR Grant N-00014-12-1-1035

12:03PM G6.00003 Ferroelectrics with a trilinear coupling of three lattice modes: Response to electrical boundary conditions from first principles, ANDREW T. MULDER, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — Recent progress in the design of functional materials has led to the discovery of several ferroelectrics with the polarization coupled trilinearly to two nonpolar lattice modes. Because nonpolar lattice modes in perovskites play a key role in determining electronic and magnetic properties, these materials have a polarization that is strongly coupled to other functionality by design. But many properties of trilineral ferroelectrics remain unknown, and general design rules have been difficult to uncover. For example, the electrical properties are unclear because trilineral ferroelectrics may have a conventional ferroelectric mechanism, or may not (like an improper ferroelectric). Understanding the polarization response to electrical boundary conditions is therefore an open question that will impact the application of trilinear ferroelectrics to practical devices. In this talk, we use first principles methods to study the single domain polarization response to changing electrical boundary conditions in a variety of trilinear ferroelectrics. We clarify the design rules, the connection to phenomenological models (proper, improper, and weak ferroelectricity), and we show how epitaxial strain can tune a single trilinear ferroelectric between proper and improper ferroelectricity.
12:15PM G6.00004 Epitaxial-strain-induced insulating phase in 1:1 SrCrO$_3$/SrTiO$_3$ superlattices: A first-principles study, YUANJUN ZHOU, KARIN RABE, Rutgers University — Using first principles calculations, we studied the structure and electronic properties of the 1:1 superlattice combining the magnetic metallic oxide SrCrO$_3$ and the band insulator SrTiO$_3$. We determined the epitaxial-strain-dependent ground-state structures of the superlattice using the “stacking” method. An insulating polar ground state is found when the tensile strain is greater than 2.2%. The insulating character of this phase is related to the $d_{x^2-y^2}$, $d_{z^2}$ orbital ordering of the Cr $t_d$ electrons. Specifically, the 1:1 periodic superlattice structure eliminates the Cr-O-Cr bonds in the direction normal to the interface, which reduces the hopping of 3d electrons in this direction. The band widths of $d_{xy}$ and $d_{xz}$ for Cr are thus significantly reduced, enhancing the effect of the in-plane polar distortions in the SrCrO$_3$ layer responsible for opening the the band gap. The elucidation of this mechanism opens a new approach to band engineering, encouraging further investigations on related metallic/dielectric superlattice systems.

12:27PM G6.00005 Trilinear couplings and the multi-mode anti-ferroelectric transition of PbZrO$_3$: a first-principles investigation, JORGE INIGUEZ$^2$, ICMA-CSC, MASSIMILIANO STENGEL, ICREA and ICMA-CSC, SERGEY PROSANDEEV, LAURENT BEAULIEU, University of Arkansas — We have studied ab initio the phase transition in PbZrO$_3$, a perovskite oxide usually presented as the prototypic anti-ferroelectric. Our work reveals the crucial role that anti-ferrodistortive modes—invoking concerted rotations of the oxygen octahedra in the structure—play in the transformation, as they select the observed anti-ferroelectric phase, among competing structural variants, via a cooperative trilinear coupling. The resulting picture is that of a complex transition whose multi-mode character is essential to its very occurrence, and poses the provocative question of whether such an intricate behavior can be taken as representative of anti-ferroelectricity in perovskite oxides.

1 Supported by MINECO-Spain and ONR.
2Current address: Luxembourg Institute of Science and Technology (LIST)

12:39PM G6.00006 A new class of in-plane Ferroelectric Mott insulators via oxide heterostructuring, CHANUL KIM, Columbia Univ, HYOWON PARK, University of Illinois at Chicago, CHRIS MARIANETTI, Columbia Univ, MARIANETTI GROUP TEAM$^2$ — We propose simple design rules based on charge transfer, cation ordering, and size mismatch to design a new class of in-plane ferroelectric Mott insulators in perovskite-based transition metal oxides. Ab Initio DFT+U calculations are then used to selectively scan phase space based on these rules. We begin by exploring pairs of A-type ions (A, A’), and pairs of B-type ions (B, B’) in AAB’BO$_6$ which will have nominal charge transfer consistent with valencies that are conducive to a low Mott gap insulator. Additionally, the A-type ions are chosen to have a large size mismatch and stereochemical effect. The ordering of A/A’ and B/B’ still retains C$_4v$ symmetry which may be spontaneously broken to yield an in-plane ferroelectric. We uncover a number of materials which are strong candidates to be in-plane ferroelectric Mott insulators in experiment, including BaBiVCuO$_6$, BaBiVNiO$_6$, PbLaVCuO$_6$. Finally, we will discuss potential applications of in-plane ferroelectric Mott insulators such as ferroelectric photovoltaks, Mott FET, and optoelectronic devices.

1Semiconductor Research Corporation (FAME)
2Marianetti Group @ Department of Applied Physics and Applied Mathematics, Columbia University

12:51PM G6.00007 Why is the electrocaloric effect so small in ferroelectrics? , GIAN G. GUZMAN-VERRI, Argonne National Laboratory, PETER B. LITTLEWOOD, Argonne National Laboratory and The University of Chicago — Ferroelectrics are attractive candidate materials for environmentally friendly solid state refrigeration free of greenhouse gases. Their thermal response upon variations of external electric fields is largest in the vicinity of their phase transitions, which may occur near room temperature. The magnitude of the effect, however, is too small for useful cooling applications even when they are driven close to dielectric breakdown. Insight from microscopic theory is therefore needed to characterize materials and provide guiding principles to search for new ones with enhanced electrocaloric performance [1]. Here, we present meaningful figures of merit derived from well-known microscopic models of ferroelectricity which provide insight into the relation between the strength of the effect and the characteristic interactions of ferroelectrics such as dipole forces. We find that the long range nature of these interactions results in a small effect. A strategy is proposed to make it larger by shortening the correlation lengths of fluctuations of polarization [2].


1Work at Argonne is supported by the U.S. Department of Energy, Office of Basic Energy Sciences under contract no. DE-AC02-06CH11357.

1:03PM G6.00008 Strain–Induced Geometric Ferroelectricity in Perovskite–structured Fluoroscorpates , NENIAN CHARLES, Drexel University, JAMES RONDINELLI, Northwestern University — Using first-principles density functional theory calculations we investigate geometric ferroelectricity in epitaxially strained double-perovskite fluorides, Na$_3$ScF$_6$ and K$_2$NaScF$_6$. The experimental room temperature crystal structures of the fluoroscorpates are centrosymmetric, i.e. Na$_3$ScF$_6$ (P2$_1$/n) and K$_2$NaScF$_6$ (Fm3m). However, in their prototypical cubic geometry, we identify soft infrared active modes that are strongly sensitive to pressure: Ferroelectric instabilities are found for negative hydrostatic pressures $\sim$ 6 GPa. For Na$_3$ScF$_6$ we observe octahedral rotations ($a^* - a^* - c^*$ tilt system) are in strong competition with acentric polar distortions, and as a result exceedingly large tensile strain above 8% are required to stabilize a Pm polar phase. We demonstrate that the strain mismatch required to stabilize the ferroelectric phase can be reduced to approximately 4% with chemical substitution in (a$^$2$b^*c^*$) K$_2$NaScF$_6$ by reducing the tendency to octahedral rotations. Our study provides new insights that may prove useful in guiding experimental efforts towards identifying functional polar fluoroperovskites.

1:15PM G6.00009 Tuning the structure of oxide thin films with strain, ELIZABETH NOWADNICK, ANDREW MULDER, CRAIG FENNIE, Cornell University — Octahedral rotations are ubiquitous in perovskite oxides and play an important role in determining the functionality of these materials, for example impacting magnetism and ferroelectricity. Pressure applied to bulk perovskites, as well as biaxial strain in epitaxially grown thin films, couples to the octahedral rotations. By performing first principles density functional theory calculations for a wide variety of ABO$_3$ perovskite oxides, we present a systematic study of the structural response of these systems to pressure and strain. We find that the octahedral rotations respond to pressure and biaxial strain in distinct ways. With pressure, the relative compressibilities of the A012 and BO$_3$ polyhedra govern the response of the octahedral rotations, whereas the response to biaxial strain arises from an interplay of the out of plane axis relaxation and the polyhedral compressibilities. Our findings offer insight into how to optimize the sensitivity of octahedral rotations to strain and pressure.
1:27PM G6.00010 First-principles studies of lone-pair-induced distortions in epitaxial phases of perovskite SnTiO$_3$ and PbTiO$_3$. KRISHNA PITIKE, LYDIE LOUIS, University of Connecticut - Storrs, WILLIAM PARKER, Purdue University, SERGE NAKHMANSON, University of Connecticut - Storrs — In this project, a computational investigation utilizing density functional theory methods is carried out to elucidate the differences in stereochemical lone-pair activity of Pb and Sn A-site ions in epitaxial polar ATiO$_3$ perovskites. The contrasting tendencies for the lead- and tin-based compounds to form different phases under biaxial tension are connected to the amount of charge concentrated within the lone pair orbits. Specifically, phases are energetically more preferable when as much charge as possible is dissipated out of the lobe, thus lowering the cost of Coulomb repulsion between the lone pair and the surrounding oxygen cage. The insights gained about the electronic-level underpinnings of transitional behavior in such lone-pair active epitaxial ferroelectrics may be used in the design of a new generation of more efficient electromechanical and electrooptical devices.

1:39PM G6.00011 Tuning ferroelectric polarization in $A\prime A'MnWO_6$ double perovskites through $A$ cation substitution. JOSHUA YOUNG, Drexel University, JAMES RONDINELLI, Northwestern University — Magnetic ferroelectric materials, which exhibit simultaneous magnetic and electric polarizations, have generated significant interest for application in novel electronic devices. Recent experimental work has shown that the double perovskite NaLaMnWO$_6$ exhibits anti-ferromagnetic order, while computational studies predict it to also exhibit a spontaneous polarization of 16 $\mu$C/cm$^2$ owing to an octahedral rotation induced improper mechanism. Using first principles density functional theory calculations, we investigate nine isostructural $A\prime A'MnWO_6$ compounds through chemical substitution of alkali metal ($A\prime$=Na, K, Rb) and rare earth cations ($A$=La, Nd, Y), and find that the ferroelectric polarization can be enhanced by up to 150% by maximizing the difference in ionic size of the $A$ and $A'$ cations. We then identify the microscopic features responsible for this polarization through an examination of the tolerance factors, bond valences, and atomic displacement patterns. We anticipate that the crystal-chemistry criteria and analysis presented here can be extended to additional members of this family as well as guide the targeted design of novel multiferrics.

1:51PM G6.00012 First principles study of the band gaps and edges of (111) epitaxially strained SrTiO$_3$. SEBASTIAN E. REYES-LILLO, Molecular Foundry, Lawrence Berkeley National Laboratory, ROBERT F. BERGER, Department of Chemistry, Western Washington University, JEFFREY B. NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory; Department of Physics, University of California-Berkeley — SrTiO$_3$ is a tunable material with potential use in energy applications. Previous experimental and first principles results demonstrated controllable manipulation of the electronic band gap in (001) biaxially strained, and predicted a large room-temperature band gap reduction (0.3 eV) for (111) epitaxial growth at small and large strains. In this work, we revisit and examine the effect of (111) epitaxial strain on the structural and electronic properties of SrTiO$_3$ using density functional theory calculations at low and room temperatures. Under (111) epitaxial strain at low temperature, we find that SrTiO$_3$ has an antiferrodistortive ground state at large compressive strains ($\sim-1\%$) and a ferroelectric phase transition between $-1\% < \eta < 4\%$ biaxial strains. While structural distortions widen the band gap compared to the paraelectric phase, an effective reduction of band gap is observed for the distorted structure at large compressive strains compared to bulk. This work is supported by DOE, computational resources are provided by NERSC.

2:03PM G6.00013 First principles investigations of structural, elastic, dielectric and piezoelectric properties of {Ba,Sr,Pb}TiO$_3$, {Ba,Sr,Pb}ZrO$_3$ and {Ba,Sr,Pb}{Zr,Ti}O$_3$ ceramics. BERNA AKGENC, Kırklareli University Department of Physics, Faculty of Science, Kavaklı, 39060, Kırklareli, Turkey, CETIN TASSEVEN, Department of Physics, Faculty of Science, Yildiz Technical University, Davutpaşa Campus, Esenler, 34210, Istanbul, Turkey, TAHIR CĄĠIN, Department of Materials Science and Engineering, Texas A&M University, College Station, TX 77843-3003, USA — We use first-principle density-functional study of structural, anisotropic mechanical, dielectric, and piezoelectric properties of {Ba,Sr,Pb}TiO$_3$, {Ba,Sr,Pb}ZrO$_3$ and {Ba,Sr,Pb}{Zr,Ti}O$_3$ alloys in cubic perovskite structures at zero temperature. Because there is significant interest in finding new piezoelectrics that do not contain toxic elements such as lead. In this study, we compare piezoelectric response of those alloys to synthesize outstanding piezoelectric materials. In perovskite structures, the spontaneous polarization is due to enormous values of Born effective charges computed by linear response within density functional perturbation theory, which are much larger than predicted nominal charge. We deeply investigated the effects of composition, order and site defects structure on piezoelectric constants.


11:15AM G7.00001 Possible Chern insulators based on novel ferromagnetic substrates. JIANPENG LIU, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University — Previous work has opened the possibility that one can obtain non-zero Chern numbers from the surface bands of atomic layers with strong spin-orbit coupling deposited on insulating ferromagnetic thin films. Following this idea, we carry out a theoretical search for Chern (i.e., quantum anomalous Hall) insulators formed by depositing heavy adatoms on top of stable insulating ferromagnetic substrates such as CrSiTe$_3$ and CrGeTe$_3$. These materials have a layered structure with weak van der Waals interlayer coupling, so it seems likely that thin films with clean surfaces will be experimentally stable. Moreover, the insulating character of these materials, with magnetization normal to the surface, are promising for realizing Chern-insulator states when adatoms are added. By searching over a series of heavy elements, we found non-zero Chern numbers in Bi and Tl-deposited CrSiTe$_3$ thin films, although with slightly negative indirect energy gaps. We expect that a global energy gap could be opened up by some further engineering, such as by applying epitaxial strain or additional atomic substitution.

11:27AM G7.00002 Tunable topological electronic structure of silicene on semiconducting Bi/Si(111)-root3xroot3 substrate: a first-principles. CHIA-HSIU HSU, ZHI-QUAN HUANG, BO-HUNG CHOU, FENGCHUAN CHUANG, Natl. Sun Yat-sen U., HSIN LIN, Natl. U. of Singapore, ARUN BANSIL, Northeastern U. — Using first-principles calculations to obtain the crystal and electronic structures, we show that the 1x1 phase of silicene is energetically more favorable than the root3xroot3 silicene superstructure on a semiconducting Bi/Si(111)- root3xroot3 substrate. The band gap of the system is found to be influenced strongly through the participation of Bi-orbitals, which possess a larger spin-orbit coupling strength compared to Si. In particular, the non-trivial (topological) band gap of a few meV in freestanding 1x1 silicene enlarges to 150 meV and becomes trivial in the presence of the substrate. We further show how an out-of-the-plane external electric field can be used to tune the band gap and restore the non-trivial topological phase.
Amplified topological characteristics of MBE-grown Bi$_2$Se$_3$/II-VI semiconductor superlattices \(^1\), Zhiyi Chen, Lukas Zhao, Inna Korzhovska, Maria Tamargo, Lia Krusic, City College of New York - CUNY — Access to charge transport in Dirac surface states of topological insulators (TIs) such as Bi$_2$Se$_3$ is faced with two big challenges: one is significant bulk conduction and another is intermixing of topological states with nontopological 2DEG quantum well states formed by bending of bulk electronic bands near the surface. The latter effect is thought to arise via charge transfer from surface adatoms and, therefore, the choice of layers abutting topological surfaces can be critical. Here we report a successful molecular beam epitaxy growth of Bi$_2$Se$_3$ on ZnS/CD$_3$Se$_{1-x}$Se superlattices that improve topological characteristics of individual 8 - 10 nm thick TI layers. We show that in these superlattices the two-dimensional (2D) weak antilocalization quantum correction to classical magnetoresistance, associated with topological Berry phase, scales with the number of TI layers, with one quantum channel per layer. The Berry phase of \(\pi\) obtained independently from Shubnikov de Haas quantum oscillations demonstrates robust topological interfaces in the multilayer structure.

\(^1\)Supported by NSF-DMR-1122594 and DOD-W911NF-13-1-0159

Quantum Anomalous Hall Effect in Magnetic Semiconductors \(^1\), Chaoxing Liu, The Department of Physics, Pennsylvania State University — In the quantum anomalous Hall effect, dissipationless charge currents are carried by chiral edge states and the Hall conductance is quantized, similar to the quantum Hall effect. Different from the conventional quantum Hall effect that requires strong magnetic fields, the quantum anomalous Hall effect is induced by strong exchange coupling between electron spin and magnetic moments in magnetic materials, so it can be realized at zero magnetic field, enabling the potential application of electronic devices with low energy consumption. Recent experiments on Cr-doped MnTe \(^2\) and V doped BiSbTe \(^3\) thin films has observed the quantized Hall conductance at zero magnetic field and confirmed this novel effect. In this talk, I would like to discuss our recent work on the quantum anomalous Hall effect in magnetic semiconductors. I will first introduce two key ingredients, inverted band structures and ferromagnetic insulators, for the quantum anomalous Hall effect in realistic characteristics of magnetic materials. Then, based on these two ingredients, I will discuss different classes of materials for the quantum anomalous Hall effect, focusing on magnetically doped InAs/GaSb quantum wells and magnetically doped LaOSe$_2$ films. For magnetically doped InAs/GaSb quantum wells, we will show how band edge singularity can enhance spin susceptibility and lead to the quantum anomalous Hall state at a relatively high critical temperature. For magnetically doped LaOSe$_2$ films, we find the quantum anomalous Hall effect can be tuned electrically by a gate voltage and identify layer dependent spin texture as the underlying physical reason. Finally, we will also discuss disordered transport and anisotropic magnetoresistance in the quantum anomalous Hall regime.


12:27PM G7.00005 ABSTRACT WITHDRAWN

12:39PM G7.00006 Electrically tunable multiple Dirac cones in thin films of (LaO)$_2$(SbSe)$_2$ family of materials \(^1\), Xiaoyu Dong, Jianfeng Wang, Department of Physics and State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University, Beijing 100084, China, RuiXing Zhang, Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802-6300, USA, - Wenhui Duan, Bangfen Zhu, Department of Physics and State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University, Beijing 100084, China, Jorge Sofo, Chaoxing Liu, Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802-6300, USA — Two-dimensional Dirac physics has aroused great interests in condensed matter physics due to its importance in both fundamental physics and device applications. The ability to control the properties of Dirac cones is essential for the occurrence of various new phenomena and the development of next-generation electronic devices. Based on first-principles calculations and an analytical effective model, we propose a new Dirac system with eight Dirac cones in thin films of the (LaO)$_2$(SbSe)$_2$ family of materials with an external gate voltage. The advantage of this system lies in its tunability: the existence of gapless Dirac cones, their positions, Fermi velocities and anisotropy all can be controlled by an experimentally feasible gate voltage. We identify the layer dependent spin texture induced by spin-orbit coupling as the underlying physical reason for the tunability of Dirac cones in this system. As a consequence, we show that the electrically tunable quantum anomalous Hall effect with a high Chern number can be induced by introducing magnetization into this system.

12:51PM G7.00007 An Efficient numerical method to calculate the conductivity tensor for disordered topological matter \(^1\), Jose H. Garcia, Universidade Federal do Rio de Janeiro, Lucian Covaci, Universiteit Antwerpen, Tatiana G. Rapporto, Universidade Federal do Rio de Janeiro — We propose a new efficient numerical approach to calculate the conductivity tensor in solids. We use a real-space implementation of the Kubo formalism where both diagonal and off-diagonal conductivities are treated in the same footing. We adopt a formulation of the Kubo theory that is known as Bostain formula and expand the Green’s functions involved in terms of Chebyshev polynomials using the kernel polynomial method. Within this method, all the computational effort is on the calculation of the expansion coefficients. It also has the advantage of obtaining both conductivities in a single calculation step and for various values of temperature and chemical potential, capturing the topology of the band-structure. Our numerical technique is very general and is suitable for the calculation of transport properties of disordered systems. We analyze how the method’s accuracy varies with the number of moments used in the expansion and illustrate our approach by calculating the transverse conductivity of different topological systems.

1T.G.R, J.H.G and L.C. acknowledge Brazilian agencies CNPq, FAPERJ and INCT de Nanoestruturas de Carbono, Flemish Science Foundation for financial support.

12:03PM G7.00008 Topological phases in rocksalt rare-earth binary compounds \(^1\), Hsin Lin, Mingen Zhang, Guoqing Chang, National University of Singapore, Yu-An Chen, Timothy Hsieh, Massachusetts Institute of Technology, Arun Bansil, Northeastern University, Liang Fu, Massachusetts Institute of Technology — Using first-principles calculations, we have investigated the electronic properties of bulk lanthanum monopnictides (LaX, X = N, P, As, Sb, Bi) and their thin films. We predict that lanthanum nitride (LaN) harbors a three-dimensional (3D) Dirac semimetal phase, and undergoes a phase transition driven by Coulomb interaction. Other lanthanum monopnictides are found to be semimetals with a nontrivial Z2 band topology. Furthermore, we find both two-dimensional (2D) Dirac semimetal and topological insulator phases in thin films of lanthanum monopnictides. The gapless Dirac states in bulk lanthanum monopnictides and their thin films can be attributed to the crystalline symmetry protection.

\(^1\)Support by the Singapore National Research Foundation under NRF Award No. NRF-NRFF2013-03 and USDOE is acknowledged.
1:15PM G7.00009 Giant magnetoresistance and band structure of topological semimetal RhSb₃
KEFENG WANG, LIMIN WANG, Y. NAKAJIMA, RENXIONG WANG, JIE YONG, J. PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland College Park — Recently materials with skutterudite structure such as CoSb₃ were predicted to provide a promising platform for the realization of new topological materials such as topological insulators and Dirac-Weyl semimetals. Here we report a detailed study of the electronic structure and magnetotransport properties of high quality RhSb₃ single crystals. First-principles electronic structure calculations reveal a highly dispersive band with Sb-p and Rh-3d weight that shows apparent band inversion. Inclusion of spin-orbit coupling leaves the Fermi level pinned to a doublet, indicating a topological semimetal. Our synthesized high-quality single crystals show typical metallic behavior but with very small residual resistivity ratio, a sign of semimetal behavior, in zero field. We will present magnetotransport data that exhibits a very large magnetoresistance that hints of a very sensitive evolution of electronic properties and Dirac-like spectrum.

1:27PM G7.00010 SmO thin films: a flexible route to correlated flat bands with nontrivial topology
DEEPA KASINATHAN, Max Planck Institute for Chemical Physics of Solids, Dresden, KLAUS KOEPERNIK, IFW Dresden, P.O. Box 270116, D-01171 Dresden, LIU HAO TJENG, MAURITIS HAVERKORT, Max Planck Institute for Chemical Physics of Solids, Dresden — Using density functional theory based calculations, we show that the correlated mixed-valent compound SmO is a 3D strongly topological semi-metal as a result of a 4f-5d band inversion at the X point. We also show that the topological non-triviality in SmO is very robust and prevails for a wide range of lattice parameters, making it an ideal candidate to investigate topological nontrivial correlated flat bands in thin-film form. Moreover, the electron filling is tunable by strain. In addition, we find conditions for which the inversion is of the 4f-6s type, making SmO to be a rather unique system. The similarities of the crystal symmetry and the lattice constant of SmO to the well studied ferromagnetic semiconductor EuO, makes SmO/EuO thin film interfaces an excellent contender towards realizing the quantum anomalous Hall effect in a strongly correlated electron system.

1:39PM G7.00011 Topological transport and atomic tunneling-clustering dynamics for aged Cu-doped Bi₂Te₃ crystals
FENGQI SONG, TAISHI CHEN, WENKAI HUANG, ZHAOGUO LI, XUEFENG WANG, Nanjing University, COLLABORATIVE INNOVATION CENTER OF ADVANCED MICROSTRUCTURES COLLABORATION — Here we report the suppression of the bulk conductance of the material by four orders of magnitude by intense aging in (Cu₀.₁Bi₀.₉)₂Te₃₀₀ crystals. The weak antilocalization analysis, Shubnikov de Haas oscillations and scanning tunneling spectroscopy corroborate the transport of the topological surface states. The aging method therefore leads to an optimized band-insulating Ti crystal and appeals to a free-of-IB crystal. STM visualizes the novel defect features of Cu dopants and their dynamics during the aging process, based on which the details of the aging process are further revealed by ab initio calculations. These calculations suggest that there exists a diffusion barrier at the interface of the Bi₂Te₃ QLS. During the aging process, Cu atoms freely migrate inside the QLS and frequently hit the barrier. The dopant atoms will also form clusters in between the QLS, leaving disorder within the QLS. This leads to a pronounced mobility suppression of the bulk electrons, finally allowing the observation of the TSS-related electron transport in bulk crystal samples. An atomic tunneling-clustering picture across a diffusion barrier of 0.57eV is proposed. (Nature Commun. 5, 5022(2014))

2:03PM G7.00013 Surface Shubnikov-de Haas oscillations of the topological hole conduction in the bulk insulator Tl₁−ₓBi₁+xSe₂
GAKU EGUCHI¹, KYOTO UNIV, KENTO KURODA², MAURITIS HAVERKORT, Max Planck Institute for Chemical Physics of Solids, Dresden — Density functional theory calculations predict that Bi₃Te₃ is a 3D topological insulator. Here, we report our study on Bi₂Se₃ thin films using scanning tunneling microscopy. Using the results on Bi₂Se₃, we fabricate thin Tl₁−ₓBi₁+xSe₂, grown from a liquid precursors, within which the Bi₂Se₃ surface is quenched. The Tl₁−ₓBi₁+xSe₂ constitutes a 3D Dirac fermion fluid that shows a strong antilocalization behavior, which is caused by the spin-orbit coupling and many-body effects. The results suggest that topological superconductors can be engineered with Dirac fermions.

1Funding by the DFG within FOR 1346 is acknowledged
2Supported by NSF (DMR-1105839).

Tuesday, March 3, 2015 11:15AM - 2:15PM
Session G8 DCMP: From Single Molecules to Molecular Assemblies on Surfaces II 006C - Pengpeng Zhang, Michigan State University
11:15AM G8.00001 Self-Assembly and Molecular Dynamics Studies: Ab Initio and Molecular Dynamics Studies, ALEXANDER ST. JOHN, CARLOS WEXLER, Univ of Missouri - Columbia — Spontaneous molecular self-assembly is a promising route for bottom-up manufacturing of two-dimensional (2D) nanostructures with specific topologies on atomically flat surfaces. Of particular interest is the possibility of selective lock-and-key interaction of guest molecules inside cavities formed by complex self-assembled host structures. Our host structure is a monolayer consisting of interdigitated 1,3,5-tristryrylbenzene substituted by alkoxy peripheral chains containing n = 6, 8, 10, 12, or 14 carbon atoms (TSB3,5-CN) deposited on a highly ordered pyrolytic graphite (HOPG) surface. Using ab initio methods from quantum chemistry and molecular dynamics simulations, we construct and analyze the structure and functionality of the TSB3,5-CN monolayer as a molecular sieve.

Supported by ACS-PRF 52096-ND5

11:27AM G8.00002 Highly-Oriented Molecular Assembly on Monolayer Graphene for Boosting Photon Harvesting in Bilayer Organic Solar Cells, KILWON CHO, Department of Chemical Engineering, Pohang University of Science and Technology — A novel approach to dramatically enhance the photon harvesting in organic solar cells was demonstrated by utilizing a graphene-organic heterointerface. A large area, residue-free monolayer graphene was inserted at anodic interface to serve as an atomically thin, transparent and highly conductive epitaxial template for organic crystal growth with specific orientation. The anisotropic nature of optoelectronic properties of organic semiconductor molecules provided a significant enhancement in exciton diffusion length, optical absorption, charge carrier lifetime as well as the energy level alignment at metal-organic and organic-organic interfaces. Especially, the exciton diffusion length increases up to nearly 100 nm, which allows the device thickness to be doubled to yield 5 times higher power conversion efficiency in comparison to conventional planar heterojunction organic photovoltaic cells. Theoretical simulations as well as systematic studies on the film structure and optoelectrical properties were performed to corroborate our new findings.

11:39AM G8.00003 Ultrastron exciton-photon coupling in single and coupled organic microcavities, BIN LIU, ROSEMARY BRAMANTE, BRENT VALLE, KENNETH SINGER, Case Western Reserve University, TAWFIK KHATTAB, JARROD WILLIAMS, ROBERT TWIEC, Kent State University — We have demonstrated ultrastron light-matter coupling in organic planar microcavities composed of a neat glassy organic dye film between two metallic (aluminum) mirrors in a half-cavity configuration. Such cavities are characterized by Q factors around 10. Tuning the thickness of the organic layer enables the observation of the ultrastron coupling regime. Via reflectivity measurements, we observe a very large Rabi splitting around 1.227 eV between upper and lower polariton branches at room temperature, and we detect polariton emission from the lower polariton branch via photoluminescence measurements. The large splitting is due to the large oscillator strength of the neat dye glass, and to the match of the cavity Q-factor with the width of the dye material. We also investigated the ultrastron coupling between excitonic states of neat glassy organic dye and cavity modes within coupled microcavity structures. The high-reflectivity mirrors are formed from distributed Bragg reflectors (DBR), which are multilayered films fabricated using the coextrusion process, containing alternating layers of high (SAN25, n=1.57) and low (Dyneon THV 220G, n=1.37) refractive index dielectric polymers. Nonlinear optical measurements will be discussed.

This research was supported by the National Science Foundation Center for Layered Polymer Systems (CLiPS) under grant number DMR-0423914.

11:51AM G8.00004 Single molecule dissociation by tunneling electrons in NO-Co-Porphyrin complex on Au(111): A novel mechanics revealed by scanning tunneling spectroscopy and first-principles thermodynamic simulation, YUNHEE CHANG, Graduate School of Nanoscience and Technology, KAIST, HOWON KIM, Dept. of Physics, Korea University, EUI-SUP LEE, Graduate School of Nanoscience and Technology, KAIST, WON-JUN JANG, Dept. of Physics, Korea University, YONG-HYUN KIM, Graduate School of Nanoscience and Technology, KAIST, SE-JONG KAHNG, Dept. of Physics, Korea University — To microscopically understand the mechanisms of electron-induced NO dissociations, we performed first-principles density-functional theory (DFT) calculations for NO-CoTPP on Au(111). We explain the scanning tunneling microscopy (STM) results that the dissociations of NO were induced by both positive and negative voltage pulses with threshold voltages, ~0.68 V and 0.74 V, respectively, at 0.1 nA tunneling current, showing power law relations between tunneling current and dissociation yield. To evaluate first-principles thermodynamics of the NO dissociation, we considered not only adsorption-desorption energetics, zero-point energy, and vibrational free energy at experiment temperature from first-principles, but also the chemical potential of NO gas at the cryogenic ultra-high vacuum condition. Using first-principles thermodynamics for the NO dissociation, we argue that the dissociations are induced with inelastic electron tunneling through molecular orbital resonances.

12:03PM G8.00005 Growth of Thin, Anisotropic, π-Conjugated Molecular Films by Step-Wise ‘Click’ Assembly of Molecular Building Blocks: Characterizing Reaction Yield, Surface Coverage, and Film Thickness vs. Addition Step Number, ABEL DEMISSIE, GREG HAUGSTAD, C. DANIEL FRISBIE, University of Minnesota — Molecular electronics is an active field of nanotechnology that has gained much interest due to the advent of modern microscopy techniques, and thin film synthesis using click chemistry — an approach which has enabled scientists to achieve a sub-angstrom control of monolayer length. Among the major challenges to grow oriented, surface-confined wires by click chemistry is development of synthetic routes that yield monodisperse wires, and lack of systematic way to measure the surface coverage of molecules. In this work, we report a comprehensive characterization of π-conjugated oligophenylene imine (OPI) wires synthesized step-wise by imine condensation click chemistry. OPI wire synthesis began with a self-assembled monolayer (SAM) of 4-formyliphenol or 4-aminothiophenol on Au, followed by alternate addition of terephthaldehyde or phenylenediamine. OPI wires were characterized after each monomer addition using Rutherford backscattering spectrometry, x-ray photoelectron spectroscopy, cyclic voltammetry, reflection-absorption infra-red spectroscopy, and nuclear reaction analysis. We have determined an average extent of reaction greater than 98% completion for each growth step using five different techniques. Overall, these nanoscale scale surface characterization techniques proved to be an extremely sufficient method for monitoring wire growth and surface coverage.

12:15PM G8.00006 Direct Patterning of Organic Self-Assembled Monolayer (SAM) on GaAs Surfaces via Dip-Pen Nanolithography (DPN), PENG XIONG, TIMOTHY KEIPER, Department of Physics, Florida State University, XIAOLEI WANG, JIANHUA ZHAO, Institute of Semiconductors, CAS — Hybrid structures of functional molecules and solid-state (SS) materials have attracted extensive interest in surface nanoscience and molecular electronics. The formation and micro/nano patterning of organic SAMs on SS surfaces are a key step in fabricating such devices. Here we report realization of high quality MHA SAMs on GaAs and direct formation of micro/nanoscale patterns of MHA SAM on the surface by micro-contact printing (µCP) and DPN. The process begins with the preparation of an oxide-free surface of GaAs, for which we employed treatment by an ammonium polysulfide ((NH₄)₂S₉) solution. The treatment strips native oxides from GaAs creating an atomic layer of sulfur covalently bonded to the fresh surface. Formation of high-quality SAMs of thiol molecules on GaAs then proceeds through exchange of the sulfur and the thiol terminal of the molecules. The effects of the sulfur-passivation and formation of MHA SAM on the treated surface were confirmed by XPS, HRTEM, and DPN. To the best of our knowledge, this is a first realization of direct DPN of nanoscale organic SAM on a semiconductor free of surface oxide. We further evidence the utility of the hybrid platform by demonstrating directed self-assembly of Au nanoparticles onto MHA/ODT SAM templates on GaAs.
12:27PM G8.00007 The S(2p) Core Level Binding Energies for Alternative Adsorption Sites and the Example of Thiol Self Assembly*, JUANJUAN JIA, VLADIMIR ESAULOV, Universite Paris Sud, ABDELKADER KARA1, University of Central Florida — Results of an investigation of the characteristics of thiol SAMs obtained by vacuum evaporative adsorption, useful for reactive substrates, are presented along with core level binding energy (BE) calculations. Thiold ended SAMs of 1,4-benzenedimethanethiol (BDMT) are obtained by evaporation on Au. They display an unconventional BE structure at about 161 eV, which is close to a known BE of an S atom on Au. S(2p) core level BE calculations for molecules chemisorbed on hollow, bridge and atop sites are reported and suggest that the 161 eV peak is indeed due to an alternative adsorption site, which can be associated to an atom configuration. This must therefore not be confused with atomic sulfur and dissociation processes with S-C bond scission.

1Work partially supported by the U.S. Department of Energy Basic Energy Science under Contract No DE-FG02-11ER16243

12:39PM G8.00008 Spatial Arrangement of Organic Compounds on a Model Mineral Surface: Implications for Soil Organic Matter Stabilization*, HAIKE AMBAYE, LOUKAS PETRIDIS, ORNL, SINDHU JAGADAMMA, MICHAEL KILBEY, University of Tennessee, VALERIA LAUTER, BRADLEY LOKITZ, MELANIE MAYES, ORNL — Stability of organic carbon compounds in soil is important for global climate futures which could be affected by the complexity of the mineral-organic carbon interfaces. We examined the nanoscale structure of model interfaces by depositing films of organic carbon compounds of contrasting chemical character, hydrophilic glucose, deuterated-amphiphilic stearic acid (SA) and Natural Organic Matters (NOM) onto a soil mineral analogue (Al₃(OH)₄). The NOM was separated into its component such components as NOM-Phiic and NOM-Phobic when it is deposited onto the soil mineral. We used Neutron Reflectivity technique to understand the depth-organization of the thin films. The result indicates that glucose molecules reside in a layer between Al₂O₃ and stearic acid and SA self-assembles. No self-assembly of SA was observed when SA and NOM-Phobic was deposited on the mineral soil. Molecular dynamics simulations reveal the thermodynamic driving force behind glucose partitioning on the mineral interface.

1Funded by ORNL Director’s Research and Development Program. Research at ORNL was sponsored by the BES, DOE.

12:51PM G8.00009 Sliding friction of thick and thin oxygen layers on spin crossover materials*, ZACHARY B. FREDRICS, K. M. STEVENS, DANIEL DOUGHERTY, JACQUELINE KRIM, North Carolina State University — Friction at the nanoscale is known to encompass phononic, electrostatic, conduction electronic and magnetic effects [1], with relatively little known about magnetic contributions to friction [2]. To probe such effects we have employed a quartz crystal microbalance technique to record the sliding friction associated with thin and thick films of solid and liquid oxygen, a paramagnetic material, atop nanoscale films of the spin-crossover material Fe([H₂Bpz₂]₂)bpv, which is diamagnetic at cryogenic temperatures and paramagnetic at room temperature. Previously these systems have been shown to be frictionally sensitive to the application of small fields, for Pb(111) substrates [3]. We observe changes in dissipation as well for Fe([H₂Bpz₂]₂)bpv, in response to externally applied magnetic fields. We will report our efforts to model the frictional interaction, which is reduced in the presence of a weak applied magnetic field, and is also observed to be temperature dependent.


1:03PM G8.00010 Imaging Surface Reactions of Formaldehyde on TiO₂*, ZHENRONG ZHANG, Department of Physics, Baylor University, MIRU TANG, Department of Chemistry and Biochemistry, Southern Illinois University, ZHI-TAO WANG, Pacific Northwest National Laboratory, ZHU KE, YAOBIAO XIA, KENNETH PARK, Department of Physics, Baylor University, IGOR LYUBINETS, ZDENEK DOHÁLEK, Pacific Northwest National Laboratory, QINGFENG GE, Department of Chemistry and Biochemistry, Southern Illinois University — Formaldehyde is involved in many surface catalytic and photo-catalytic reactions on metal oxides. We studied surface reactions of formaldehyde on reduced TiO₂(110) surfaces using variable-temperature scanning tunneling microscopy (STM) and density functional theory (DFT). STM images taken from a same area at various temperatures clearly show that formaldehyde preferentially adsorbs on the bridge-bonded oxygen vacancy (V₂O) defect sites. Bias-dependent STM images suggest the bonding configurations of the Ti-bound CH₂O and the V₂O-bound CH₂O. The isothermal time dependent images show the rotation of V₂O-bound CH₂O and the two diffusion channels of formaldehyde at different temperatures. We also directly observed the formation of formaldehyde dimmer.

1:15PM G8.00011 Water adsorption on non polar ZnO surfaces: from single molecules to multilayers*, STEPHANE KENMOE, P. ULRICH BIEDERMANN, Max-Planck Institute fuer Eisenforschung — The interface between water and ZnO plays an important role in many domains of technological relevance. Following the vital role of adsorbed water on substrate properties and the fascinating properties of interfacial water, there is a great interest in characterizing this interface. We use DFT to study the possible aggregation regimes that can form on the ZnO non-polar low-index (1010) and (1120) surfaces. We study the adsorption of water monomers, small water clusters like water dimers, water chains, ladder-like water structures, water thin films and water multilayers. Based on this, trends in binding energy as well as the binding mechanisms are analyzed to understand the driving forces and the nature of the fundamental interactions that stabilize the adsorbed layers.

1:27PM G8.00012 Adsorption, vibration and diffusion of oxygen on Ag(110)*, KATAK RAWAL, SAMPOYO HONG, University of Central Florida, AKI PULKINEN, Lappeenranta University of Technology, MATTI ALATALO, University of Oulu, TALAT RAHMAN, University of Central Florida — We have performed density functional theory calculations for the adsorption, vibration and diffusion of oxygen on Ag(110). At low coverage, O₂ adsorbs at the four-fold hollow (FFH) with the molecular axis aligned along the [110] direction. The dissociation of O₂ is easier along the [001] direction than along the [110] direction. For O₂ species in FFH aligned along the [001] the O-O intra-molecular stretching mode is coupled with the substrate vibration and thus its dissociation can be induced by surface phonon. In addition, O diffusion barrier from FFH to next FFH along the [110] is small (0.07 eV only) but is by far larger (0.4 eV) along [001]. On the other hand, O species in the short-bide (SB) site prefers to diffuse along the [001] (to FFH) rather than along the [110] direction (to next SB). Finally, the preference of atomic oxygen to form O-Ag-O complex on Ag(110) is responsible for disordering of the surface by means of substantial lateral and vertical displacements of Ag atoms in the topmost layer. In fact, such disordering phase of Ag(110) may act as a precursor of the reconstructed phase of Ag(110).

1Work supported in part by NSF under grant CHE-1310327
on the adsorption energy of CO thin film. The adsorption/desorption energy for desorption was obtained. (XPS) and Auger Electron Spectroscopy (AES). Our results revealed that carbon dioxide interacts with CuFeO2 forming Fe carbonates compounds on its surface.

resulted with highly epitaxial crystal structure. The adsorption/desorption of CO2 and H2O process was also monitored with X-ray Photoelectron Spectroscopy (XPS). A standard UHV chamber, The CuFeO2 thin film grown using Pulsed Laser Deposition (PLD) over an Al2O3 (0001) substrate with controlled O2 atmosphere was employed to investigate the effective thermal conductivity (Keff) and thermal boundary resistances (Rbd) of polymer composites containing carbon nanotubes (CNTs) and inorganic nanoparticles. By considering the synergistic effect of CNTs and nanoparticles, our model more accurately predicted Keff of 3-phase composites than effective medium theories (EMTs). Complex morphology of CNTs (diameter, length) and the heat transfer at interfaces (Rbd) were quantified to study their influences on Keff. By matching the simulated Keff with the measured Keff, Rbd of polymer-CNT and polymer-nanoparticle could be estimated. The results showed that Keff of composites increases when CNT fraction increases and when Rbd of polymer-nanofillers (CNTs and nanoparticles) decreases. CNT bundle was built to investigate its effect on Keff of composites, which had not been considered in EMTs. It was found that when CNT bundles increase, Keff decreases in the composites with random and parallel CNTs, whereas, Keff increases in those with perpendicular CNTs.
11:51AM G9.00004 High-throughput computational search for new high mobility transparent (semi)conducting oxides, GEOFFROY HAUTIER, Université catholique de Louvain — Transparent conducting oxides (TCOs) are large band gap materials (to favor transparency) doped with electrons (n-type) or holes (p-type). TCOs are essential to many technologies from solar cell to transparent electronics. We will discuss several unsolved problems with promising electronic structures and present preliminary experimental results. Beyond the description of new TCO candidates, I will chemically rationalize our findings, highlighting several design strategies towards the development of future high mobility TCOs.

12:27PM G9.00005 Transparent Conductive Oxides as Near-IR Plasmonic Materials for Energy Conversion, ARRIGO CALZOLARI, CNR-NANO-S3, ALICE RUINI, Universita’ di Modena e Reggio Emilia, ALESSANDRA CATELLANI, CNR-NANO-S3, MARCO BUONGIORNO NARDELLI, University of North Texas — Using first principles calculations, we investigate the origin of near-infrared plasmonic activity in M-doped ZnO, one of the most promising transparent conducting oxide (TCO) materials. Our results [1-2] predict realistic values for the plasma frequency and the free electron density as a function of the M-doping, in agreement with recent experimental results. Then we characterize the plasmon properties of In-doped nanowires that have been envisaged as plasmonic nanoparticles for energy conversion applications.


12:39PM G9.00006 Engineering the bandgap of ferroelectric ZnSnO\textsubscript{3} via sulfur substitution, BRIAN KOLB, ALEXIE KOLPAK, MIT — Since its recent discovery, ferroelectric ZnSnO\textsubscript{3} has been investigated for utility in a number of applications. Its strong remnant polarization and good conductivity, for example, make it attractive as a photovoltaic material, but its relatively large 3 eV bandgap limits its potential usefulness. We find that the bandgap of ZnSnO\textsubscript{3} is highly sensitive to changes in lattice volume, which can be effected either with application of external strain or by substituting sulfur for oxygen. Upon forming the fully-substituted ZnSnS\textsubscript{3}, the bandgap reduces to a near-optimal 1.3 eV while retaining many of the important properties of the oxide, including a strong polarization. In this talk we describe the physics governing the tunable electronic structure of ZnSnO\textsubscript{3}, discuss the stability of the ZnSnS\textsubscript{3} analogue, and propose a route to its use in a photovoltaic cell by growth on a GaN substrate.

12:51PM G9.00007 p-type transparent conducting chalcogenides, HONGLIANG SHI, BAYRAMMURAD SAPAROV, DAVID SINGH, ATHENA SEFAT, MAO-HUA DU, Oak Ridge National Lab, MATERIALS SCIENCE & TECHNOLOGY DIVISION COLLABORATION — Transparent conducting materials are an important component in many optoelectronic devices ranging from solar cells to transparent electronics. A good transparent conducting material must allow high optical transmittance across a wide optical spectrum, requiring a large optical band gap (>3.0 eV), and have high conductivity. However, in materials high conductivity and large band gaps usually do not coexist. At present, only a few materials are known to be reasonably good n-type transparent conducting oxides (TCOs). The p-type TCOs are still plagued by their poor hole conductivity, usually two orders of magnitudes lower than the highest electron conductivity in the n-TCOs. Chalcogenides usually have better hole conductivity, but their band gaps are usually too small. In this study, first-principles calculations are used to design new chalcogenides with large band gaps. New ternary chalcogenides, i.e., C\textsubscript{5}S\textsubscript{2}Zn\textsubscript{4}Se\textsubscript{4} and C\textsubscript{5}S\textsubscript{2}Zn\textsubscript{3}Te\textsubscript{4}, are found by calculations to be chemically stable and have both large band gaps (>3.0 eV) and small effective masses. These new ternary chalcogenides are synthesized and found to be air stable.

1Part of this work was supported by the Department of Energy, BasicEnergy Sciences, Materials Sciences and Engineering Division.

1:03PM G9.00008 Comparative first principles study for Li, Na, and Mg storage at rutile, anatase, bronze, and amorphous TiO\textsubscript{2}, KONSTANTINOS KOTSIS, FLEUR LEGRAIN, SERGEI MANZHOS, National University of Singapore — TiO\textsubscript{2} has been studied very extensively and its applications in various fields, e.g. applications in energy storage and catalysis are well known [1, 2]. Crystalline, amorphous and amorphous/crystalline titania have emerged as anode materials for Li and post-Li batteries due to good capacity, high rates [2, 3], and safety. Which is why the electronic and atomic structures as well as the properties of various crystalline TiO\textsubscript{2} phases have recently attracted much research interest. Amorphous TiO\textsubscript{2} (a-TiO\textsubscript{2}) phase also looks promising based on the few available studies but is much less explored [3, 4, 5, 6]. We have previously shown that amorphization of Si improves storage energetics of Li, Na, Mg [7], and there are reasons to believe that a-TiO\textsubscript{2} will achieve the same. At high rates of charge-discharge, capacitive contribution to the specific capacity of titania electrodes becomes significant [8, 9, 10]. Therefore, interfacial effects are critical for the performance of titania-based anodes and need to be understood. We present a comparative first principles study of Li, Na, and Mg storage at rutile (R), anatase (A1), and (B) (110) surfaces) and amorphous TiO\textsubscript{2} and compare the results to Li, Na, Mg.

1:15PM G9.00009 Probing for cationic dopants in lanthanum manganite for solid oxide fuel cell applications, SRIDEVI KRISHNAN, VINITH SHARMA, Material Science and Engineering, Institute of Materials Science, University of Connecticut, Storrs, MANOJ K MAHAPATRA, PRABHAKAR SINGH, Material Science and Engineering, Center for Clean Energy Engineering, University of Connecticut, Storrs, RAMPAL RAMPRASAD, Material Science and Engineering, Institute of Materials Science, University of Connecticut, Storrs — Solid oxide fuel cells (SOFC) are an efficient source of clean energy. Long-term stability of SOFC cathodes is ensured along with thermophysical characteristics. Sr-doped LaMnO\textsubscript{3} is one of the active material for this application. A suitable choice of the dopant has a significant influence on the stability and performance of the cathode material at elevated operating temperature. Using first principles computations, we compare the stability of the LaMnO\textsubscript{3} host for a range of cationic dopants including alkali, alkaline earth metals, 3d, 4d and 5d transition metal elements in the absence and presence of an oxygen vacancy. The stability of doped LaMnO\textsubscript{3} against decomposition to various combinations of metals and oxides is assessed using a linear programming based algorithm, and the oxygen vacancy promoters are identified. Properties of the dopants like the ionic radius, oxidation state, magnetic moment and Mendeleev number are correlated with their potential usefulness. We find that the bandgap of ZnSnO\textsubscript{3} is highly sensitive to changes in lattice volume, which can be effected either with application of external strain or by substituting sulfur for oxygen. Upon forming the fully-substituted ZnSnS\textsubscript{3}, the bandgap reduces to a near-optimal 1.3 eV while retaining many of the important properties of the oxide, including a strong polarization. In this talk we describe the physics governing the tunable electronic structure of ZnSnO\textsubscript{3}, discuss the stability of the ZnSnS\textsubscript{3} analogue, and propose a route to its use in a photovoltaic cell by growth on a GaN substrate.

1:27PM G9.00010 Designing brownmillerite SrCoO\textsubscript{2.5} (BM-SCO) as a cathode material — a first principles study of oxygen diffusion process in BM-SCO, CHANDRIMA MITRA, TRICIA MEYER, HO NYUNG LEE, FERNANDO REBOREDO, Oak Ridge National Laboratory — The discovery and design of new materials for next generation energy devices are crucial steps towards addressing various energy-related issues. ABO\textsubscript{3−x} type perovskite oxides have emerged as promising candidates for cathode/electrolyte materials in solid oxide fuel cells (SOFC’s). In this work, we investigate oxygen diffusion in brownmillerite oxide SrCoO\textsubscript{2.5} (BM-SCO), employing a first principles approach. Our calculations indicate highly anisotropic diffusion pathways, which result from its anisotropic crystal structure. The one-dimensional vacancy channels are found to be reasonably good n-type transparent conducting oxides (TCOs). New ternary chalcogenides, i.e., C\textsubscript{5}S\textsubscript{2}Zn\textsubscript{4}Se\textsubscript{4} and C\textsubscript{5}S\textsubscript{2}Zn\textsubscript{3}Te\textsubscript{4}, are found by calculations to be chemically stable and have both large band gaps (>3.0 eV) and small effective masses. These new ternary chalcogenides are synthesized and found to be air stable.

1We gratefully acknowledge support from U.S Department of Energy, Basic Energy Sciences, Materials Science and Engineering Division.
1:39PM G9.00011 A DFT study of oxygen reduction reaction on single-atom Pt nanocatalyst , YOUNGJOO TAK, NORINA A. RICHTER, ALOYSIUS SOON, Global E3 Institute, Department of Materials Science and Engineering, YonseiUniversity, Seoul 120-749, Korea — Platinum is one of the most broadly used catalyst for many chemical reactions (e.g. oxygen reduction reaction). Although its great reactivity, platinum catalysis has not met enthusiastic reception from industry due to its high price. Pt/C catalyst is widely used to come over this problem, but still considered as an imperfect solution because of its poor stability [1,2]. Recently, platinum single-atom catalyst with TiN support has suggested and proved to be stable on the N vacancy site of TiN support under N-lean condition [3]. In this work, we present density-functional theory (DFT) study of the oxygen reduction reaction on single Pt atom embedded on the surfaces of TiN(100) and TiC(100) within the computational hydrogen model (CHE) [4].


1:51PM G9.00012 Gold-doped graphene as a cost-effective, highly stable and active electrocatalyst for the oxygen reduction reaction: prediction from first principles. SERGEY STOLBOV, MARIOL ALCANTARA ORTIGOZA, University of Central Florida — One of the main obstacles hindering large scale practical application of hydrogen fuel cells is a prohibited cost of the Pt (or Pt-based) catalysts for the oxygen reduction reaction (ORR) on the fuel cell cathode. In this work, we consider Au-doped graphene as an alternative to Pt for facilitating ORR. Our first-principles calculations show that Au atoms incorporated into graphene di-vacancies form a thermodynamically and electrochemically stable structure. Furthermore, calculation of the binding energies of the ORR intermediates reveals that Au-C bonding makes the C atoms neighboring to Au optimally reactive for ORR. The calculated ORR free energy diagrams suggest that the Au-graphene structures have an ORR onset potential as high as that of Pt. We also demonstrate that the linear relation among the binding energy of the reaction intermediates assumed in a number of works on computational high-throughput material screening does not hold, at least for this none purely transition-metal material.

2:03PM G9.00013 ABSTRACT WITHDRAWN

Tuesday, March 3, 2015 11:15AM - 2:15PM
Session G10 DCMP: Interacting Dirac and Parabolic Semimetals 007A - Igor Herbut, Simon Fraser University

11:15AM G10.00001 Influence of electronic band topology on phonon properties in Dirac materials1, ION GARATE, KUSH SAHA, KATHERINE LEGARE, Université de Sherbrooke — In Dirac materials, the interaction between electrons and long-wavelength phonons has been shown to induce and stabilize topological insulator [1-2]. Here report on a theoretical study of the converse effect, namely the influence of band topology on phonon properties. We calculate how electron-phonon interactions change the bulk phonon dispersion as a function of pressure and temperature, in both trivial and topological phases. We find that (i) topological insulators are more prone to lattice instabilities than trivial insulators, and (ii) Raman and neutron scattering measurements can be used to determine the electronic band topology.


1Research funded by Canada's NSERC and Quebec's RQMP

11:27AM G10.00002 Weyl Semimetal in the Limit of Strong Coulomb Interactions , AKIHKO SEKINE, KENTARO NOMURA, Institute for Materials Research, Tohoku University — Weyl semimetals have a topological property such that an energy gap opens only if the Weyl nodes with opposite chirality meet and annihilate each other. Then it is expected that Weyl semimetals are stable against perturbations. Motivated by this, we study the stability of a time-reversal symmetry broken Weyl semimetal with two nodes against strong 1/r long-range Coulomb interactions. We consider the case where magnetic impurities are doped into a 3D topological insulator, and take into account the 1/r Coulomb interactions between the bulk electrons. In this case, the system can be described by the U(1) lattice gauge theory. With the use of the strong coupling expansion of the lattice gauge theory and the mean-field approximation, we analyze the system from the strong coupling limit. It is shown that parity (spatial inversion) symmetry of the system is spontaneously broken in the strong coupling limit, and a different type of the Weyl semimetal, in which time-reversal and parity symmetries are broken, appears in the strong coupling limit.

11:39AM G10.00003 Topological Mott Insulator in Three-Dimensional Systems with Quadratic Band Touching , LUKAS JANSSSEN, IGOR HERBUT, Simon Fraser University — We will discuss the effects of the long-range Coulomb interaction in three-dimensional systems in which conduction and valence bands touch quadratically at the Fermi level. Such band structure is realized in various strongly spin-orbit-coupled materials, such as HgTe, α-Sn, and some pyrochlore iridates. We will argue that these systems may be unstable towards spontaneous formation of the strong topological Mott insulator already at weak long-range Coulomb interaction. The mechanism of the instability can be understood as the collision of a non-Fermi-liquid fixed point, discovered by Abrikosov in the 70s and revisited recently, with another, critical, fixed point, which approaches it in the coupling space as the system's dimensionality approaches a certain “critical dimension” from above. Some universal characteristics of this scenario, the width of the non-Fermi-liquid crossover regime, and the observability of the topological Mott phase will be discussed. Reference: I. F. Herbut and L. Janssen, Phys. Rev. Lett. 113, 106401 (2014).

11:51AM G10.00004 Interacting Weyl semimetals: characterization via the topological Hamiltonian and its breakdown , WILLIAM WITCZAK-KREMPA, Perimeter Institute for Theoretical Physics, MICHAEL KNAP, Harvard University, DMITRY ABANIN, Perimeter Institute for Theoretical Physics — Weyl semimetals (WSMs) have robust linearly-dispersing excitations. Unusual properties arise from the latter, such as anomalous electrodynamics responses and open Fermi arcs on boundaries. We derive a simple criterion to identify and characterize WSMs in an interacting setting using the exact electronic Green’s function at zero frequency, which defines a topological Bloch Hamiltonian. We apply this criterion by numerically analyzing, via cluster and other methods, interacting models with and without time-reversal symmetry. We thus identify mechanisms for how interactions move and renormalize Weyl fermions. Our methods remain valid in the presence of long-ranged Coulomb repulsion. Finally, we introduce a WSM-like phase for which our criterion breaks down, due to fractionalization of the electron.


12:03PM G10.00005 ABSTRACT WITHDRAWN
12:15PM G10.00006 Magnetotransport properties of three-dimensional Weyl semimetals

NAVNEETH RAMAKRISHNAN, MIRCO MILLETARI, SHAFFIQUE ADAM, Natl Univ of Singapore — We investigate theoretically the transport and magnetotransport properties of three-dimensional Weyl semimetals. We consider the RPA-Boltzmann transport theory relevant for non-interacting electrons scattering off randomly distributed charged impurities, and employ an effective medium theory to average over the resulting spatially inhomogeneous carrier density profile. Our formalism allows us to smoothly connect results for the minimum conductivity near the Dirac point with known results for the conductivity at high carrier density. In the presence of a non-quantizing magnetic field, we predict that the magnetoresistance shows a transition from quadratic at low magnetic fields to linear at higher fields. In addition, our formalism can qualitatively explain some recent unexpected experimental results on the mixed-chalcogenide compound TIBiS2Se. This work is supported by the Singapore National Research Foundation NRF-NRFF2012-01.

1:27PM G10.00007 Interaction-driven phase instabilities in two-dimensional quadratic band touching systems

JAMES MURRAY, National High Magnetic Field Laboratory, Tallahassee, KELLY PAWLAK, University of California, Santa Barbara, OSKAR VAFEK, National High Magnetic Field Laboratory and Florida State University — Quadratic band touching (QBT) systems, in which an upward-dispersing and a downward-dispersing energy band meet at a single point in momentum space, have emerged as an attractive arena in which to study multicriticality and intertwined orders driven by electron interactions. Analogous to the two-valley QBT occurring in bilayer graphene, single-valley QBTs such as those arising on checkerboard and kagome lattices exhibit phase instabilities in multiple channels even for arbitrarily weak interactions. Using a Wilsonian renormalization group procedure, we show - without requiring spin-orbit coupling or special values of the interaction - that the leading instabilities in the half-filled system are toward quantum anomalous Hall or quantum spin Hall phases. Upon doping away from half-filling, the repulsive interactions lead to superconductivity in s-wave or d-wave channels.

12:39PM G10.00008 Calculation of the magneto-optical response of Kane fermions in HgCdTe

JOHN MALCOLM, ELISABETH NICOL, University of Guelph — The concentration x = x_c ≈ 0.17 in Hg_xCd_{1-x}Te describes a critical value in the phase transition between semimetal (x < x_c) and semiconductor (x > x_c). At this critical value, the low-energy quasiparticle dispersion exhibits a node at the intersection of two doubly degenerate linear cones and an equally degenerate flat band: quasiparticles that have been dubbed Kane fermions [1]. We present our results for the calculation of the magneto-optical spectra of these Kane fermions in the three-dimensional material, which can be compared to experiment, and also for those confined to only two-dimensions. The latter allows for a direct comparison to the analogous theoretical Dirac-Weyl system in two dimensions with pseudospin one [2].


12:51PM G10.00009 Topological property and phase transition in three dimensional Dirac semimetal

YONGPING DU, BO WAN, XIANGANG WAN, Nanjing University — Based on first-principles calculations and effective model analysis, we find a new three dimensional Dirac semimetal. This material has a Dirac point protected by crystal symmetry. It can be driven into various topological phases and Weyl semimetal state by breaking symmetries. This material may have linear quantum magnetoresistance, quantum spin Hall effect.

Corresponding author

1:03PM G10.00010 Dirac Circles and Quantum Hall Effect in 3D Inversion-Symmetric Crystals

BENJAMIN J. WIEDER, Department of Physics and Astronomy, University of Pennsylvania, YOUNGKUK KIM, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, C.L. KANE, Department of Physics and Astronomy, University of Pennsylvania — In the presence of inversion and time-reversal symmetries, materials with weak spin-orbit coupling may host topologically protected Dirac line nodes. A band inversion transition in these systems can produce a line node which closes on itself and forms a protected Dirac circle. The surfaces parallel to this circle host zero-energy puddles in momentum space which are flat if the inverting bands have the same effective mass. In cases with differing effective masses, the surface modes disperse, but the bulk Dirac circle remains gapless. Adding an external magnetic field perpendicular to this circle creates surface Landau levels, whose number can be controlled by tuning the field strength. When a new level is created or destroyed, the bulk becomes gapless and the zero-temperature bulk conductivity displays a sharp peak. The sequence of conductivity peaks describes an unusual manifestation of the integer quantum hall effect. We characterize surface and bulk transport as a function of magnetic field strength and in the presence of disorder.

1:15PM G10.00011 Topological Node-Line Semimetal in Three Dimensional Graphene Networks

HONGMING WENG, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, YUNYE LIANG, New Industry Creation Hatchery Center, Tohoku University, Japan, QIUNAN XU, Institute of Physics, Chinese Academy of Sciences, RUI YU, International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science, ZHONG FANG, XI DAI, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, YOSHIYUKI KAWAZOE, New Industry Creation Hatchery Center, Tohoku University, Japan & Thermophysics Institute, Siberian Branch, Russian Academy of Sciences, Russia — Graphene, a two dimensional (2D) carbon sheet, acquires many of its amazing properties from the Dirac point nature of its electronic structures with negligible spin-orbit coupling. Extending to 3D space, graphene networks with negative curvature, called Mackay-Terrones crystals (MTC), have been proposed and experimentally explored, yet their topological properties remain to be discovered. Based on the first-principle calculations, we report an all-carbon MTC with topologically non-trivial electronic states by exhibiting node-lines in bulk. When the node-lines are projected on to surfaces to form circles, “drumhead” like flat surface bands nestled inside of the circles are formed. The bulk node-line can evolve into 3D Dirac point in the absence of inversion symmetry, which has shown its plausible existence in recent experiments.

1:27PM G10.00012 Topological states of Sb thin films over doped graphene

CHI-HSUAN LEE, CHIH-KAI YANG, National Chengchi University — Electronic properties of Sb thin films on pure, boron-doped, and nitrogen-doped graphene are investigated using density functional calculations. Various stacking configurations are taken into consideration. Sb films on boron-doped graphene have stronger interaction than those on pure or nitrogen-doped graphene. Dirac cones also occur in these systems and can serve as conduits for spin-polarized conduction. The results are useful for applications in topological transport and spintronics.

1:39PM G10.00013 ABSTRACT WITHDRAWN
1:51PM G10.00014 Phonon analogue of topological nodal semimetals. HOI CHUN PO, YASAMAN BAHRI, ASHVIN VISHWANATH, Univ of California - Berkeley — Recently, Kane and Lubensky proposed a mapping between bosonic phonon problems on isostatic lattices to chiral fermion systems based on factorization of the dynamical matrix [Nat. Phys. 10, 39 (2014)]. The existence of topologically protected zero modes in such mechanical problems is related to their presence in the fermionic system and is dictated by a local index theorem. Here we adopt the proposed mapping to construct a two-dimensional mechanical analogue of a fermionic topological nodal semimetal that hosts a robust bulk node in its linearized phonon spectrum. Such topologically protected soft modes with tunable wavevector may be useful in designing mechanical structures with fault-tolerant properties.

2:03PM G10.00015 Photoinduced Topological phase Transition in a 2D Fermi System with a Quadratic Band Crossing. XIAOTING ZHOU, GREGORY A. FIETE, Department of Physics, Univ of Texas, Austin — Recent years, physicists have been gripped by the topological phases in condensed matter systems, and many attentions have been concentrated on the pursuit of new topological matters. The achievement of the topological control by the external fields provides a new direction. Using Floquet theory, we demonstrate that, a topologically stable quadratic band-crossing point (QBCP), carrying a Berry flux $\pm 2\pi i$ (or $-2\pi i$), would be splitted into 2 Dirac points with Berry flux $\pi$ (or $-\pi$), by the irradiation of a linearly polarized light. And the QBCP will either be lifted due to the breaking of the time-reversal symmetry, or go to a trivial QBCP with distinct topological properties, by introducing a circularly polarized light. Therefore, the manipulation of band structure could be realized.

Tuesday, March 3, 2015 11:15AM - 2:15PM – Session G11 DMP: Focus Session: Superconductivity in the 2D Limit

11:15AM G11.00001 Superconductivity in Electric Double Layer Capacitor under Pressure. M. MCCANN, MARTIN MISEK, KONSTANTIN KAMENEV, ANDREW HUXLEY, Centre for Science at Extreme Conditions, The University of Edinburgh — Chemical doping generally provides the most common method for tuning into the superconducting state of a material yet can be difficult to control and also potentially introduces structural disorder complicating the underlying physics. Electric Double Layer devices however provide a means to electrostatically dope materials with high electric fields allowing continuous tuning of a 2D superconducting state thus avoiding such issues. One such device is the Electric Double Layer Capacitor which can detect the onset of superconductivity through AC magnetisation measurements. We make use of a similar device in an attempt to electrostatically dope and tune the superconductivity in the cuprate compound La$_1.9$Sr$_0.07$CuO$_4$ as well as investigating whether application of pressure improves its efficiency.

11:27AM G11.00002 Doping evolution and polar surface reconstruction of the infinite-layer cuprate Sr$_{1−x}$La$_x$CuO$_2$. JOHN HARTER, Department of Physics, Cornell University, LUIGI MARITATO, DARRELL SCHLOM, Department of Materials Science and Engineering, Cornell University, KYLE SHEN, Department of Physics, Cornell University — We use angle-resolved photoemission spectroscopy to study the doping evolution of infinite-layer Sr$_{1−x}$La$_x$CuO$_2$ thin films grown by molecular-beam epitaxy. At low doping, the material exhibits a dispersive lower Hubbard band typical of the superconducting cuprate parent compounds. Electron diffraction probes reveal a $p(2 \times 2)$ reconstruction of the surface. Using a number of simple assumptions, we develop a model of this reconstruction based on the polar nature of the infinite-layer material. As carriers are added to the system, a continuous evolution from Mott insulator to superconducting metal is observed as a coherent low-energy band develops with a concomitant remnant lower Hubbard band, gradually lifting in the Mott gap. This two-component spectral function emphasizes the important role that strong local electron correlations play in the electronic structure of Sr$_{1−x}$La$_x$CuO$_2$ even at relatively high doping levels. Finally, we confirm the theoretical prediction of a thickness-controlled transition in ultrathin films of SrCuO$_2$ grown on nonpolar SrTiO$_3$, highlighting the diverse structural changes that can occur in polar complex oxide thin films.

11:39AM G11.00003 Oxygen redistribution and induced high-Tc superconductivity at the CaCuO$_2$/SrTiO$_3$ interface. CLAUDIA CANTONI, Oak Ridge National Laboratory, DANIELE DI CASTRO, CNR-SPIN and Dipartimento di Ingegneria Civile e Ingegneria Informatica, Universitá' di Roma Tor Vergata, Via del Politecnico 1, I-00133 Roma, Italy, CARMELA ARUTA, CNR-SPIN, Dipartimento di Scienze Fisiche, Via Cintia, Mont S. Angelo, 80126 Napoli, Italy, GIUSEPPE BAILESTRINO, CNR-SPIN and Dipartimento di Ingegneria Civile e Ingegneria Informatica, Universitá’ di Roma Tor Vergata, Via del Politecnico 1, I-00133 Roma, Italy — High-Tc cuprate superconductors (HTS) can be extended and anisotropy of the 2D-superconductivity and the Rashba spin-orbit field can be largely modulated by controlling the 2D-QW subband filling. Our results indicate a route to manipulate selectively the electronic properties of QWs at the LaAlO$_3$/SrTiO$_3$ interface, naturally suggesting the opportunity to exploit similar interfaces as a charge reservoir to dope a cuprate IL. We have explored the system in which LAO is replaced by the insulating IL CaCuO$_2$ (CCO/STO interface) and found a Tc of 50 K. This interface closely reproduces the IL/CR native interface of HTS and can be used to extract important information on the physical processes occurring in HTS. Present atomicly resolved ABF-STEM and EELS measurements, which combined with XAS uncover the existence of interfacial apical O atoms. We will discuss their electronic signature for superconductivity.

11:51AM G11.00004 Engineering LaAlO$_3$/SrTiO$_3$ quantum wells by selective orbital occupancy. GERVASI HERRANZ, Institute for Materials Science of Barcelona ICMAB-CSIC — The two-dimensional confinement of electrons in quantum wells (QWs) along the interface between two semiconductors such as Si or GaAs has been fundamental for technology as well for the development of new fundamental concepts. More recently, the discovery of 2D-QWs in oxides, with the flagship interface between LaAlO$_3$ and SrTiO$_3$, has been heralded as a milestone in the research of 2D electron systems. Unlike more conventional 2D-QWs based on III-V or II-VI semiconductors, carriers at LaAlO$_3$/SrTiO$_3$ populate narrow 3d-bands, where strong correlations underlie complex phases not present in conventional semiconductors. In LaAlO$_3$/SrTiO$_3$ not all the electrons reside in the same QW subband and, indeed, they behave differently depending on which orbital are they occupying. Here we demonstrate that the symmetry of the conduction band inside the QWs can be selected, disclosing unprecedented ways to tailor the electron properties. More specifically, we show that the spatial extension and anisotropy of the 2D-superconductivity and the Rashba spin-orbit field can be largely modulated by controlling the 2D-QW subband filling. Our results indicate a route to manipulate selectively the electronic properties of QWs at the LaAlO$_3$/SrTiO$_3$ interface, opening new prospects to understand the link between orbital symmetry and 2D-superconductivity and to achieve enhanced properties suitable for spin-dependent transport.
12:27PM G11.00005 Top gating control of superconductivity at the LaAlO3/SrTiO3 interfaces. ALEXIS JOUAN, SIMON HURAND, CHERYL FEUILLET-PALMA, GYANENDRA SINGH, JEROME LESUEUR, NICOLAS BERGAL, Laboratoire de Physique et d’Etude des Matériaux - CNRS - ESPCI ParisTech - UPMC, EDOUARD LESNE, NICOLAS REYREN, Unite Mixte de Physique CNRS-Thales, 1 Av. A. Fresnel, 91767 Palaiseau, France — Transition metal oxides display a great variety of quantum electronic behaviors. Epitaxial interfaces involving such materials give a unique opportunity to engineer artificial materials where new electronic order parameters take place. It has been shown that a superconducting two-dimensional electron gas could form at the interface of two insulators such as LaAlO3 and SrTiO3 [1], or LaTiO3 and SrTiO3 [2]. An important feature of these interfaces lies in the possibility to control their electronic properties, including superconductivity and spin-orbit coupling (SOC) with field effect [3-5]. However, experiments have been performed almost exclusively with a metallic gate on the back of the sample. In this presentation, we will report on the realization of a top-gated LaAlO3/SrTiO3 device whose physical properties, including superconductivity and SOC, can be tuned over a wide range of electrostatic doping. In particular, we will present a phase diagram of the interface and compare the effect of the top-gate and back-gate. Finally, we will discuss the field-effect modulation of the Rashba spin-splitting energy extracted from the analysis of magneto-transport measurements. Our result paves the way for the realization of mesoscopic devices where both superconductivity and SOC can be tuned locally.

12:39PM G11.00006 Electric field modulation of superconductivity and kondo effect in LaAl1−xCrxO2/SrTiO3 interfaces, GYANENDRA SINGH, ALEXIS JOUAN, SIMON HURAND, CHERYL PALMA, LPEM -CNRS-ESPCI ParisTech-UPMC, 10 Rue Vauquelin - 75005 Paris, France, PRAMOD KUMAR, ANJANA DOGRA, RAMESH BUDHANI, National Physical Laboratory, New Delhi 110012, India, JEROME LESUEUR, NICOLAS BERGAL, LPEM -CNRS-ESPCI ParisTech-UPMC, 10 Rue Vauquelin - 75005 Paris, France — Two-dimensional electron gas exhibit superconductivity and spin orbit coupling (SOC) at the interfaces of two insulators LaOx/SrTiO3 (where x = Al, Ti and Ga) [1-3], whereas no conductivity is seen when X is replaced by Cr and Mn [4]. We present low temperature measurements of LaAl1−xCrxO2/SrTiO3 interfaces for Cr doping of x = 0, 0.1, 0.2. We show a sharp superconducting transition (Tc) at 175 mK for undoped sample (x = 0) which becomes broader for the Cr doping of x = 0.1 with Tc of 100 mK. Further Cr doping to x = 0.2 indicate no sign of superconductivity. We have analyzed the results with hallmark carrier density and SOC as a function of Cr doping. The temperature dependent sheet resistance below 50 K display an upturn for x = 0 which becomes more pronounced with Cr doping. We discuss the results on the basis of kondo scattering which can be modulated by varying the carrier density.


12:51PM G11.00007 Enhanced transition temperature due to tetragonal domains in two-dimensional superconducting strontium titanate, HILARY NOAD, SIMES, SLAC National Accelerator Laboratory; Department of Applied Physics, Stanford University, KATJA NOWACK, Department of Applied Physics, Stanford University, ERIC SPANTON, SIMES, SLAC National Accelerator Laboratory; Department of Applied Physics, Stanford University, HISASHI INOUE, Department of Applied Physics, Stanford University, MINU KIM, CHRIS BELL, YASUYUKI HIKITA, SIMES, SLAC National Accelerator Laboratory, HAROLD Y. HWANG, SIMES, SLAC National Accelerator Laboratory; Department of Physics and Applied Physics, Stanford University, KATHRYN MOLER, SIMES, SLAC National Accelerator Laboratory; Departments of Physics and Applied Physics, Stanford University, MATS HORSDAL, University of Oslo, Norway, TIMO HYART, University of Jyväskyla, Finland, GINIYAT KHALILULLIN, Max Planck Institute for Solid State Research, Germany, BERND ROSENOW, Leipzig University, Germany — We show, how in principle, a coherent coupling between two superconductors of opposite parity can be realised in a three-layer oxide heterostructure. Due to strong intrasubband spin-orbit coupling in the middle layer singlet Cooper pairs are converted into triplet ones, and vice versa. The result is a large enhancement of the triplet order parameter that persist well beyond the native triplet critical temperature.

1Research Council of Norway

1:03PM G11.00008 Enhancing Triplet Superconductivity by the Proximity to a Singlet Superconductor in Oxide Heterostructures1, MATS HORSDAL, University of Oslo, Norway, TIMO HYART, University of Jyväskyla, Finland, GINIYAT KHALILULLIN, Max Planck Institute for Solid State Research, Germany, BERND ROSENOW, Leipzig University, Germany — We propose a new mechanism of the interfacial superconductivity observed in many heterostructures composed of different materials including high-temperature superconductors. Our proposal is based on the use of the Ginzburg–Landau equations applicable to a wide class of systems. The system under consideration is assumed to have, alongside the superconducting order parameter, also another competing order that might be a charge- or spin-density wave. At certain temperatures or doping level the superconducting state is not realized (thus, “hidden”), while the amplitude of another order parameter corresponds to a minimum of the free energy. We also assume that at an interface or at a defect, the non-superconducting order parameter is suppressed (strongly or weakly), e.g., due to an enhanced impurity scattering. The local superconductivity is shown to emerge at the interface, and the spatial dependence of the corresponding order parameter is described by the Gross–Pitaevskii equation. The quantized values of the temperature and doping levels, at which Δ(x) arises, are determined by the “energy” levels of the linearized Gross–Pitaevskii equation, i.e., of the Schrodinger equation. Interestingly, the local superconductivity arises even at a small suppression of the rival order.

1We appreciate the support from DFG via the Projekt EF 11/8-1; K. B. E. gratefully acknowledges the financial support of the Ministry of Education and Science of the Russian Federation in the framework of Increase Competitiveness Program of NUST “MISIS.”

1:15PM G11.00009 Hidden Order as a Source of Interface Superconductivity1, ANDREAS MOOR, ANATOLY VOLKOV, KONSTANTIN EFETOV, Institut für Theoretische Physik III, Ruhr-University Bochum — We propose a new mechanism of the interfacial superconductivity observed in many heterostructures composed of different materials including high-temperature superconductors. Our proposal is based on the use of the Ginzburg–Landau equations applicable to a wide class of systems. The system under consideration is assumed to have, alongside the superconducting order parameter, also another competing order that might be a charge- or spin-density wave. At certain temperatures or doping level the superconducting state is not realized (thus, “hidden”), while the amplitude of another order parameter corresponds to a minimum of the free energy. We also assume that at an interface or at a defect, the non-superconducting order parameter is suppressed (strongly or weakly), e.g., due to an enhanced impurity scattering. The local superconductivity is shown to emerge at the interface, and the spatial dependence of the corresponding order parameter is described by the Gross–Pitaevskii equation. The quantized values of the temperature and doping levels, at which Δ(x) arises, are determined by the “energy” levels of the linearized Gross–Pitaevskii equation, i.e., of the Schrodinger equation. Interestingly, the local superconductivity arises even at a small suppression of the rival order.

1We appreciate the support from DFG via the Projekt EF 11/8-1; K. B. E. gratefully acknowledges the financial support of the Ministry of Education and Science of the Russian Federation in the framework of Increase Competitiveness Program of NUST “MISIS.”

1:27PM G11.00010 A The effects of non-linear electron-phonon interactions on superconductivity and charge-density-wave correlations, SHAOZHI LI, STEVE JOHNSTON, Department of physics and Astronomy, Univ of Tennessee, Knoxville — Linear treatments of the electron-phonon (e-ph) interaction, derived from Taylor expansions of the lattice potential, often predict large lattice distortions in the strong coupling limit; however, the prediction of large lattice displacements violates the assumptions underlying the linear model, indicating that the higher-order non-linear terms should also be included. In this talk, we examine non-linear e-ph interactions in a two-dimensional Holstein-like model using non-perturbative determinant quantum Monte Carlo. We show that even small non-linear interactions dramatically suppress charge-density-wave formation and s-wave superconductivity that are predicted by the linear e-ph model. These effects are attributed to a combined hardening of the phonon frequency and a renormalization of the effective linear coupling to weaker values.
To test this, we compare the behavior of edge and corner junctions on a patterned bilayer of Nb and Bi$_2$ phase-sensitive Josephson interferometry. It is predicted that the proximity region should have p-wave pairing symmetry with spin-dependent chiral components.

We are exploring the nature of the proximity-induced order in 3D topological insulators in contact with an s-wave superconductor by group methods to extract universal transport characteristics of superconductor/quantum spin Hall heterostructures where the native edge states serve as a group method.

Institute of Technology, Pasadena, CA 91125, USA — Interfacing s-wave superconductors with quantum spin Hall systems provides a promising route to "engineering" topological superconductivity. Given exciting recent progress on the fabrication side, identifying experiments that definitively expose the topological superconducting phase (and clearly distinguish it from a trivial state) raises an increasingly important problem. With this goal in mind we use renormalization group methods to extract universal transport characteristics of superconductor/quantum spin Hall heterostructures where the native edge states serve as a lead. Interestingly, arbitrarily weak interactions induce qualitative changes in the behavior relative to the free-fermion limit, leading to a sharp dichotomy in conductance for the trivial (narrow superconductor) and topological (wide superconductor) cases. Furthermore, we find that strong interactions can in principle induce power-law-localized "parafermion" excitations at a superconductor/quatum spin Hall junction.

Layered group-VI dichalcogenides are two dimensional materials that engender novel coupled spin and valley physics. Characterized by strong spin-orbit coupling and inversion symmetry breaking, they give rise to novel phenomena such as the spin Hall effect and valley Hall effect. In this talk, we focus on the intrinsic and substrate induced superconducting phases expected in this new class of materials. Generically, two types are expected: (1) Cooper pairing with finite center-of-mass momentum, and (2) zero momentum pairs analogous to the conventional BCS phase. We establish the conditions for the realization of each type. Time permitting, we will discuss the nature of the quasiparticles resulting from valley-discriminating pair-breaking processes.

Though precise superconducting nature of the system is still under theoretical debate, the observation motivates the study of superconductivity in this atomic layer system. In particular, the valley-spins locking of the p-doped MoS$_2$ monolayer suggests possibility of exotic type of superconductivity in the system. We use two-step perturbative renormalization group treatment to study superconducting instabilities in various channels and discuss the possibility of an exotic modulated superconductor.

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The practicality and robustness of this novel scheme for producing a 1D p-wave superconductor is discussed [2].

The superconducting proximity effect in a synthetic helical liquid, formed in a quantum wire in the presence of a spatially periodic Rashba interaction [1]. The implications for transport in normal-superconductor junctions in this system will be discussed.

The presence of a vortex in the order parameter winding around the wire is essential to have a non-trivial invariant. In addition, we present a full phase diagram of the model as a function of chemical potential, flux and superconducting pairing, emphasizing that not all regions present a fully gapped superconducting state.

By computing the topological invariant of the system from both a continuum Dirac fermion model and a lattice realization of a TI. We demonstrate that the presence of a vortex in the order parameter winding around the wire is essential to have a non-trivial invariant. In addition, we present a full phase diagram of the model as a function of chemical potential, flux and superconducting pairing, emphasizing that not all regions present a fully gapped superconducting state.

In recent work, we showed how a topological state can be induced from regular or irregular scattering in (i) p-wave superconducting wires and (ii) Rashba wires in proximity to an s-wave superconductor. We also related the topological properties of such nanowires to their normal state properties as well as conductance [2]. In the present work, we build on these results and study the correlation between parity-crossings in the superconducting state and the normal state properties of a hybrid nanostructure. Surprisingly, we find that the crossing points are not as well defined as the statistics are for other universality classes. We obtain formulae for mean spacing between parity crossings as well as crossing statistics in disordered wires/cavities. We finally discuss under what conditions these crossings signal Majorana fermions. [1] I. Adagideli et al. [2] I. Adagideli, M. Wimmer, A. Teker, Phys Rev B 89, 144506 (2014)

12:03PM G12.00005 Probing the Superconducting Proximity Effect in a Topological Insulator using Scanning Tunneling Microscopy

IAN DAYTON, Department of Physics and Astronomy, Michigan State University, DUCK-YOUNG CHUNG, Materials Science Division, Argonne National Laboratory, THOMAS CHASAPIS, Department of Chemistry, Northwestern University, ERIC GOODWIN, REZA LOOOLEE, Department of Physics and Astronomy, Michigan State University, MERCOURI KANATZIDIS, Department of Chemistry, Northwestern University, STUART TESSMER, Department of Physics and Astronomy, Michigan State University — Topological insulators (TI) embody a new state of quantum matter characterized by topological invariants; this contrasts with superconductors (S), as superconductivity arises from a spontaneously broken symmetry of the underlying electron system. When a superconductor is placed on the surface of a topological insulator, the behavior of the superconducting condensate across the S/TI interface offers the opportunity to study the interplay between these two distinct quantum states. In this talk, we present our progress in applying cryogenic Scanning Tunneling Microscopy measurements to probe the local density of states in proximity to Pb/Bi2Se3 interfaces.

12:15PM G12.00006 Non-contact current-phase measurements of topological weak links with scanning SQUID

C.A. WATSON, I. SOCHNIKOV, J.R. KIRITLEY, K.A. MOLER, Stanford University, M. DENG, W. CHANG, P. KROGSTRUP, T.S. JESPERSEN, J. NYGARD, C.M. MARCUS, University of Copenhagen, I. MAIER, C. GOULD, G. TKACHOV, E.M. HANKIEWICZ, C. BRÜNE, H. BUHMANN, L.W. MOLENKAMP, University of Würzburg — Topological superconductivity has recently generated substantial interest as a pathway to Majorana physics in the solid state. Experimental efforts have focused on the superconducting proximity effect in topologically non-trivial junctions, but proof of the topological nature of the induced superconductivity remains elusive. We employ scanning superconducting quantum interference device (SQUID) susceptometry to study conventional superconducting Nb rings interrupted by weak links of 3D topological insulator HgTe and Al rings with InAs nanowire junctions. Varying the flux through each ring, we directly measure the current-phase relation (CPR) of the junction. Forward skewness in the CPR of 3D-HgTe which persists even in junctions long compared to the mean free path suggests that helicity may play a role in the high transmittance of Andreev Bound States that carry the Josephson current. Progress In InAs nanowire junction CPR measurements is also discussed. These measurements showcase the CPR as a fundamental characteristic of superconducting weak links and establish scanning SQUID microscopy as a powerful probe for performing such measurements.

12:27PM G12.00007 Observation of anomalous current phase relation on Pb-Bi2Te3 Josephson devices

YUAN PANG, JIE SHEN, JUNHUA WANG, JUNYA FENG, FANMING QU, ZHAOZHEN LU, JIE FAN, GUANGTONG LIU, ZHONGQING JI, XIUNIAN JING, CHANGLI YANG, Institute of Physics, CAS, QINGFENG SUN, X. C. XIE, ICQM, Peking University, LIANG FU, Department of Physics, Massachusetts Institute of Technology, LI LU, Institute of Physics, CAS — Josephson devices based on s-wave superconductor Pb and 3D topological insulator Bi2Te3 have been fabricated and investigated down to low temperatures. Anomalous current phase relation (CPR) was observed, indicating the existence of an unconventional component of superconductivity. Our experiment demonstrates that hybrid devices based on s-wave superconductor and 3D topological insulator might provide a platform for searching for and manipulating Majorana bound state.

12:39PM G12.00008 Anomalous Resistance Increase on Topological Insulator Bi2Te3 Nanotubes with Superconductor Contacts

RENZHONG DU, YUEWEI YIN, LUDI MIAO, AOKUI SUN, QI LI, Department of Physics, Pennsylvania State University — Topological superconductivity has gained much attention in recent years since it has been predicted to exhibit exotic behaviors and host the Majorana states. We report transport studies on topological insulator Bi2Te3 nanotube with Nb superconductor contacts. The Bi2Te3 nanotubes were synthesized by solution phase method and have previously been proved to possess robust surface states with long phase coherency against strong bulk disorders. Superconducting Nb contacts on the nanotubes were fabricated by electron beam lithography process. An anomalous resistance upturn of the resistance in the nanotube was observed when the contacts became superconducting. When applying a magnetic field, the resistance upturn is reduced gradually and disappears when the magnetic field exceeds the Hc2 of Nb. From both the temperature and magnetic field dependence of the resistance upturn, we conclude that the resistance upturn is associated superconducting transition of the contact leads. Combination of Au and Nb leads have been fabricated with different channel length and the detailed experimental results will be discussed.

12:51PM G12.00009 Phase diagram for topological superconductivity in topological insulator nanowires

FERNANDO DE JUAN, University of California Berkeley, JENS BARDARSON, Max Planck Institute for Complex Systems, Dresden, RONI ILAN, University of California Berkeley — A topological insulator nanowire can be used as a platform to produce one dimensional topological superconductivity in the presence of magnetic fields and the proximity effect from a nearby superconductor. In this work, we discuss the conditions under which this can happen by computing the topological invariant of the system from both a continuum Dirac fermion model and a lattice realization of a TI. We demonstrate that the presence of a vortex in the order parameter winding around the wire is essential to have a non-trivial invariant. In addition, we present a full phase diagram of the model as a function of chemical potential, flux and superconducting pairing, emphasizing that not all regions present a fully gapped superconducting state. Implications for transport in normal-superconductor junctions in this system will be discussed.

1:03PM G12.00010 Superconducting proximity effect in a synthetic helical liquid

MARIANA MALARD, University of Brasilia, GEORGE JAPARIDZE, Ilia State University, HENRIK JOHANNESSON, University of Gothenburg — We explore the possibility of a superconducting proximity effect in a synthetic helical liquid, formed in a quantum wire in the presence of a spatially periodic Rashba interaction [1]. The practicality and robustness of this novel scheme for producing a 1D p-wave superconductor is discussed [2].


1:27PM G12.000012 Fermion Fractionalization to Majorana Fermions in Dimerized Kitaev Superconductor, RYOHEI WAKATSUKI, MOTOHIKO EZAWA, University of Tokyo, YUKIIO TANAKA, Nagoya University, NAOTO NAGAOSA, University of Tokyo, RIKEN CEMS — We study theoretically a one-dimensional dimerized Kitaev superconductor model which belongs to BDI class with time-reversal, particle-hole, and chiral symmetries. There are two sources of the particle-hole symmetry, i.e., the sublattice symmetry and superconductivity. Accordingly, we define two types of topological numbers with respect to the chiral indices of normal and Majorana fermions, which offers an ideal laboratory to examine the interference between the two different physics within the same symmetry class. Phase diagram, zero-energy bound states, and conductance at normal metal/superconductor junction of this model are unveiled from this viewpoint. Especially, the electron fractionalization to the Majorana fermions showing the splitting of the local density of states is realized at the soliton of the dimerization in this model.


1:39PM G12.00013 Majorana edge states in single layer graphene, LIN WANG, MINGWEI WU, University of Science and Technology of China, 96 JinZhai Road, Hefei, Anhui 230026 — We investigate the Majorana edge states in single layer graphene near the Dirac point with the Rashba spin-orbit coupling. We find that there exist naturally induced out-of-plane Zeeman splitting in the proximity of an s-wave superconductor. By calculating the topological invariant, we show the topological phase diagram. In the topological nontrivial regime, we study the Majorana edge states in the case of zigzag or armchair ribbon. For these two cases, both have two Majorana edge states along one edge. However, there exist strong anisotropies in the localization length, the group velocity and the momentum of the Majorana fermions in two ribbons. In addition, the effects of the in-plane Zeeman splitting and the disorder on the Majorana edge states are also discussed.

5:11PM G12.00014 Time-Reversal-Invariant $Z_4$ Fractional Josephson Effect, FAN ZHANG, University of Texas, Dallas, CHARLES KANE, University of Pennsylvania — We study the Josephson junction mediated by the quantum spin Hall edge states and show that electron-electron interactions lead to a dissipationless fractional Josephson effect in the presence of time-reversal symmetry. Surprisingly, the periodicity is $\pi$, corresponding to a Josephson frequency $eV/2h$. We estimate the magnitude of interaction-induced many-body level splitting responsible for this effect and argue that it can be measured by using tunneling spectroscopy. For strong interactions we show that the Josephson effect is associated with the weak tunneling of charge e/2 quasiparticles between the superconductors. Our theory describes a fourfold ground state degeneracy that is similar to that of coupled "fractional" Majorana modes but is protected by time-reversal symmetry. [Reference: PRL 113, 036401 (2014).]

2:03PM G12.00015 Magnetotransport response in the 3D topological insulator Bi2Te3 with indium superconducting electrodes, ZHUO WANG, TIANYU YE, RAMESH MANI, Georgia State University — 3D Topological insulators (TIs) include novel surface states which are protected by time reversal symmetry from backscattering by impurities. Recently, the superconducting proximity effect at the interface between a TI and a superconductor has been a focus of attention. Hence, our study explores the magnetotransport behavior of thin Bi$_2$Te$_3$ flakes with superconducting electrodes in a Hall bar configuration. Such specimens exhibit a magnetotransport anomaly resulting from the proximity effect. To better understand this magnetotransport anomaly, we examine here the effect of biasing thin Bi$_2$Te$_3$ flakes samples of different thicknesses simultaneously with both a dc and a low-frequency ac current through the same pair of contacts at the ends of the device. Here, we report the role of finite bias and electron heating on the observed effects.

Tuesday, March 3, 2015 11:15AM - 2:15PM – Session G13 DMP: Focus Session: Electrostatic Control of Phenomena at Complex Oxide Interfaces 007D - Rositsa Pentcheva, University of Duisburg-Essen

11:15AM G13.00001 Interrelation of polarity, screening, structure, and electronic states at nickelate interfaces, SOHRAB ISMAIL-BEIJI, Yale University — A basic property of metal oxides is ionicity: the metal (cation) and oxygen (anion) sites have different electron densities and thus different charge states. This then permits the existence of polarity whether (1) in static form deriving from the choice of the terminating atomic plane at an interface, or (2) in dynamic form through the existence of ferroelectricity which permits switching of the polarity at an interface. The polarity drives the accumulation of charge, modification of the atomic-scale structure, and alteration of the electronic states at an interface. Here we describe an interconnected body of recent collaborative work on nickelate interfaces where electronic transport is strongly modified by the presence of ferroelectricity and induced out-of-plane Zeeman splitting in the proximity of a s-wave superconductor. By calculating the topological invariant, we show the topological phase diagram. In the topological nontrivial regime, we study the Majorana edge states in the case of zigzag or armchair ribbon. For these two cases, both have two Majorana edge states along one edge. However, there exist strong anisotropies in the localization length, the group velocity and the momentum of the Majorana fermions in two ribbons. In addition, the effects of the in-plane Zeeman splitting and the disorder on the Majorana edge states are also discussed.


1 Primary support for this work is provided by the NSF via grant MRSEC DMR-1119826.
11:51AM G13.00002 Electrolyte Gating of SrTiO$_3$ Nanostructures, SAM STANWYCK, Department of Applied Physics, Stanford University, Stanford, CA, 94305, USA, PATRICK GALLAGHER, MENEYOUNG LEE, DAVID GOLDBER-GORDON, Department of Physics, Stanford University, Stanford, CA, 94305, USA — We report low-temperature transport measurements of a two-dimensional electron system (2DES) at the surface of Strontium Titanate. We use electrolyte gating to create the 2DES, and nanopatterning techniques to create gate-tunable submicron constrictions. We observe universal conductance fluctuations, from which we extract an electron dephasing rate linear in temperature, characteristic of electron-electron interaction in a disordered conductor. Furthermore, the dephasing rate has a temperature-independent offset, suggestive of unscreened local magnetic moments in the sample. Finally, we demonstrate that protecting the Strontium Titanate with a thin layer of hexagonal Boron Nitride allows us to create a 2DES with dramatically increased mobility, while also preventing surface electrochemistry.

12:03PM G13.00003 A high-mobility electronic system at an electrolyte-gated oxide surface, PATRICK GALLAGHER, MENEYOUNG LEE, TREVOR PETACH, Department of Physics, Stanford University, Stanford, California 94305, USA, SAM STANWYCK, Department of Applied Physics, Stanford University, Stanford, California 94305, USA, JAMES WILLIAMS, Department of Physics, Stanford University, Stanford, California 94305, USA, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan, DAVID GOLDBER-GORDON, Department of Physics, Stanford University, Stanford, California 94305, USA — Electrolyte gating is a powerful technique for accumulating large carrier densities in surface two-dimensional electron systems (2DES). Yet this approach suffers from significant sources of disorder: electrochemical reactions can damage or alter the surface of interest, and the ions of the electrolyte and various dissolved contaminants sit Angstroms from the 2DES. In this talk, we demonstrate that this disorder can be minimized by protecting the sample with a chemically inert, atomically smooth sheet of hexagonal boron nitride (BN). We illustrate our technique with electrolyte-gated strontium titanate, whose mobility improves more than tenfold when protected with BN. We find this improvement even for our thinnest BN, of measured thickness 6 Angstrom, with which we can accumulate electron densities nearing $10^{14}$ cm$^{-2}$. Our technique is portable to other materials, and should enable future studies where high carrier density modulation is required but electrochemical reactions and surface disorder must be minimized.

12:15PM G13.00004 LaAlO$_3$/SrTiO$_3$ field-effect nanodevices using in-situ-grown Au top gates$^1$, YUN-YI PAI, MENCHEH HUANG, Univ of Pittsburgh, HYUWONG WEE, LEE, CHANG-BEMO EOM, Univ of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Univ of Pittsburgh — Conductive atomic force microscope (c-AFM) lithography can create a wide range of nanostructures based on the LaAlO$_3$/SrTiO$_3$ system, including field effect transistor$^2$, single-electron transistor$^2$ and superconducting nanoelectronic$^3$. However, the operating range of gated devices is often limited by tunneling through insulating barriers. Using in-situ Au deposited on top of LaAlO$_3$, we create vertical field-effect devices with significantly lower leakage due to the large bandgap of LaAlO$_3$. We describe the fabrication process for vertical field-effect nanodevices and show representative transport measurements both at room temperature and low temperatures.

$^1$We gratefully acknowledge support for this work from NSF (DMR-1124131 and DMR-0704022 and DMR-1234096) and AFOSR (FA9550-10-1-0524 and FA9550-12-1-0342).


12:27PM G13.00005 Large Thermopower of δ-doped LaTiO$_3$/SrTiO$_3$ Interfaces and it’s Field Dependence$^1$, R.C. BUDHANI, Indian Institute of Technology, Kanpur & National Physical Laboratory, New Delhi, SHUBHANKAR DAS, P.C. JOSHI, A. RASTOGI, Z. HOSSAIN, Indian Institute of Technology, Kanpur — We will present the magneto-thermopower (S(T, H)) of interfacial delta LaTiO$_3$/SrTiO$_3$ heterostructure by an iso-structural antiferromagnetic perovskite LaCrO$_3$. The thermoelectric power of 2-dimensional electron gas (2DEG) of pure LaTiO$_3$/SrTiO$_3$ at 300 K is $\approx 118 \mu V/K$, but increases dramatically to 337 $\mu V/K$ on inserting 5 uc LaCrO$_3$ at the interface. The negative sign of the thermoelectric power confirms the electron as major carriers in these interfaces. A linear temperature dependence of S(T) has been observed in the temperature range 100 K to 300 K which is in agreement with the theory of diffusion thermopower of 2DEG. The S(T) shows a distinct enhancement at temperature $< 100$ K, where a Kondo-type minimum has been observed in sheet resistance. We attribute this maximum in S(T) to Kondo scattering of conduction electron by localized impurity spin at the interface. The S in this temperature range is suppressed significantly ($< 20\%$) by moderate magnetic field ($\lesssim 13 T$) applied either perpendicular or parallel to the film surface. The isotropic nature of the suppression of S by magnetic field further strengthen the Kondo based interpretation of S(T, H).

$^1$We acknowledge IIT Kanpur and CSIR India for funding this research work.

12:39PM G13.00006 Contrasting electrostatic tuning of the superconducting LaAlO$_3$/SrTiO$_3$ interface by top and back gating, ZHUOYU CHEN, HISASHI INOUE, YANWU XIE, HONGTAO YUAN, Stanford Univ, YASUYUKI HIKITA, SLAC Nat Acc Lab, HAROLD Y. HWANG, Stanford Univ & SLAC Nat Acc Lab, HWANG TEAM — We report an experimental study of electrostatic tuning of the superconducting interface in dual gated LaAlO$_3$/SrTiO$_3$ controlled by the electric field effect. The dual gate devices are formed by simultaneously gating from the top of the epitaxial LaAlO$_3$ layer and the back of the SrTiO$_3$ substrate. Along with electrostatic doping to tune the carrier density, the quantum well profile of the interface electron system is modified due to the inversion asymmetry of the structure, resulting in the modulation of the effective disorder of the system (carrier mobility). We find therefore a strong contrast in the superconducting phase transition by top versus back gating. Simultaneous gating provides a unique opportunity to tune both the carrier density and disorder in this 2D superconducting system.

12:51PM G13.00007 Electric field control of thermoelectric effect in oxide interface LaAlO$_3$/SrTiO$_3$, TOMOYA ASABA, FAN YU, GANG LI, BENJAMIN LAWSON, COLIN TINSMAN, University of Michigan, JOCHEN MANNHART, Max Planck Institute for Solid State Research, LU LI, University of Michigan — Oxide interface LaAlO$_3$/SrTiO$_3$ (LAO/STO) has been attracting huge interest and the origin of the magnetic-field-induced phase transition is yet to be understood. However, thermoelectric power studies, a powerful tool for detecting phase transitions, have been sparsely reported so far. In this study we measured the carrier density dependence of thermopower to understand the origin of this phase transition. Below critical carrier density, thermopower is found to increase dramatically while the interface is still conductive. These results may not only help in understanding the physics around the phase transition but also shed light on the significance of this system as a thermoelectric material.
Vis a well-established, potentially quite exotic, feature. We measure the resistance of the LAO/STO interface in an in-plane magnetic field perpendicular to well have more in common with each other than with LAO/STO. In these two systems, spin-orbit coupling effects are for many purposes unimportant or negligibly confined by at least one order of magnitude, in a regime closer to that achieved in graphene. Nonetheless, graphene and, for example, GaAs/AlGaAs quantum confinement of electrons is no longer synonymous with semiconducting quantum well. The mobile electrons at the metallic LAO/STO interface are better of Technology, E. COBANERA, Utrecht University, T. HYART, University of Jyväskylä, A.D. CAVIGLIA, Delft University of Technology — Today, the planar structures, we have investigated the possible coupling of the two superconducting sheets, tuning one of the two by electric field. We have also realized bilayer interfaces, where two superconducting liquids are separated by the LaAlO interfaces characteristic lengths (the coherence length and the superconducting thickness) as a function of the gate voltage by measuring the critical magnetic fields in 3 parallel and perpendicular geometry. We have also realized bilayer interfaces, where two superconducting liquids are separated by the LaAlO interfaces. In this work, we have mapped the evolution of the superconducting properties upon gate voltage tuning, revealing a surprising change in thickness of the superconducting layer across the phase diagram. Using a single LaAlO/SrTiO interface, we have realized field effect transistors and estimated the origin of such properties and explore potential application. We demonstrate the modulation of electrical transport properties in LAO/STO interface by electric field effect using electric double layer transistor (EDLT) configuration. In initially metallic samples, reversible metallic-insulating phase transition, field-effect transistor operation and electron mobility enhancement were observed in liquid-gated LaAlO/SrTiO interface. Due to enhancement of mobility, we can observe quantum oscillations of the conductance at liquid-gated LAO/STO interface.

1:03PM G13.00008 Link Between Mobile Band Population and Superconductivity in SrTiO3/LaAlO3 Interface, ERAN MANIV, MOSHE BEN SHALOM, ALON RON, IZHAR NEDER, MOSHE GOLDSSTEIN, ALEXANDER PALEVSKI, YORAM DAGAN, Tel Aviv University — The entire superconducting phase diagram of SrTiO3/LaAlO is scanned using back gate voltage. The superconducting transition temperature Tc and critical field Hc are recorded along with the Hall resistance and Shubnikov-de Haas (SdH) effect. The latter is sensitive only to the density of the mobile band while the former probes all bands. We find that Tc and Hc follow a similar non-monotonic gate voltage dependence as the SDH frequency and the low field Hall. This suggests that the mobile band is getting depopulated at high gate voltages resulting in the reduction of Tc on the overdoped side. We discuss a possible scenario for this peculiar behavior.

1:15PM G13.00009 External voltage control of LaAlO/SrTiO3 interface structure, HIROMASA FUJII, Osaka Univ., MAKOTO MINOHARA, KEK, CHRISTOPHER BELL, YASUYUKI HIKITA, HAROLD Y. HWANG, Stanford Univ., TSUYOSHI KIMURA, YUSUKE WAKABAYASHI, Osaka Univ. — Physical properties of the LaAlO (LAO)/SrTiO3 (STO) interface are controlled by external voltage such as voltage-induced metal-insulator transition [1] and superconductivity-insulator transition [2]. The modulated parameters by external voltage are not only the carrier density but also the Hall mobility [3]. In order to clarify local electric field and polarization around the interface, we have investigated the effect of external voltage on the interface structure at room temperature by means of a surface x-ray diffraction technique, crystal truncation rod (CTR) scattering. Our measurements were performed at BL-4C of the Photon Factory, KEK, Japan. A 5-unit-cell thick sample was prepared using the pulsed laser deposition technique. The scattered x-ray intensity profile shows slight external voltage dependence, which means that the interface structure is changed by the external voltage. We also found that the voltage dependence of the scattering intensity exhibits hysteresis. Least squares refinement revealed that main atomic displacement induced by the external voltage occur in the LAO. The displacements in STO at the interface are of the order of sub-pm, which is much larger than expected for bulk STO (∼0.01 pm).


1:27PM G13.00010 Superconducting properties of single and bilayer LaAlO/SrTiO3 interfaces, STEFANO GARIGLIO, ALEXANDRE FETE, DANFENG LI, WEI LIU, MARGHERITA BOSELLI, DQMP, University of Geneva, NICOLA LAS REYREN, Unite Mixte de Physique CNRS-Thales, JEAN-MARC TRISCON, DQMP, University of Geneva — The two-dimensional electron liquid present at the LaAlO/SrTiO3 interface exhibits superconductivity and hosts a large spin-orbit interaction. Quite remarkably, both phenomena can be controlled by an electric field. In this work, we have mapped the evolution of the superconducting properties upon gate voltage tuning, revealing a surprising change in thickness of the superconducting layer across the phase diagram. Using a single LaAlO/SrTiO interface, we have realized field effect transistors and estimated the characteristic lengths (the coherence length and the superconducting thickness) as a function of the gate voltage by measuring the critical magnetic fields in parallel and perpendicular geometry. We have also realized bilayer interfaces, where two superconducting liquids are separated by the LaAlO interfaces. In such structures, we have investigated the possible coupling of the two superconducting sheets, tuning one of the two by electric field.

1:39PM G13.00011 Domination of spin-orbit coupling in magnetotransport at the LaAlO/SrTiO3 interface, M. DIEZ, University of Leiden, A.M.R.V.L. MONTEIRO, G. MATTONI, E. MULAZIMOGLU, Delft University of Technology, E. COBANERA, Utrecht University, T. HYART, University of Jyväskylä, A.D. CAVIGLIA, Delft University of Technology — Today, the planar confinement of electrons is no longer synonymous with semiconducting quantum wells. The mobile electrons at the metallic LAO/STO interface are better confined by at least one order of magnitude, in a regime closer to that achieved in graphene. Nonetheless, graphene and, for example, GaAs/AlGaAs quantum well have more in common with each other than with LAO/STO. In these two systems, spin-orbit coupling effects are for many purposes unimportant or negligibly weak, and neither system has ever shown superconductivity. In contrast, spin-orbit coupling effects are strong at the LAO/STO interface, and superconductivity is a well established, potentially quite exotic, feature. We measure the resistance of the LAO/STO interface in an in-plane magnetic field perpendicular to the current, for a wide range of applied fields B, temperatures, and carrier densities controlled by a back-gate voltage Vg. Our measurements show dramatic, fast and very large drops in magnetoresistance, either as a function of B or Vg, decrease slowly with temperature and seem suggestive of magnetic ordering. However, we compare very well with an alternative explanation that strongly suggests that the effect of spin-orbit coupling on the band structure alone can dominate magnetotransport.
Tuesday, March 3, 2015 11:15AM - 2:15PM —
Session G14 DMP: Focus Session: Mesoscopic Materials and Devices 008A - Nina Markovic, Johns Hopkins University

11:15AM G14.00001 Nano-Josephson Superconducting Tunnel Junctions Direct-patterned in Y-Ba-Cu-O with a Focused Helium Ion Beam. SHANE CYBART, UC San Diego — Functional oxide materials are very sensitive to disorder and many transition from metal to insulator as disorder increases. This phenomenon has been used for many years to fabricate Josephson junctions in cuprate high-transition-temperature \( T_c \) superconductors like \( \text{YBa}_2\text{Cu}_3\text{O}_7 \) (YBCO). In this approach, ion irradiation is used to selectively disorder a nanoscale region of material between two superconducting electrodes, that serves as a Josephson barrier. Historically, the barriers created in this manner have been tens of nanometers in length which only allowed for the creation of superconductor-reduced-\( T_c \)-superconductor-junctions. We have reduced the length of the Josephson barriers to just a few nm by using a 500 pm diameter focused beam of helium ions. The smaller length of these barriers allows us to change the properties continuously from reduced \( T_c \) superconductor to normal metal, to insulator as a function of irradiation dose. We present data for several Josephson junctions fabricated in this manner using controlled doses. Our results are well-described by the Blonder, Tinkham, Klapwijk model (BTK) for microscopc electrical transport at an interface between a superconductor and a normal material. This model uses a single parameter related to barrier strength (irradiation dose in our experiments) and can describe current-voltage characteristics for barriers ranging from a strong barrier, such as an insulator in a tunnel junction, to a weak barrier like a normal metal. In the case of a strong barrier (a tunnel barrier) the only transport mechanism for Cooper pairs is direct Josephson tunneling whereas in the case of weaker barriers both tunneling and Andreev reflection occur. This technique could provide a reliable method for the realization of reproducible high-\( T_c \) Josephson junctions. I will present details of the technique and analysis of the results.

11:51AM G14.00002 Controlled fabrication of sub-15nm nanostructures of an arbitrary conductive material1. HANNAH HUGHES, TYLER MORGAN-WALL, NIKOLAUS HARTMAN, NINA MARKOVIC, Johns Hopkins University — Traditional lithographic techniques that are used to produce low-dimensional nanostructures are often limited in both the minimum achievable size and the control over the final resistance of the device. To achieve such control, we had developed a wet etching method with in-situ monitoring of resistance, but this method relies on an oxide layer to electrically isolate the monitoring circuit from the etching solution. We will present a more general method for fabricating sub-15 nm nanostructures out of various conductive materials without a need for an oxide layer.

1This work was supported by NSF DMR-1106167.

12:03PM G14.00003 Black Silicon Formation in Cryogenic Reactive Ion Etching. DAVID ABI SAAB, PHILIPPE BASSET, Universite Paris Est, ESIEE Paris, ESYCOM, MATTHEW J. PIEROTTI, MATTHEW L. TRAWICK, University of Richmond, DAN E. ANGELESCU, Universite Paris Est, ESIEE Paris, ESYCOM — We present both experimental data and computational modeling that explain some aspects of the formation of black silicon during cryogenic reactive ion etching (RIE) processes. We generate a phase diagram that predicts combinations of RIE parameters that lead to different black silicon geometries. We also show that the combination of needle- and hole-like features of various heights and depths in black silicon creates a uniquely smooth transition in refractive index that is responsible for the material’s low optical reflectivity. These details are captured by our model and confirmed by focused ion beam (FIB) nanotomography and scanning electron microscopy of black silicon surfaces during various stages of development. The model also correctly describes dynamical characteristics such as the dependence of aspect ratio on process time, and the prediction of new etching fronts appearing at topographical saddle points.

12:15PM G14.00004 Spin-filtering in nickel-oxide atomic junctions . RAN VARDIMON, MARINA KLIONSKY, OREN TAL, Weizmann Institute of Science, OREN TAL GROUP TEAM — Generating a highly spin-polarized current governed by electrons of a single spin type is of central importance for realization of nanoscale spintronics. We report on the detection of up to 100% spin-polarized currents across nickel-oxide atomic junctions formed between two nickel electrodes under cryogenic vacuum conditions. The degree of spin polarization is probed by analyzing the quantum shot noise resulting from the discrete statistics of electron transport. In sharp contrast to the insulating character of bulk nickel-oxide, our results can be explained by the emergence of a local half-metallic electronic structure, stemming from the distinct orbital hybridization of the low-coordinated junction atoms. These findings illuminate new directions for spin transport manipulations by atomic-scale material design.

12:27PM G14.00005 Evolution of Ni nanofilaments and electromagnetic coupling in the resistive switching of NiO1. YUXIANG LUO, Tsinghua University, China, DEPARTMENT OF PHYSICS, TSINGHUA UNIVERSITY, BEIJING, CHINA TEAM — Resistive switching effect in conductor/insulator/conductor thin-film stacks is promising for resistance random access memory with high-density, fast speed, low power dissipation and high endurance, as well as novel computer logic architectures. NiO is a model system for the resistive switching effect and the formation/rupture of Ni nanofilaments is considered to be essential. However, it is not clear how the nanofilaments evolve in the switching process. Moreover, since Ni nanofilaments should be ferromagnetic, it provides an opportunity to explore the electromagnetic coupling in this system. Here, we report a direct observation of Ni nanofilaments and their specific evolution process for the first time by a combination of various measurements and theoretical calculation. We found that multi-nanofilaments are involved in the low resistance state and the nanofilaments become thin and rupture separately in the RESET process with subsequent increase of the rupture gaps. Theoretical calculations reveal the role of oxygen vacancy amount in the evolution of Ni nanofilaments. We also demonstrate electromagnetic coupling in this system, which opens a new avenue for multifunctional devices.

1This work was supported by the National Science Foundation of China (Grant Nos. 11134007, 10721404) and Special Found of Tsinghua for basic research (Grant No. 201110810625).

12:39PM G14.00006 Electronic Transport properties of SET and REST states of interfacial phase-change memory , HISAOK NAKAMURA, JUNJI TOMINAGA, YOSHIHIRO ASAI, AIST, IVAN RUNGGER, AWADHESH NARAYAN, STEFANO SANVITO, School of Physcs. AMBER and CRANN, Trinity College — The phase change memory (PCM) is one of most promising nonvolatile information storage technologies. Recently, the superlattice structure of GeTe/Sb2Te3 is proposed as PCM to reduce the resistive switching energy. This PCM is called interfacial PCM (IPCM) and it is considered that SET and RESET states are realized only by the flip-flop transition of Ge atoms in crystal phase because of small loss of entropy. Furthermore, the GeTe is sandwiched by Sb2Te3 topological insulator. In this study, we performed the first principles electric transport calculations including spin-orbit interactions. We presents the mechanism of resistive switch by the transition of Ge atoms as well as the volume change effect and the role of spin-orbit interaction to resistance ration of SET and RESE states.
12:51PM G14.00007 A mesoscopic magnetron as an open quantum system. TADEUSZ PUDLIK, Physics Department, Boston University, ANTONIO CASTRO NETO, Physics Department, Boston University; Department of Physics, National University of Singapore, DAVID CAMPBELL, Physics Department, Boston University — The emergence of materials with room temperature electron mean free paths of a micron or more opens up new possibilities in the design of solid state devices. One such potential new paradigm are solid state quasi-free electron devices, which promise to combine the wide frequency tunability of classical vacuum tube devices with the small size and low costs of semiconductor technology. As a step towards realistic models of these devices, we develop a quantum mechanical description of a mesoscopic magnetron, in which the vacuum chamber of traditional magnetron is replaced with a semiconductor. We show that the problem can be mapped to a Bose-Hubbard dimer coupled to a dissipative bath and study the effect of the band structure of the medium on device performance.

1:03PM G14.00008 Interplay between magnetic anisotropy and vibron-assisted tunneling in a single-molecule magnet transistor1, KYUNGWA PARK, ALEXANDER MCCASKY, YOH YAMAMOTO, MICHAEL WARNOCK, Virginia Tech, ENRIQUE BURZURI, HERRE VAN DER ZANT, TU Delft — Molecules trapped in single-molecule devices vibrate with discrete frequencies characteristic to the molecules, and the molecular vibrations can couple to electronic charge and/or spin degrees of freedom. For a significant electron-vibron coupling, electrons may tunnel via the vibrational excitations unique to the molecules. Recently, electron transport via individual anisotropic magnetic molecules (referred to as single-molecule influences electrons transport via a single-molecule magnet Fe₄, by using a model Hamiltonian with parameter values obtained from density-functional theory (arXiv:1411.2677). We show that the magnetic anisotropy of the Fe₄ induces new features in vibrational conductance peaks and creates vibrational satellite peaks. The main and satellite peak heights have a strong, unusual dependence on the direction and magnitude of applied magnetic field, because the magnetic anisotropy barrier is comparable to vibrational energies.

1:15PM G14.00009 Single Molecule Magnetic Force Detection with a Carbon Nanotube Resonator1, KYLE WILICK, SEAN WALKER, JONATHAN BAUGH, Institute for Quantum Computing, University of Waterloo — Single molecule magnets (SMMs) sit at the boundary between macroscopic magnetic behaviour and quantum phenomena. Detecting the magnetic moment of an individual SMM would allow exploration of this boundary, and could enable technological applications based on SMMs such as quantum information processing. Detection of these magnetic moments remains an experimental challenge, particularly at the time scales of relaxation and decoherence. We present a technique for sensitive magnetic force detection that should permit such measurements. A suspended carbon nanotube (CNT) mechanical resonator is combined with a magnetic field gradient generated by a ferromagnetic gate electrode, which couples the magnetic moment of a nanomagnet to the resonant motion of the CNT. Numerical calculations of the mechanical resonance show that resonant frequency shifts on the order of a few kHz arise due to single Bohr magneton changes in magnetic moment. A signal-to-noise analysis based on thermomechanical noise shows that magnetic switching at the level of a Bohr magneton can be measured in a single shot on timescales as short as 10μs. This sensitivity should enable studies of the spin dynamics of an isolated SMM, within the spin relaxation timescales for many available SMMs.

1Supported by NSERC

1:27PM G14.00010 Leakage radiation microscopy for observation of non-transparent samples. JUAN M. MERLO, FAN YE1, MICHAEL J. BURNS, MICHAEL J. NAUGHTON2, Boston College — Surface plasmon interactions are confined to be proximate to the surface on which they are excited, such that common optical microscopic imaging is precluded. In order to overcome this limitation, the leakage radiation microscopy technique can be employed to obtain images of interactions at a metallic surface where the surface plasmon propagates [1]. A disadvantage of this configuration is that the metallic layer must be optically thin, resulting in the (additional) direct observation of the excitation source. Here, we describe a leakage radiation microscope that can be used to observe plasmonic interactions in optically non-transparent samples [2]. We show that theoretically-calculated values of the surface plasmon wavelength and propagation length agree with the measured values. This configuration opens the possibility to study important effects where samples are optically non-transparent, as in plasmonic cavities, without the use of time-consuming near-field scanning optical microscopy.

1Supported by W.M. Keck Foundation.

1:39PM G14.00011 Random Telegraph Signal in a Metallic Double-Dot System1, YUVAL VARDI, AVRAHAM GUTTMAN, ISRAEL BAR-JOSEPH, Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel — Double quantum dot systems offer a unique opportunity for studying the world of quantum transport. This stems from the ability to localize an electron in a limited region in space on the dot, and monitor its presence and properties. Another system, in which electrons can be stored and measured, is an electronic trap in solid. The electrons in such a trap are better isolated from the environment. However, their measurement and control are more difficult. Here we demonstrate how these two systems, metallic double-dots and electronic traps, are combined to yield a hybrid structure in which an electron can be stored for long durations and can be easily detected and measured. We investigate the dynamics of a single electron surface trap, embedded in a self-assembly metallic double-dot system. The charging and discharging of the trap by a single electron is manifested as a random telegraph signal of the current through the double-dot device. We find that we can control the duration that an electron resides in the trap through the current, varying it between fractions of a second to more than an hour, at the Coulomb blockade region. We suggest that the observed switching is the electrical manifestation of the optical blinking phenomenon, commonly observed in semiconductor quantum dots.

1Supported by the W.M. Keck Foundation.

this technique should be applicable to other nanoscale devices, providing a general route for tuning device properties. We reproducibly achieve high rectification ratios at low operating voltages for molecular junctions based on a family of symmetric small-gap molecules. This establishes the feasibility of exploiting quantum transport to transform the performance horizons of Si devices fabricated in an industrially scalable manner.

1:51PM G14.00012 Negative Differential Transconductance in Silicon Quantum Well MOSFET/Bipolar Hybrid Transistors

11:15AM G15.00001 Ultrafast mid-infrared intraexcitonic spectroscopy of monolayer MoS2

11:27AM G15.00002 Infrared nano-imaging of plasmonic hotspots on graphene nano-bubbles

11:39AM G15.00003 Temperature-induced plasma excitations in gapped graphene and silicene

12:03PM G15.00005 Dynamics of Ion-Gating 2D Crystals Using a Solid Polymer Electrolyte


Supported by Semiconductor Research Council Task Number 1836.145

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008B - Hayk Harutyunyan, Emory University

11:15AM G15.00001 Ultrafast mid-infrared intraexcitonic spectroscopy of monolayer MoS2

SOONYOUNG CHA, School of Electrical and Electronic Engineering, Yonsei University, Seoul, Korea, JI HO SUNG, MOON-HO JO, Division of Advanced Materials Science, Pohang University of Science and Technology (POSTECH), Pohang, Korea, HYUNYOUNG CHOI, School of Electrical and Electronic Engineering, Yonsei University, Seoul, Korea. — The optical properties of transition metal dichalcogenide (TMD) are currently active research topics for understanding the two-dimensional nature of carrier dynamics. For monolayer TMDs, reduced dielectric screening invokes strong Coulomb interactions, which lead to the large exciton binding energy. Recent theory predicts that the subset of excitons is much richer, such that internal transitions between excitons (ex. 1s, 2s, 2p) should prevail the photo-induced optical response. We performed ultrafast optical pump and mid-infrared (IR) probe spectroscopy to investigate transient intraexcitonic dynamics in a monolayer MoS2. To obtain a complete excitonic dynamics, the probe photon energy is tuned over a broad range from mid-IR to IR, 0.24 eV to 0.66 eV. Our study reveals that the mid-IR responses exhibit photo-induced absorption after 3.1 eV pump excitation, which then relax within tens of picosecond and show multiple intraexcitonic and interexcitonic transitions. Our experiment shows that the fast decay component of the dynamics closely follows transient dynamics of so called A-exciton population, suggesting the photo-induced absorption indeed originates from the internal excitonic transitions.

11:27AM G15.00002 Infrared nano-imaging of plasmonic hotspots on graphene nano-bubbles

ZH FEI, UC San Diego & Argonne Natl Lab, JONATHAN FOLEY, Argonne Natl Lab, WILL GANNETT, ALEX ZETTL, UC Berkeley, MENGKUN LIU, Stony Brook University, GUANGXIN NI, SIYUAN DAI, UC San Diego, FRITZ KEILMANN, Ludwigs-Maximilians-Universität, ANTONIO CASTRO NETO, National University of Singapore, STEPHEN GRAY, GARY WIEDERRECHT, Argonne Natl Lab, MICHAEL FOGLER, DIMITRI BASOV, UC San Diego — One of the most interesting phenomena in plasmonics is the appearance of strong enhancements of electromagnetic energy by forming plasmonic hot spots for various applications including bio-sensing, single molecule fingerprinting, surface enhanced spectroscopy, and etc. Here, we demonstrate by infrared nano-imaging that nano-bubbles formed on graphene/hexagonal boron nitride heterostructures are ideal for trapping electromagnetic energy thus forming ultra-confined plasmonic hot spots. The distributions of these hot spots are sensitively dependent on the size and shape of these nano-bubbles as well as the ingredients inside. Further analysis indicates that the observed plasmonic hotspots are formed due to a significant enhancement of the plasmon wavelength and intensity above graphene nano-bubbles filled with air or other low-k dielectric materials. Our work presents a novel scheme for plasmonic hot spots formation and sheds light on future applications of graphene nano-bubbles for plasmon-enhanced single molecule characterization.

11:39AM G15.00003 Temperature-induced plasma excitations in gapped graphene and silicene

ANDRII IUROV, University of New Mexico and Hunter College, CUNY, GODFREY GUMBS, Hunter College, CUNY and Donostia International Physics Center (DIPC), DANHONG HUANG, Air Force Research Laboratory, Space Vehicles Directorate — Both closed-form analytic and numerical results are presented for the polarization function, as well as the plasma excitations of gapped graphene and silicene. The calculations are carried out within the random phase approximation (RPA). We investigate the behavior of the plasmon dispersion as a function of sublattice potential difference in silicene. These results could be used to compare the effective mass model with the tight-binding approximation at finite temperature in which spin-orbit coupling is included.

12:03PM G15.00005 Dynamics of Ion-Gating 2D Crystals Using a Solid Polymer Electrolyte

HU-MIN LI, BUCHANAN BOURDON, University of Notre Dame, YU-CHUAN LIN, JOSHUA ROBINSON, The Pennsylvania State University, ALAN SEABAGH, University of Notre Dame, CENTER FOR LOW ENERGY SYSTEMS TECHNOLOGY (LEAST) TEAM — Ion-gating can significantly increase the static carrier density of graphene due to the formation of an electric double layer (EDL); however, the dynamics of ion-gating have not been extensively reported. A comprehensive understanding of ion dynamics is important because it establishes the timescales required to achieve EDL equilibrium, and directly affects the operating speed of devices and circuits employing electrolytic gates. Here, ion dynamics are measured on epitaxial graphene Hall-bar devices that are electrolytically gated with polyethylene oxide and lithium perchlorate. The time constants for EDL formation and dissipation are measured as a function of temperature. The measured formation time is longer than the dissipation time, because ion diffusion resulting from a concentration gradient must be opposed during EDL formation. These results quantitatively agree with COMSOL multiphysics simulations. EDL dissipation follows a stretched exponential decay described by the Kohlraus-Williams-Watts (KWW) equation. The temperature-dependent relaxation times extracted from the KWW fit follow the Vogel-Fulcher-Tammann (VFT) temperature dependence. At temperatures approaching the glass transition temperature of the electrolyte, the relaxation times exceed several hours, demonstrating the long timescales over which the EDL can persist in the absence of a gate bias.
Electronic transport in graphene/CdSe nanoparticle monolayer/graphene tunneling devices, DATONG ZHANG, Columbia University, CHENGLIANG LU, National Center for Nanoscience and Technology, AREND VAN DER ZANDE, PHILIP KIM, IRVING P. HERMAN, Columbia University — We fabricated graphene/CdSe nanoparticle monolayer/graphene sandwich device structures. The CdSe nanoparticle monolayer is formed on a liquid-air surface before transferring it onto the bottom graphene layer that had been micro-exfoliated onto a 285 nm SiO2/Si substrate. The top graphene layer is transferred to the targeted area on the CdSe nanoparticle monolayer via a dry transfer technique. Tunneling-type vertical transport is observed, which is fitted by tunneling models that suggest that ligand shell instead of nanoparticle core is the major barrier of tunneling. Photoconductivity is enhanced but with low exciton separation efficiency when the laser is on the junction area, also suggesting that ligand shell is the major barrier of electronic transport in the sandwich structure.

PVA:LiClO4: a robust, high T_g polymer electrolyte for adjustable ion gating of 2D materials, ERICH KINDER, SUSAN FULLERTON, Univ of Notre Dame, Dept. of Electrical Engineering, CENTER FOR LOW ENERGY SYSTEMS TECHNOLOGY TEAM — Polymer electrolytes are an effective way to gate organic semiconductors and nanomaterials, such as nanotubes and 2D materials, by establishing an electrostatic double layer with large capacitance. Widely used solid electrolytes, such as those based on polyethylene oxide, have a glass transition temperature below room temperature. This permits relatively fast ion mobility at T = 23 °C, but requires a constant applied field to maintain a doping profile. Moreover, PEO-based electrolytes cannot withstand a variety of solvents, limiting its use. Here, we demonstrate a polymer electrolyte using polyvinyl alcohol (PVA) with T_g > 23 °C, through which a doping profile can be defined by a potential applied when the polymer is heated above T_g, then “locked-in” by cooling the electrolyte to room temperature (< T_g) to limit ion mobility. Current-voltage measurements of a graphene field effect transistor verify the “lock-in” process, showing constant drain current regardless of the applied electrolyte gate bias. Hall bar measurements are used to quantify the charge carrier density. Owing to PVA’s chemical stability, photolithography can be performed directly on the polymer electrolyte, which allows for the deposition of a patterned, metal gate directly on the electrolyte, as well as the ability to pattern the electrolyte itself.

Near-field optical second-harmonic technique for detection and characterization of semiconductor thin film electron-scattering domain boundaries, FARZAD SHAHIF, The University of Texas at Austin, TOMMASO ORZALI, Gennadi Bersuker, Sematech, DOWNER MICHAEL, The University of Texas at Austin — Understanding electron transport in epitaxial semiconductor thin films and low dimension systems is crucial for new electro-optic devices. III-V films grown on Si integrate high carrier mobility into the established Si platform, but are susceptible to formation of sub-micron anti-phase domains that possess unwanted Ga-Ga or As-As electron-scattering defects at their boundaries. Optical second-harmonic generation provides sensitive, specific and noninvasive but so far only spatially-integrated characterization for these defects [1]. We introduce a fiber based nearfield scanning optical second harmonic microscopy for the first time to fully resolve the electron scattering boundaries on III-V/Si films. This technique reveal variations in electron scattering boundaries structure as growth conditions, epitaxial film composition, and substrate vary, and are compared with surface topography, darkfield transmission electron microscopy and electron back scatter diffraction. Suppression of the electron-scattering boundaries has been explored.

Semiclassical Boltzmann Theory Studies of the Electronic Resistances of Multilayered Silicene Junctions, YUNPENG WANG, X-G. ZHANG, JAMES FRY, HAI-PING CHENG, University of Florida — A layer-by-layer investigation is carried out to understand electron transport across metal-semiconductor-metal junctions. Structures of junctions are optimized using first-principles density functional theory with the generalized gradient approximation. The semiclassical Boltzmann theory of the electronic transport is revisited and applied to multilayer silicene and hexagonal BN based junctions. The calculated resistance is smaller than, but converges to that calculated by the Landauer formula. Owing to the thickness of the barrier increases. Our calculation results provide an upper limit on the transmission coefficient per channel, ~ 0.05, below which the Landauer formula is applicable for calculating the resistance. In addition, we find that the resistance of a junction is not determined entirely by the average transmission, but also by the distribution of the transmission over the first Brillouin zone.

Localized surface plasmon effects of two dimensional lattice of metal nanoslads, YUKARI ODA, RYOKO SHIMADA, Japan Women’s University, JAPAN WOMEN’S UNIVERSITY TEAM — Localized surface plasmon (LSP) of metal nanoparticles results from non-propagating excitation of their conduction electrons coupled to the electromagnetic field. LSP localizes the electric field and enhances light emission from fluorescent materials. In this study, a two dimensional (2D) lattice of silver (Ag) nanoslads was fabricated by nanosphere lithography (NSL) method utilizing self-assembled, close-packed hexagonal structures of polystyrene spheres as the masking etching. This 2D lattice was subjected to the electric field for investigating a role of the periodicity of metal islands in the LSP effect. 9,10-di(2-naphthyl)anthracene (ADN), a well-known blue-emitting material in the field of electroluminescence, was used for the study of the enhancement of emission due to the LSP effect. Hybrid thin films of poly(methyl methacrylate) containing ADN were prepared with spin-casting onto the 2D lattice of Ag nanoslads. Transmission and photoluminescence measurements were conducted for these hybrid thin films at room temperature. Detailed results will be presented on site.

Spatially indirect exciton condensate in bilayer systems, FEI XUE, FENGCHENG WU, ALLAN MACDONALD, Department of Physics, University of Texas at Austin — Bilayer equilibrium exciton condensates have attracted attention in recent years because of their interesting and anomalous transport properties. Here we report on the microscopic derivation of bosonic effective Hamiltonians which include exciton-exciton interaction terms and account realistically for band-structure and dielectric environment effects. We describe in detail the microscopic origin of different contributions to exciton-exciton interaction. We apply our theory to the case of transition metal dichalcogenides, addressing specifically the role of the excitonic flavor multiplicity in that system.

Coulomb drag in coupled electronic systems of different dimensionalities, BEN YU-KUANG HU, The University of Akron — Coulomb drag occurs when two electrically independent electronic systems are situated in close enough proximity to each other that the Coulomb coupling between the two systems causes an electric current in one system to drag along a carriers in the other system. The magnitude of this effect is quantified by the drag rate. We derive the formalism to determine the drag rate in systems of different dimensionalities (for example, one-dimensional quantum wires coupled to two-dimensional quantum wells), based on coupled transport equations. We discuss how the hybrid coupled plasmons of the systems of different dimensionalities can affect the drag, and we investigate the effect that plasmons in the higher-dimensional system can have on the drag rate of the carriers in the lower-dimensional system.
1:39PM G15.00013 Three-dimensional plane-wave full-band quantum transport using empirical pseudopotentials1. JINGTIAN FANG, WILLIAM VANDENBERGHE, MASSIMO FISCHETTI, Univ of Texas, Dallas — We study theoretically the ballistic performance of future sub-5 nm Field-Effect Transistors (FETs) using an atomic quantum transport formalism based on empirical pseudopotentials, with armchair Graphene Nanoribbons (aGNRs), Silicon Nanowires (SiNWs) and zigzag Carbon Nanotubes (zCNTs) as channel structures. Due to the heavy computational burden from the plane-wave basis set, we restrict our study to ultrasmall devices, characterized by 5 nm channel lengths and 0.7 nm × 0.7 nm cross-sectional areas. Band structure calculations show that aGNRs have an oscillating chirality-dependent band gap. SiNWs with dimer lines N=3p+1 have large band gaps and aGNRFETs show promising device performance in terms of high Ion/Ioff, small drain-induced barrier lowering and limited short channel effects due to their very thin body and associated excellent electrostatic control. N=3p+2 aGNRs have small band gaps and band-to-band tunneling generates a large current at high bias. We also discuss spurious solutions introduced by the envelope function approximation. Device characteristics of SiNWFETs and zCNTFETs are compared to aGNRFETs as well.

1We acknowledge the support of Nanoelectronics Research Initiative's (NRI's) Southwest Academy of Nanoelectronics (SWAN).

1:51PM G15.00014 Dynamic Control of Thermal Emission with Plasmonically Active Graphene Metasurfaces, VICTOR BRAR, MICHELLE SHERROTT, Caltech, MIN JANG, Seoul National University, SEYoon KIM, Laura Kim, Josue Lopez, Caltech, MANSoo ChoI, Seoul National University, LUKE SWEATLOCK, Northrop Grumman Aerospace Systems, HARRY ATWATER, Caltech — Thermal emission is typically viewed to be broadband, unpolarized and isotropic, with a spectral profile and intensity that depend on the emissivity of the material, and that vary only with changes in temperature. In this talk we demonstrate that the intensity, polarization and spectrum of thermal emission at constant temperature can be dynamically controlled through electrostatic gating of plasmonic graphene resonators on a heated SiNx substrate. We show that the plasmonic resonances in graphene act as antenna that to out-couple the thermal energy of substrate phonons and graphene electrons to create narrow, mid-infrared spectral features in the thermal emission profile. By varying the gate voltage and resonator width, we show that these features can be effectively turned on and off at kHz rates, and tuned across a broad frequency range. Our measurements show that at 7μm the emissivity of the surface can be varied by 0.02, and that the emitted radiation is polarized, with a modulated power density of 0.02W/m2 over 100cm-1 of bandwidth.

2:03PM G15.00015 Graphene-enabled electrically switchable radar absorbing surfaces, OSman Balci, Emre Ozan Polat, Nurbek Kakenov, CosKun Kocabas, Bilkent University — Radar absorbing materials are used in stealth technologies for concealment of an object from radar detection. Resistive and/or magnetic composite materials are used to reduce the backscattered microwave signals. Inability to control electrical properties of these materials however, hinders the realization of active camouflage systems which require adaptive surfaces operating in microwave frequencies. Here, using large-area graphene electrodes, we demonstrate a new class of active surfaces which enables unprecedented ability to control reflection, transmission and absorption of microwaves by electric means. Instead of tuning bulk material property, our strategy relies on electrostatic tuning of the charge density on an atomically thin electrode which operates as a tunable metal in microwave frequencies. Notably, we fabricated large area adaptive radar absorbing surfaces with tunable reflection suppression ratio up to 50 dB with operation voltages less than 5 V. These electrically switchable radar absorbing surfaces provide a significant step in realization of active camouflage systems and adaptive cloaking in microwave frequencies, which cannot be realized by conventional materials.

Tuesday, March 3, 2015 11:15AM - 2:15PM
Session G16 DMP: Comp: Focus Session: Iron Based Superconductors: Local Probes 101AB
- Alexander Balatsky, Los Alamos National Laboratory/Nordita

11:15AM G16.00001 Quasiparticle interference (QPI) as a model-free phase sensitive tool to determine the pairing symmetry in Fe based superconductors (FeBS). IGOR MAZIN, Naval Research Lab, PETER HIRSCHFELD, University of Florida, ILYA EREMEN, University of Bochum — QPI has been successfully used to identify the d-wave pairing in high-Tc cuprates[1]. However, applying the same technique to FeBS has been confounded by difficulties not present in in cuprates, where QPI is dominated by several hot spots, thus calling for a more detailed analysis. This talk aims at providing such theoretical framework and clarifying some misconceptions regarding QPI in superconductors (partially pointed out before, but not generally appreciated). We emphasize that detailed comparison of the calculated model QPI maps with the experiment, as often attempted, is hardly helpful because the result depends not only on the assumed pairing symmetry but of numerous uncontrolled approximations. Instead, we suggest that the T dependence (but not the detailed q dependence at any given T) bears clear qualitative fingerprints of the s± or d± symmetry, independent of the details of impurity scattering, electronic structure etc. We propose an experiment that should unambiguously distinguish between the two symmetries in question. [1] Hanaguri et al, Science, 323, 923 (2009)

11:27AM G16.00002 STM investigation of FeSe1-xSx.1+ M. IAVARONE, S.A. MOORE, E. LECHNER, Department of Physics, Temple University, Philadelphia, PA 19122. J. CURTIS, Department of Physics, Drexel University, Philadelphia, PA 19104, O.S. VOLKova, A.N. VASILIEV, Low Temperature Physics and Superconductivity Department, Physics Faculty, M.V. Lomonosov Moscow State University, Moscow 119991, Russia, D.A. CHAREEV, Institute of Experimental Mineralogy, Russian Academy of Sciences, 142432 Chernogolovka, Moscow District, Russia, G. KARAPETROV, Department of Physics, Drexel University, Philadelphia, PA 19104 — FeSe has the simplest structure among the Fe-based superconductors, and this very simplicity could provide the most appropriate venue of understanding the superconducting mechanism of Fe-based superconductors. High quality FeSe single crystals were grown in evacuated quartz ampoules using a KCl/AlCl flux and the structure of tetragonal P4/nmm was demonstrated by x-ray diffraction. Low temperature STM measurements were performed on FeSe1-x-Sx with x=0.04 and 0.09. Effects of multiband superconductivity and vortex matter as a function of doping will be presented.

G.K. and A.N.V. acknowledge the support by a grant from U.S. Civilian Research & Development Foundation (CRDF Global).

11:39AM G16.00003 Real Space Imaging of the Atomic-Scale Magnetic Structure of Fe1y+Te, PETER WAHL, University of St Andrews, MOSTFA ENAYAT, ZHI-XIANG SUN, UDAI RAJ SINGH, RAMAKRISCHNA ALURU, STEFAN SCHMAUS, ALEXANDER YARESKO, YONG LIU, CHENGTIAN LIN, MAX-Plank-Institut fuer Festkoerperforschung, VLADIMIR TSURKAN, ALOIS LOIDL, JOACHIM DEISENHOFER, Universitaet Augsburg — High temperature superconductivity, both in cuprate as well as iron pnictide materials, occurs in close proximity to the superconducting transition temperatures. A detailed understanding of the superconducting mechanism of Fe1y+Te, the non-superconducting parent compound of the iron chalcogenides, by spin-polarized low temperature scanning tunneling microscopy. Our images of the magnetic structure reveal that magnetic order in the monoclinic phase is truly a unidirectional stripe order, whereas in the orthorhombic phase at higher excess iron concentrations (y > 0.12), a transition to a phase with coexistence of stripes in both directions is observed.
11:51AM 16.00004 Visualization of electronic nematicity in the iron pnictides, ETHAN ROSENTHAL, Columbia University — The nematic state from which superconductivity emerges in the iron pnictides continues to confound. We use scanning tunneling microscopy (STM) and spectroscopy (STS) to image both long-range nematic order and nematic fluctuations across the doping phase diagram in Co-doped NaFeAs. We associate twinning domains with long-range order and directly visualize the temperature and doping dependence of these features. Anisotropic electronic structure is found to persist outside of the ordered nematic phase. With the aid of a novel experimental setup which combines simultaneous STS and variable, uniaxial strain, we determine the relationship between strain and nematic fluctuations which gives rise to the anisotropy.

12:27PM 16.00005 Observation of van Hove singularity and quasiparticle interference in KFe2As2 superconductors revealed by STM/STS measurements, HAI-HU WEN, DELONG FANG, ZENGYI DU, ZHENYU WANG, HUAN YANG, XIAOXIN DING, Nanjing University — We have conducted STM/STS investigations on the KFe2As2 superconducting single crystals down to 0.45 K under magnetic field. Clear electronic standing waves have been observed allowing us to investigate the quasiparticle interference (QPI). Interestingly we observed a sharp peak of local density of states (LDOS) near the Fermi energy showing evidence of strongly enhanced DOS both below and above Tc. We also found a peak at xopt and a Tc vs λab dependence similar on both sides of xopt. Near the underdoped edge of the dome λab increases sharply, suggesting that superconductivity competes with another phase. Indeed MFM vortex imaging shows correlated defects parallel to twin boundaries only in underdoped samples and not for x ≥ xopt. Furthermore, in underdoped samples we report stripes parallel to twin boundaries that are visible even in the absence of vortices.

12:39PM 16.00006 Local characterization of superconductivity in BaFe2(As1−xPax)2, OPHIR AUSSLANDER, YUVAL LAMHOT, ALON YAGIL, NADAV SHAPIRA, Technion – Israel Institute of Technology, SHIGERU KASAHARA, TATSUYA WATASHIGE, Kyoto University, Japan, TAKASADA SHIBAUCHI, University of Tokyo, Japan, YUJI MATSUDA, Kyoto University, Japan — We use magnetic force microscopy (MFM) to characterize superconductivity across the superconducting dome in BaFe2(As1−xPax)2, an isovalently doped pnictide that exhibits a peak in the penetration depth (λab) at optimal doping (xopt), as shown previously in sample-wide measurements. Our local measurements show a peak at xopt and a Tc vs λab dependence similar on both sides of xopt. Near the underdoped edge of the dome λab increases sharply, suggesting that superconductivity competes with another phase. Indeed MFM vortex imaging shows correlated defects parallel to twin boundaries only in underdoped samples and not for x ≥ xopt. Furthermore, in underdoped samples we report stripes parallel to twin boundaries that are visible even in the absence of vortices.

12:51PM 16.00007 ABSTRACT WITHDRAWN —
1:39PM G16.00011 57As and 59Co NMR studies of SrCo$_2$As$_2$\textsuperscript{1}, YUJI FURUKAWA, Ames Laboratory, Dept. of Phys. and Astro, Iowa State Univ., VASILY OGLOBLINCHEV, Institute of Metal Physics, Ural Div. of Russian Academy of Sci., Ekaterinburg, Russia, ABHISEK PANDEY, DAVID C. JOHNSTON, Ames Laboratory, Dept. of Phys. and Astro, Iowa State Univ. — After the discovery of unconventional superconductivity in Fe pnictides with the ThCr$_2$Si$_2$-type structure, much attention has been paid to the related materials AM$_2$As$_2$ (A = Ca, Sr, and Ba, and M = Co, Ni, Mn, and Cu). We have been studying the electronic and magnetic properties of these related materials systematically. Among them, metallic SrCo$_2$As$_2$ is an interesting system [1] because inelastic neutron scattering measurements indicate strong stripe-type antiferromagnetic correlations [2], similar to the Fe pnictide superconductors. In order to investigate the magnetic and electronic properties of SrCo$_2$As$_2$ from a microscopic point of view, we carried out 57As and 59Co NMR in the temperature range T = 1.3 – 300 K. In this talk, based on 59Co NMR data including 75As NMR results published previously [1], we discuss the characteristic magnetic fluctuations in the system and compare them with those measured from NMR data for another cobalt arsenide BaCo$_2$As$_2$.


1Supported by USDOE under Contract No. DE-AC02-07CH11358.

1:51PM G16.00012 57Fe Mössbauer study of iron-silicide superconductor Lu$_3$Fe$_2$Si$_2$\textsuperscript{1}, XIAOMING MA, Ames Laboratory/ Iowa State University, Ames, IA 50011, USA and Institute of Applied Magnetics/ Lanzhou University, Lanzhou, Gansu 730000, China, SHENG RAN, Ames Laboratory/ Iowa State University, Ames, IA 50011, USA, HUA PANG, FASHEN LI, Institute of Applied Magnetics/ Lanzhou University, Lanzhou, Gansu 730000, China, PAUL CANFIELD, SERGEY BUD’KO, Ames Laboratory/ Iowa State University, Ames, IA 50011, USA — In order to investigate the changes of the hyperfine parameters of a compound when it goes into a superconducting state from a normal state, we studied Lu$_3$Fe$_2$Si$_2$, Lu$_2$Fe$_2$Si$_3$, and LuFe$_2$Si$_3$, which is a superconductor with a transition temperature, T$_C$ ∼ 6 K and the Fe has been proved to be non-magnetic in a previous Mössbauer study\textsuperscript{[1]}. We performed detailed 57Fe Mössbauer spectra measurement on Lu$_2$Fe$_2$Si$_3$, from room temperature down to 4.4 K with particular attention paid to region near T$_C$. No clear feature that can be associated with the superconducting transition was found in the hyperfine parameters. Detailed hyperfine parameters and recoilless fraction as a function of temperature will be presented and discussed.

[1] The authors gratefully acknowledge the financial support of the University Fellowship Scholarship Council and this work is supported by the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

Tuesday, March 3, 2015 11:15AM - 2:15PM –
Session G17 DCMP: Graphene: Quantum Hall Effects
102AB - Fan Zhang, University of Texas at Dallas

11:15AM G17.00001 Collective Edge Modes near the onset of a graphene quantum spin Hall state, GANPATHY MURTHY, Department of Physics and Astronomy, University of Kentucky, Lexington KY 40506-0055, USA, EFRAT SHIMSHONI, Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel, HERBERT FERTIG, Department of Physics, Indiana University, Bloomington, IN 47405, USA — Graphene subject to a strong, tilted magnetic field exhibits an insulator-metal transition tuneable by tilt-angle, which is attributed to the transition from a canted antiferromagnetic (CAF) to a ferromagnetic (FM) bulk state at filling factor ν = 0. We develop a theoretical description for the spin and valley edge textures in the two phases, and the implied evolution in the nature of edge modes through the transition. Based upon numerical Hartree-Fock calculations, we derive a simple description of the spin-valley domain wall for arbitrary Zeeman energy E$_z$, parameterized by two canting angles. Low-energy charged excitations can be constructed by imposing a slowly varying spin rotation on this state. In the CAF, these involve binding a vortex (meron) of the bulk state to a spin twist at the edge, so that the bulk spin stiffness controls the excitation energy. As the CAF-FM transition is approached (E$_z$ → E$_z^*$), the bulk stiffness vanishes linearly with (E$_z^*$ − E$_z$) and the vortex unbinds from the edge, yielding a gapless edge excitation characteristic of a quantum spin Hall state. Our model predicts the E$_z$-dependence of the activation gap in edge transport, and offers a qualitative picture of how this transport should evolve with filling factor.

11:27AM G17.00002 Oscillatory magnetotransport between co-propagating quantum Hall edge channels in graphene p-n junctions, SEI MORIKAWA, SATORU MASUBUCHI, RAI MORIYA, Institute of Industrial Science, University of Tokyo, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, TOMOKI MACHIDA, Institute of Industrial Science, University of Tokyo — We conducted magnetotransport measurements in high-quality dual-gated graphene p-n-junctions. As we used hexagonal boron nitride as a dielectric layer, Fabry-Perot interference patterns\textsuperscript{2} can be observed clearly in zero magnetic fields, owing to the extremely high carrier mobility of our devices\textsuperscript{3}. Moreover, the two-terminal resistance R exhibited oscillatory behavior as a function of the magnetic field B, whose oscillation period ∆B differed from both the conventional Shubnikov-de Haas effect (∆B ∝ B) and the Aharonov-Bohm effect with magnetic flux penetrating through the gated region (∆B = const). The oscillatory behavior of R was well reproduced by our numerical calculation under the assumption that R oscillated as a function of the magnetic flux penetrating through the insulating region between the co-propagating p and n quantum Hall edge channels\textsuperscript{4}.

11:39AM G17.00003 Ising quantum Hall ferromagnetic states in bilayer graphene. RENÉ CÔTE, WENCHEン LUO, ALEXANDRE BÉDARD-VALLÉE, University of Sherbrooke — We present a study of the phase diagram of the chiral two-dimensional electron gas (C2DEG) in the higher Landau levels, $|N| \geq 1$, of a chirally stacked bilayer graphene as a function of magnetic field $B$ and interlayer electrical bias $\Delta V$. In the Hartree-Fock approximation, the ground states of the C2DEG are respectively valley-pseudospin or spin Ising quantum Hall ferromagnets at odd or even filling factors of the quartet of states in levels $|N| \geq 1$ [1]. Changing the magnetic field or the bias introduces first order phase transitions between the different Ising ground states that are characterized by a discontinuity in the transport gap $\Delta t$. The C2DEG shows a hysteretic behavior with respect to the bias $\Delta V$ with a marked difference between positive $N > 0$ and negative $N < 0$ Landau levels [2]. We discuss the relevance of our results with recent experimental measurements of broken-symmetry gaps in bilayer graphene [3].

11:51AM G17.00004 Quantum Hall ferromagnetism in gapped bilayer graphene with trigonal warping effects. XIAO LI, Condensed Matter Theory Center, University of Maryland, FAN ZHANG, Department of Physics, The University of Texas at Dallas, QIAN NIU, ALLAN MACDONALD, Department of Physics, The University of Texas at Austin — The interplay between nontrivial Fermi surface topology and electron-electron interactions often leads to interesting phenomena in the quantum Hall regime. Bilayer graphene provides a unique platform to explore such physics, because the combined effects of trigonal warping and interlayer bias give rise to a nontrivial bandstructure at low energies. In the presence of a small perpendicular magnetic field, the highest valence-band Landau level of gapped bilayer graphene becomes three-fold degenerate excluding the spin degrees of freedom, with the three Landau levels corresponding to semiclassical orbits centered on different points in momentum space. Such a Landau level structure has been observed in a recent experiment [Phys. Rev. Lett. 113, 116602 (2014)]. In this work we construct a theory to show how the electron-electron interactions break this three-fold orbital degeneracy, and give rise to a gapped quantum Hall state at all intermediate integer filling factors. We further demonstrate that the resulting ground state breaks rotational symmetry and discuss some experimental consequences.

12:03PM G17.00005 Chiral symmetry breaking and the Quantum Hall Effect in monolayer graphene1, MALCOLM KENNETT, Physics Department, Simon Fraser University, BITAN ROY, Condensed Matter Theory Center, University of Maryland — Monolayer graphene in a strong magnetic field exhibits quantum Hall states at filling fractions $\nu = 0$ and $\nu = \pm 1$ that are not explained within a picture of non-interacting electrons. We propose that these states arise from interaction induced chiral symmetry breaking orders. We argue that when the chemical potential is at the Dirac point, weak onsite repulsion supports an easy-plane antiferromagnet state, which simultaneously gives rise to ferromagnetism oriented parallel to the magnetic field direction, whereas for $|\nu| > 1$, easy-axis antiferromagnetism and charge-density-wave order coexist. We perform self-consistent calculations of the magnetic field dependence of the activation gap for the $\nu = 0$ and $|\nu| = 1$ states and obtain excellent agreement with recent experimental results.

1Supported by NSF-JQI-PFC, LPS-CMTC, NSERC

12:15PM G17.00006 Quantum Hall Effect (QHE) in ABA stacked trilayer graphene. PETR STEPANOV, YAFIS BARLAS, NATHANIEL GILLGREEN, University of California, Riverside, TAKASHI TANIGUCHI, National Institute for Materials Science, JEANIE LAU, University of California, Riverside — Since its experimental discovery in 2004 graphene was under extensive research as a promising counterpart of silicon for the future electronics application as well as an excellent model of 2 dimensional electron gas. Here we investigate quantum Hall effect in ABA trilayer graphene – hexagonal boron nitride heterostructures. Landau Levels (LL) crossings at low filling factors were observed and explored at different external electric fields. The formation of the QH states as an interaction of monlayer-like and bilayer-like branches will be discussed. We will present the most recent experimental results.

12:27PM G17.00007 Optical study of nonuniform quantum-Hall ferromagnetic states in bilayer and trilayer graphene. MANUEL BARRETTE, RENÉ CÔTE, Université de Sherbrooke — The chiral two-dimensional electron gas in the $N = 0$ Landau level of a Bernal-stacked bilayer graphene is host to a variety of broken-symmetry ground states that can be described as layer, spin, or orbital quantum Hall ferromagnets (QHFs). At filling factors $\nu = 1, 3$, an externally applied electric field between the two layers can induce a transition from uniform to nonuniform orbital QHF states with an helical oriskyrtomic texture of electric dipoles [1]. A similar skyrmionic texture can also arise in the $N = 0$ Landau level of an ABC-stacked trilayer graphene. In this talk, we discuss the optical properties of these textured ground states. We compute their electromagnetic absorption as well as the Kerr and Faraday rotations induced by their collective excitations and show that each textured phase has a distinct optical signature.


12:39PM G17.00008 Broken Symmetry States in Twisted Bilayer Graphene. YOUNGWOOK KIM, JONG MOK OK, JUN SUNG KIM, Department of Physics, Pohang University of Science and Technology, Korea, JAESUNG PARK, SUYONG JUNG, Center for Quantum Measurements, Korea Research Institute of Standards and Science, Korea, DONG SU LEE, Soft Innovative Materials Research Center, Korea Institute of Science and Technology, Korea, INTEK SONG, HEE CHEUL CHOI, Department of Chemistry and Division of Advanced Materials Science, Pohang University of Science and Technology, Korea, K. WATANABE, T. TANIGUCHI, National Institute for Materials Science, Japan — Graphene bilayer with multiple degeneracy provides an access to rich quantum Hall states (QHS) with broken symmetry, arising from electron-electron interactions and Zeeman splitting. Here, we present quantum Hall effect in high-quality twisted bilayer graphene. At high density regime, we found several QH plateaus are suppressed or emerged with magnetic fields, indicating transitions between different QH states. We ascribe this to imperfect screening of twisted bilayer, which results in different Landau levels formation on each layer and their mixings. As low density regime, odd integer QHS are observed, suggesting an important role of the interlayer charge transfer for stabilizing broken symmetry QHS.
12:51PM G17.00009 Collective spin excitations in magnetically ordered graphene Quantum Hall insulator¹, JOSE LADO, JOAQUIN FERNANDEZ-ROSSIER, International Iberian Nanotechnology Laboratory — At half filling, the application of a perpendicular magnetic field in graphene results in a very large density of states at the Fermi energy, due to the n=0 Landau levels. Interactions are known to lead to some sort of electronic order that leads to a band-gap opening. Experimental evidence [1] suggest that electronic order is antiferromagnetic, and can be tuned into ferromagnetic upon application of a large in-plane field. This behaviour is properly captured by mean field Hubbard model [2]. In this talk, by using tight binding models and calculating responses within the random phase approximation [3], we show the different collective modes of bulk and edges associated to the different electronically ordered phases. Furthermore, we discuss the coupling of these spin waves to quasiparticles transport at the edges and discuss how this can affect local spin transport.

¹ We acknowledge financial support from Spinograph.


1:03PM G17.00010 Imaging the charge profile of graphene in quantum Hall states, YONGTAO CUI, ERIC MA, GEORGI DANKOV, FRANÇOIS AMET, Stanford Univ, VITTO HAN, Columbia Univ, MICHAEL KELLY, DAVID GOLDhaber-Gordon, Stanford Univ, CORY DEAN, Columbia Univ, ZHI-XUN SHEN, Stanford Univ — Under quantum Hall conditions, discrete energy levels (Landau levels) form in a two dimensional electron gas (2DEG) system. Spatial reconstructions of carriers due to electrostatics can occur for a non-uniform charge profile, giving rise to highly insulating incompressible regions. In this work we use microwave impedance microscope to image the quantum Hall states in graphene devices. First, scanning images clearly show dividing regions of insulating bulk and conductive edges. We study the evolution of the edge patterns as the carrier density is tuned through multiple Landau levels. Furthermore, a finite voltage bias on the tip can induce a local charge perturbation, which leads to an extra incompressible ring that moves along with the tip during scanning. Such incompressible ring can be used to probe the variations of the local carrier profile. Our results indicate that the carrier density in graphene tuned by the back gate tends to increase toward the edge due to electrostatic screening. This is in contrast to the case of conventional semiconductor 2DEG systems, where the carrier density always decreases toward the edge due to charge depletion. We will discuss how this charge profile affects the formation of the incompressible stripes.

1:15PM G17.00011 Measurement of energy gaps of integer and fractional quantum Hall states in suspended bilayer graphene devices, YANMENG SHI, YONGJIN LEE, SHI CHE, ZIQI PI, TIM ESPIRITU, KEVIN MYHRO, PETR STEPANOV, NATHANIAL GILLGREEN, Univ of California - Riverside, DMITRY SMIRNOV, National High Magnetic Field Laboratory, FL, CHUN NING LAU, Univ of California - Riverside — Coulomb drag between electrons in closely spaced two-dimensional electron systems has provided an exciting avenue for research on quantum Hall systems. Employing dual-gated, encapsulated graphene double layers separated by a thin hBN dielectric, we investigate density tunable magneto and Hall drag in quantum Hall bilayer systems. Large variations of magneto-drag and Hall-drag are observed, which can be related to the Landau level (LL) filling status of both driving and drag layers. The measured drag resistivity tensor can be associated with the tensor product of the differential magneto- and Hall-drag in quantum Hall bilayer systems. Large variations of magneto-drag and Hall-drag are observed, which can be related to the Landau level (LL) filling status of both driving and drag layers. The measured drag resistivity tensor can be associated with the tensor product of the differential magneto-resistivity tensors of the drive and drag layers [1]. The temperature and field dependence of magneto-drag can be described in terms of the phase space for Coulomb scattering between LLs in the drag and drive layers. In the strong interaction regime and ultra-low temperature, we observe the effect of symmetry broken integer Quantum Hall States in magneto and Hall drag signals. [1] F. von Oppen, S. Simon, and A. Stern, Phys. Rev. Lett. 87, 106803 (2001).

1:27PM G17.00012 Wess-Zumino-Witten terms in graphene Landau levels, JUNHYUN LEE, SUBIR SACHDEV, Department of Physics, Harvard University — We consider the interplay between the antiferromagnetic and Kekulé valence bond solid orderings in the zero energy Landau levels of neutral monolayer and bilayer graphene. We establish the presence of Wess-Zumino-Witten terms between these orders: this implies that quantum fluctuations are described by the deconfined critical theories of quantum spin systems. We present implications for experiments, including the possible presence of excitonic superfluidity in bilayer graphene.

1:39PM G17.00013 Coulomb drag in graphene quantum Hall bilayer systems, XIAOMENG LIU, Harvard University, LEI WANG, Columbia University, KIN CHUNG FONG, Raytheon BBN Technologies, YUANDA GAO, PATRICK MAHER, Columbia University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, JAMES HONE, CORY DEAN, Columbia University, PHILIP KIM, Harvard University — Coulomb drag between electrons in closely spaced two-dimensional electron systems has provided an exciting avenue for research on quantum Hall systems. Employing dual-gated, encapsulated graphene double layers separated by a thin hBN dielectric, we investigate density tunable magneto and Hall drag in quantum Hall bilayer systems. Large variations of magneto-drag and Hall-drag are observed, which can be related to the Landau level (LL) filling status of both driving and drag layers. The measured drag resistivity tensor can be associated with the tensor product of the differential magneto-resistivity tensors of the drive and drag layers [1]. The temperature and field dependence of magneto-drag can be described in terms of the phase space for Coulomb scattering between LLs in the drag and drive layers. In the strong interaction regime and ultra-low temperature, we observe the effect of symmetry broken integer Quantum Hall States in magneto and Hall drag signals. [1] F. von Oppen, S. Simon, and A. Stern, Phys. Rev. Lett. 87, 106803 (2001).

1:51PM G17.00014 Fractional Quantum Hall Effect in the Second Landau Level of bilayer graphene, GEORGI DANKOV, FRANCOIS AMET, MENCYOUNG LEE, ANDREW BESTWICK, KEVIN THARRATT, CHI-TE LIANG, DAVID GOLDhaber-Gordon, Stanford University — Bilayer graphene exhibits rich Quantum Hall physics due to valley, spin and orbital degrees of freedom that lead to a variety of polarization states. We study the Fractional Quantum Hall Effect (FQHE) in ultra-clean multiterminal bilayer graphene devices on boron nitride with a local graphite gate at magnetic fields of up to 45 T. We measure mobility of up to 1 million cm²/V·s and very low disorder. In addition to the broken-symmetry integer states, we unambiguously resolve a variety of fractions and focus on a series of fractions in the Second Landau Level, which do not follow particle-hole asymmetry. From the magnetic field dependence of the fractions, we find that some of these fractions have spin-polarized ground states while others are unpolarized, and we present a possible explanation for this difference. This work provides insights into how the symmetry-breaking electron-electron interactions and Zeeman splitting interact to produce a rich landscape of composite fermions in the Second Landau Level of bilayer graphene.

2:03PM G17.00015 Effect of tunable superlattice on quantum Hall effect in graphene, SUDIPTA DUBEY, MANDAR DESHMKH, Tata Institute of Fundamental Research — We have studied quantum Hall effect in tunable superlattice in graphene created using combination of back gate and an array of top-gates pinned to the same potential. In our device we are in the regime when superlattice period is larger than the magnetic length and superlattice amplitude can be tuned to be larger than Landau level spacing. We observe robust plateaus when charge carrier in adjacent region is of the same polarity. However when we have a series of p-n junction, the high superlattice amplitude leads to large local electric field in p-n junction causing collapse of Landau level and hence incomplete equilibration. We have also studied charge transport at low magnetic field where we have higher number of edge states circulating within a strip of back-gated or top-gated region.

Tuesday, March 3, 2015 11:15AM - 2:15PM — Session G18 DCMP GQI: Invited Session: Quantum Trajectories and State Estimation Mission Room 103A - Klaus Moelmer, Aarhus University, Denmark
11:15AM G18.00001 Stochastic action principle approach to continuous quantum measurement
ANDREW JORDAN, University of Rochester — New features in fundamental quantum physics appear in generalized (or weakened) measurements that are no longer simple projections. A sequence of weak measurements can also be made effectively continuous, producing monitored state evolution in the form of a quantum stochastic process. Previous theoretical investigations of this topic have mainly focused on using Langevin-type Stochastic Schrodinger equations to generate and study the quantum trajectories. Here, we reformulate the theory of continuous quantum measurement as a stochastic path integral, describing all possible quantum trajectories moving between initial and final quantum states. In order to do this, an auxiliary set of variables is introduced to impose the intrinsic state disturbance, doubling the state space of the system. The stochastic action encodes both the Hamiltonian and measurement dynamics. This formulation is well suited to finding the most-likely quantum path between chosen boundary conditions on the quantum states separated in time via a principle of least action. This action principle leads to a set of coupled nonlinear ordinary differential equations for the most likely path, structurally similar to Hamilton’s equations. I will present predictions for the single and multiple qubit cases. Comparison to recent experiments with superconducting transmon qubits will be discussed. This formalism sheds new light on the conditional dynamics of monitored open quantum systems.

11:51AM G18.00002 Ensembles of quantum trajectories— a window into qubit measurement dynamics
STEVEN WEBER, UC Berkeley — A central feature of quantum mechanics is that a measurement result is intrinsically probabilistic. Consequently, continuously monitoring a quantum system will randomly perturb its natural unitary evolution. An accurate measurement record documents this stochastic evolution and can be used to reconstruct the quantum trajectory of the system state in a single experimental iteration. We use weak measurements to track the individual quantum trajectories of a superconducting qubit that evolves under the competing influences of continuous weak measurement and Rabi drive. We analyze large ensembles of such trajectories to examine their characteristics and to determine their statistical properties. For example, by considering only the subset of trajectories that evolve between any chosen initial and final states, we can deduce the most probably path through quantum state space.

12:27PM G18.00003 Quantum State Smoothing1, HOWARD WISEMAN, Centre for Quantum Dynamics, Griffith University — Under noisy observations, one can estimate the state of the measured system, if its a priori statistics are given. In the continuous time situation, three different types of estimation can be distinguished: filtering, which is estimating of the state at time t from earlier records; retro-filtering, which is estimating it from later records; and smoothing, which is estimating it from both earlier and later records. Of the three, smoothing allows the greatest precision. Smoothing has been well developed in classical systems, but its application to quantum systems is very recent. Previous works have used the term “quantum smoothing” to mean estimating classical parameters, [Tsang, Phys. Rev. Lett 102, 250403 (2009); Yonezawa et al., Science 337, 1514-1517 (2012)]. This is essentially classical smoothing in which the noisy observation of the classical parameters is mediated by a quantum system. Here we introduce quantum state smoothing, where the state of a partially observed open quantum system itself is smoothed. We achieve this by applying classical smoothing to a hypothetical unobserved noisy measurement record that induces (in part) the stochastic dynamics (“quantum trajectories”) of the system. Using the formalism of linear quantum trajectories, we simulate quantum state smoothing for a qubit, and quantify how well it works. Our investigations shed new light on the nature of open quantum systems and the applicability of classical concepts. Applications to continuous measurement of solid-state qubits will be presented.

1 supported by the Australian Research Council Centre for Quantum Computation and Communication Technology

1:03PM G18.00004 Unravelling quantum jumps by watching the fluorescence of a qubit, PHILIPPE CAMPAGNE-IBARCO, Laboratoire Pierre Aigrain, Ecole Normale Superieure, Paris — When the main source of qubit relaxation comes from its coupling to a photonic channel, each relaxation event is associated with the release of a photon. The corresponding discrete quantum jumps of the qubit state can be observed by counting the number of photons released. This discreetness of the quantum jumps is in fact related to the nature of the light detector. What does the evolution of the qubit state become if fluorescence is measured using a heterodyne detector instead? In this talk, an experiment will be discussed, in which the records of heterodyne measurements of fluorescence is used to reconstruct the quantum trajectories of a qubit during relaxation. Using a large number of experiments, it is shown that these trajectories can be used to better predict the probability to find given measurement outcomes during the evolution. This heterodyne measurement of the fluorescence is a quantum demolition continuous measurement, which is very different from the more common dispersive measurement sensitive to qubit occupation. These trajectories are thus expected to exhibit some exotic properties, particularly when using past and future knowledge. Besides, using measurement based feedback based on the fluorescence signal alone, it is possible to stabilize any chosen qubit state. This work thus demonstrates that relaxation into an efficiently monitored channel is not a limit for quantum information protocols but can instead be a resource.

1:39PM G18.00005 Prediction, Retrodiction, and Smoothing for a Continuously Monitored Superconducting qubit, KATER MURCH, Physics Department, Washington University, St. Louis — The quantum state of a superconducting transmon qubit inside a three-dimensional cavity is monitored by reflection of a microwave field on the cavity. Measurement outcomes at different times are correlated, and knowledge of later measurement outcomes can be used to provide statistical information about earlier probe results. For a driven, damped and continuously monitored quantum system, the information inferred from measurement data yields a quantum trajectory given by the matrix \( \rho \), which is conditioned on probe results up to \( t \). Further probing after the time \( t \) can be incorporated into an auxiliary matrix \( E_t \). We show that the combination of \( \rho \) and \( E_t \) makes nontrivially different and more precise predictions for the outcomes of measurements in the past. Our experiments verify the predictions of both projective and weak value (weak) measurements conditioned on full measurement records.

Tuesday, March 3, 2015 11:15AM - 2:15PM –
Session G19 FLAP DMP: Invited Session: Caloric Materials and Advances in Solid State Cooling Technologies
Mission Room 103B - Jun Cui, Pacific Northwest National Laboratory

11:15AM G19.00001 Magnetocaloric cooling: the phenomenon and materials1, VITALIJ PECHARSKY, Ames Laboratory and Department of Materials Science and Engineering, Iowa State University — The discovery of the giant magnetocaloric effect in Gd2Si2Ge2 and other R2T1 compounds (R = rare earth metal and T = a Group 14 element) generated a broad interest in the magnetocaloric effect and magnetic refrigeration near room temperature in particular, and in magnetostuctural transitions in general. Reports on the giant magnetocaloric effect in other systems soon followed. These include MnFeP4-xAs1-x and related compounds, La(Fe1-xSi1-x)3, and their hydrides, Mn(As1-xSb1-x), CoMnSi1-xGe1-x and related compounds, Ni2MnGa and some closely related Heusler phases, and a few non-metallic systems. A common feature observed in all giant magnetocaloric effect materials is the enhancement of the magnetic entropy change by the overlapping contribution from the lattice. In addition to the interplay between magnetic and lattice entropies, both of which are intrinsic materials’ parameters that in principle can be modeled theoretically from first principles, extrinsic parameters such as microstructure and nanostructure, have been found to play a role in controlling both the magnetostuctural transition(s) and magnetocaloric effect. Both the intrinsic and extrinsic parameters are, therefore, important in order to maximize magnetocaloric effect. The role of different control parameters and the potential pathways towards materials exhibiting advanced magnetocaloric effect will be discussed.

1 This work is supported by the Division of Materials Science and Engineering, Office of Basic Energy Sciences of the U.S. Department of Energy under contract No. DE-AC02-07CH11358 with Iowa State University.
11:51 AM G19.00002 Elastocaloric cooling materials and systems, ICHIRO TAKEUCHI, University of Maryland and Maryland Energy and Sensor Technologies — We are actively pursuing applications of thermoelastic (elastocaloric) cooling using shape memory alloys. Latent heat associated with martensitic transformation of shape memory alloys can be used to run cooling cycles with stress-inducing mechanical drives [1]. The coefficient of performance of thermoelastic cooling materials can be as high as 11 with the directly measured DT of around 17 °C. Depending on the stress application mode, the number of cycles to fatigue can be as large as of the order of 10^5. Efforts to design and develop thermoelastic alloys with long fatigue life will be discussed. The current project at the University of Maryland is focused on development of building air-conditioners, and at Maryland Energy and Sensor Technologies, smaller scale commercial applications are being pursued. This work is carried out in collaboration with Jun Cui, Yiming Wu, Suxin Qian, Yunho Hwang, Jan Muehlbauer, and Reinhard Radermacher, and it is funded by the ARPA-E BEETIT program and the State of Maryland.


12:27PM G19.00003 Modeling and design aspects of active caloric regenerators, KURT ENGELBRECHT, Technical University of Denmark — A cooling device based on a solid caloric material using, for example, the elastocaloric, magnetocaloric, barocaloric or electrorcaloric effect has the potential to replace vapor-compression based systems for a variety of applications. Any caloric device using a solid refrigerant may benefit from using a regenerative cycle to increase the operating temperature span. This presentation shows how all active caloric regenerators can be modeled using similar techniques and how they are related to passive regenerator performance. The advantages and disadvantages of using a regenerative cycle are also discussed. The issue of hysteresis in caloric materials is investigated from a system/thermodynamic standpoint and the effects on cooling power and efficiency are quantified using a numerical model of an active regenerator using model caloric materials with assumed properties. The implementation in a working device will be discussed for elastocaloric and magnetocaloric cooling devices. It is shown that demagnetization effects for magnetocaloric systems and stress concentration effects in elastocaloric system reduce the overall effect in the regenerator and care must be taken in regenerator design for both technologies. Other loss mechanisms outside the regenerator such as heat leaks are also discussed. Finally, experimental results for active magnetic regenerative cooler are given for a range of operating conditions. The most recently published device uses a regenerator consisting of Gd and three alloys of GdY and has demonstrated a COP over 3.

1:03PM G19.00004 ABSTRACT WITHDRAWN —

1:39PM G19.00005 Effective Mass of Thermoelectric Materials with Non-Parabolic Kane Bands, G. JEFFREY SNYDER, Northwestern University MSE — Effective mass is a concept commonly used to describe electronic transport in semiconductors using a classical analogy to the kinetic theory of gases. We describe many important electronic transport parameters explicitly with an electronic band mass including: Density of states, charge carrier concentration, mobility, and in particular for thermoelectrics, the Seebeck coefficient. For systems with known electronic band structures these properties can be calculated leading to subtly different definitions of effective mass. In the free electron or parabolic band model the effective masses are the same and we use the term effective mass interchangeably. However the differences between these definitions or uses of effective mass become apparent in non-parabolic band structures where it is desirable to describe the transport in terms of a effective mass that changes with energy (or Fermi Level). For example Kane bands, which become more linear and less parabolic at higher energy, have an increased density of states and therefore higher DOS effective mass than a parabolic band. While it is often assumed that also results in a higher thermopower (Seebeck coefficient), calculations of thermopower and Hall carrier concentration from the Kane model show the thermopower is actually reduced. Examples in thermoelectric materials will be discussed.


11:15AM G20.00001 Big science with little data: separating random waves from vortices in atmosphere and ocean fluid dynamics1, OLIVER BUHLER, Courant Institute of Mathematical Sciences, New York University — How to extract physical and conceptual meaning from limited data sets has been a perennial problem in atmosphere ocean science. This is especially pressing in the current era of large-scale numerical models that seek, for the first time, to simulate directly all the most energetic scales in these systems. This effort requires observational guidance at unprecedented small spatial scales. Progress in extracting physical meaning from data is therefore inseparable from progress in climate simulation and forecasting overall. For example, the successful planning of costly satellite missions depends crucially on the physical nature of the expected motions that are to be observed. In many cases, data are obtained along one-dimensional ship or flight tracks, in which case there are both kinematic and dynamic aliasing effects that obscure the physical meaning of the data. Here kinematic refers to well-known aliasing effects that arise when three-dimensional flow fields are observed only along a line. Dynamics aliasing refers to the more subtle situation when physically different processes project into the same data stream. Indeed, it is well known in atmosphere ocean science that random waves and vortices overlap and intermingle in a complex wave-turbulence jigsaw puzzle, which we need to solve! This talk describes recent progress on this problem, which led to a new method to decompose one-dimensional data into its wave and vortex constituents. The new method works by combining a new Helmholtz decomposition method for one-dimensional velocity spectra with a theoretical energy equi-partition result that allows fingerprinting and identifying the random wave component in the track data. Applications of the new method to oceanic data sets and to the famous Gage–Nastrom spectrum in the atmosphere are presented, with surprising results.

1This work was supported by NSF grants CMG-1024180, DMS-1312159, and DMS-1009213.

11:51AM G20.00002 Convection, Stability, and Turbulence1, CHARLES R. DOERING2, University of Michigan — Many natural flows are driven by buoyancy forces, perhaps the most familiar being those resulting from density variations due to temperature or compositional differences in the presence of a gravitational field. Buoyancy-driven flows of this sort play a major role in geophysical fluid mechanical processes and their transport properties and are central to climate dynamics. The simplest setting to study this phenomena is so-called Rayleigh–Bénard convection, the buoyancy driven flow in a horizontal layer of fluid heated from below and cooled from above. This seminal problem has received tremendous attention over the last century but many riddles remain, especially regarding strongly nonlinear turbulent convection. In this presentation, following an introduction to the phenomena and its applications along with a review of the current state of theory and experiments on high Rayleigh number convection, I will describe some recent results that mathematical analysis has contributed to our understanding of turbulent heat transport.

1Supported in part by NSF Mathematical Physics Award PHY-1205219
22014 Simons Fellow in Theoretical Physics
12:27PM G20.00003 A look at two disparate limits of the climate system: oceanic submesoscales and global energy balance1. BALU NADIGA, LANL — A common theme underlying this journey across scales is that of energy balance. The first topic considers scales from a few tens of meters to a few tens of kilometers and grapples with a fundamental question that concerns energetics of ocean circulation: how does ocean circulation equilibrate in the presence of continuous large-scale forcing and a tendency of geostrophic turbulence to confine energy to large and intermediate scales. In particular, interior instabilities are shown to provide an energy pathway between the largely-balanced, energetic oceanic mesoscales and smaller unbalanced scales (J. Fluid Mech. (2014), vol. 756, pp. 965-1006; doi:10.1017/jfm.2014.464). The second topic zooms out to the global scale and considers global warming from an energy balance perspective. With the global ocean sequestering in excess of 90% of the recent warming due to energy imbalance at the top of the atmosphere, sensitivity of warming and depth of penetration of warming are characterized in a probabilistic fashion.

1Supported in part by the LDRD program at LANL (project number 20110150ER)

1:03PM G20.00004 Stochastic models for tropical convection and extreme rainfall events1, SAMUEL STECHMANN, University of Wisconsin-Madison — In the Tropics, storms and convection occur intermittently and have a major impact on weather and climate. In recent years, tropical rainfall statistics have been shown to conform to paradigms of critical phenomena and statistical physics. To gain further insights into these statistics and extreme events, this talk presents simple stochastic models for the statistics of precipitation events and water vapor dynamics (local in space, and evolving in time). Through exact solutions and simple numerics, a suite of observed rainfall statistics is reproduced by the model, including power-law distributions and long-range correlations. The key ingredients of the model are the dynamics of column water vapor, governed by a combination of Gaussian stochastic forcing and nonlinearities provided via a threshold and/or stochastic trigger. Finally, these statistics are being explored in climate model simulations with collaborators.

1The research of S.N.S. is partially supported by Office of Naval Research grants ONR N000141210744 and ONR N000141210912.

1:39PM G20.00005 Climate Variability and Nonequilibrium Steady-States1, JEFFREY WEISS, University of Colorado, Boulder — The climate system is forced by incoming solar radiation and damped by outgoing long-wave radiation. As a result, the climate system is not in thermodynamic equilibrium but is better conceptualized as residing in a nonequilibrium statistically steady-state. Nonequilibrium steady-states have internal fluctuations which appear as natural variability of the climate system. Additionally, the phase space has nonzero probability current loops which are manifested as preferred patterns of natural climate variability. Nonequilibrium steady-states are often modeled by stochastic Langevin dynamics, and many aspects of the physics of these models are well understood. Simple stochastic models have been applied to a variety of climate phenomena including El-Niño, the North Atlantic Gulf Stream, surface temperature patterns, ocean heat content, and atmospheric Storm Tracks. In their simplest form, these models describe a stable steady-state with linear nonconservative damping perturbed by additive Gaussian white noise and thus fall into the class of models capturing nonequilibrium steady-states where previous results from Langevin models apply while the climate context motivates additional new questions.

1This work supported by the National Science Foundation under Grant No. OCE-1245944.


11:15AM G21.00001 An ultra-low field electron paramagnetic resonance technique for biomedical research. P. BHUPATHI, Physics Department, California Institute of Technology, I. HAHN, Jet Propulsion Laboratory, California Institute of Technology — Conventional electron paramagnetic resonance (EPR) imaging systems use high magnetic fields confined to small spaces and therefore have limitations on the sample size and safety issues related to the high level of radiation. We are developing an ultra-low field SQUID (Superconducting Quantum Interference Device)-magnetometer system for EPR detection from room temperature samples in magnetic fields of a few Gauss, corresponding to EPR frequencies of a few MHz. Operation at low EPR excitation frequencies of a few MHz ensures negligible sample heating and high penetration depth in biological systems. A new measurement system consists of a specially designed low noise, non-magnetic 4K dewar with a hollow tail housing a superconducting second order gradiometer inductively coupled to a two-stage dc SQUID amplifier. This unique gradiometer design allows a sample at room temperature to be positioned at the middle turns, which significantly improves the signal-to-noise ratio. We present preliminary results and discuss the prospects for in vivo biomedical EPR imaging.

11:27AM G21.00002 A Nanocoaxial-Based Electrochemical Sensor for the Detection of Cholera Toxin1, MICHELLE M. ARCHIBALD, BINOD RIZAL, TIMOTHY CONNOLLY, MICHAEL J. BURNS, MICHAEL J. NAUGHTON, THOMAS C. CHILES, Boston College — Sensitive, real-time detection of biomarkers is of critical importance for rapid and accurate diagnosis of disease for point of care (POC) technologies. Current methods do not allow for POC applications due to several limitations, including sophisticated instrumentation, high reagent consumption, limited multiplexing capability, and cost. Here, we report a nanocoaxial-based electrochemical sensor for the detection of bacterial toxins using an electrochemical enzyme-linked immunosorbent assay (ELISA) and differential pulse voltammetry (DPV). Proof-of-concept was demonstrated for the detection of choler toxin (CT). The linear dynamic range of detection was 10 ng/ml – 1 µg/ml, and the limit of detection (LOD) was found to be 2 ng/ml. This level of sensitivity is comparable to the standard optical ELISA used widely in clinical applications. In addition to matching the detection profile of the standard ELISA, the nanocoaxial array provides a simple electrochemical readout and a miniaturized platform with multiplexing capabilities for the simultaneous detection of multiple biomarkers, giving the nanocoax a desirable advantage over the standard method towards POC applications.

1This work was supported by the National Institutes of Health (National Cancer Institute award No. CA137681 and National Institute of Allergy and Infectious Diseases award No. AI100216).

11:39AM G21.00003 Symmetric and Asymmetric Split Ring Resonators for Biosensing at Terahertz Frequencies1, GUILLERMO NARANJO, XOMALIN PERALTA, Univ of Texas, San Antonio — Food allergies have become a major health concern around the world. Peanut allergies are particularly important because they affect over 5 million people in the United States. We are proposing to develop a metamaterial-based sensor for peanut allergens. The detection mechanism we will tap into is the change in a metamaterial’s resonant response due to the presence of a biomolecule in the gap region. Using a commercial-grade simulator based on the finite-difference time-domain method, we have simulated the terahertz transmission and reflection spectra of three different split-ring resonator designs with and without a biomolecule present. By modifying the overall symmetry of the resonator and the geometry of the gap region, we have modified the resonant response and increased its sensitivity. The increased sensitivity is demonstrated by repeating the simulations with a layer of peroxidase conjugated immunoglobulin G (PX-IgG) in the gap region and quantifying the resulting resonant shift. These results are the basis for the proposed allergen sensors.

1UTSA MBRS-RISE Research Training Program.
11:51AM G21.00004 On-chip cell sorting via patterned magnetic traps . TOM BYVANK, MICHAEL PRIKOCKIS, AARON CHEN, BRANDON MILLER, JEFFREY CHALMERS, RATNASINGHAM SOORYAKUMAR, Ohio State University — Due to their importance in research for the diagnosis and treatment of cancer, numerous schemes have been developed to sort rare cell populations, e.g., circulating tumor cells (CTCs), from a larger ensemble of cells. Here, we improve upon a previously developed microfluidic device (Lab Chip 13, 1172, (2013)) to increase throughput and sorting purity of magnetically labeled cells. The separation mechanism involves controlling magnetic forces by manipulating the magnetic domain structures of the embedded permalloy microdisks with weak external fields. These forces move labeled cells from the input flow stream into an adjacent buffer flow stream. Such magnetically activated transfer separates the magnetic entities from their non-magnetic counterparts as the two flow streams split apart and move toward their respective outputs. Purity of the magnetic output is modulated by the withdrawal rate of the non-magnetic output relative to the inputs. A proof of concept shows that CTCs from metastatic breast cancer patients can be sorted, recovered from the device, and confirmed as CTCs using separate immunofluorescence staining and analysis. With further optimizations, the channel could become a useful device for high purity final sorting of enriched patient cell samples.

12:03PM G21.00005 Neuroelectronic device based on nanocoax arrays . JEFFREY R. NAUGHTON, JACLYN N. LUNDBERG, JUAN A. VARELA, MICHAEL J. BURNS, THOMAS C. CHILES, JOHN P. CHRISTIANSON, MICHAEL J. NAUGHTON, Boston College — We report on development of a nanocoax-based neuroelectric array. The device has been used in real time to noninvasively couple to a ganglion sac located along the main nerve cord of the leech Hirudo medicinalis. This allowed for extracellular recording of synaptic activity in the form of spontaneous synapse firing in pre- and post-synaptic somata, with the next target being recording of local field potentials from rat hippocampal cells. We also discuss an alteration of the architecture to facilitate optical integration of the nanoarray, toward utilizing the so-modified device to elicit / inhibit action potentials in optogenetically-modified cells.

12:15PM G21.00006 Intracavity Microfluidic Laser Device for Single Cell Analysis , PAUL COURLEY, HighLight Research Lab — An intracavity microfluidic laser device has been developed to study bioparticles ranging in size from 50 nm to 20 µm (virions to organelles to whole cells). The versatile device can be operated used in several modes including static or flowing fluids, with or without molecular labels, and microscopic imaging and/or spectroscopy. It enables advantageous new ways to perform analyses of bioparticles for applications including cell biology, detection of disease and pathogens, environmental monitoring, pharmaceuticals, agriculture, and food processing. This talk will briefly summarize the physics of the device including its laser optics, fluid dynamics, and intracavity light interaction with cells. The talk will then focus on results of a study of mitochondria in normal and cancer liver cells. The study examines the transformation of intracellular and isolated mitochondria from the normal to disease state. The results highlight the unique utility of the device to rapidly assess biophysical changes arising from altered biomolecular states of cells and organelles.

12:27PM G21.00007 Individual Mammalian Cell Magnetic Measurements with a Superconducting Quantum Interference Device . JOHANNA C. PALMSTROM, Gabilan Stanford Graduate Fellow, Geballe Laboratory for Advanced Materials, Stanford University, KIMBERLY BREWER, SUI SENG TEE, Department of Radiology, Stanford University School of Medicine, ERIC THEIS, Geballe Laboratory for Advanced Materials, Stanford University, BRIAN RUTT, Department of Radiology, Stanford University School of Medicine, KATHRYN A. MOLER, Geballe Laboratory for Advanced Materials, Stanford University — Magnetism can be introduced into otherwise nonmagnetic cells by the uptake of superparamagnetic iron oxide (SPION) nanoparticles. SPION nanoparticles are used in numerous biomedical applications including cellular therapies and targeted drug delivery. Currently there are few tools capable of characterizing individual magnetic nanoparticles and the magnetic properties of individual mammalian cells loaded with SPION. Our scanning superconducting quantum interference devices (SQUIDs) are good candidates for these measurements due to their high sensitivity to magnetic dipole moments (approx. 200 µm/√Hz). In this study, we use a scanning SQUID to image the magnetic flux from SPION loaded H1299 lung cancer cells. We find that the magnetic moment spatially varies inside the cell with each cell having a unique distribution of moments. We also correlate these magnetic images with optical and scanning electron microscope images. These results show that the SQUID is a useful tool for imaging biological magnetism. The visualization of single cell magnetism and the quantification of magnetic dipole moments in magnetically labeled cells can be used to optimize conventional biological magnetic imaging techniques, such as MRI.

12:39PM G21.00008 Interaction-Free Quantum Electron Microscope in Free-Space1 . YUJIA YANG, CHUNG-SOO KIM, RICHARD HOBBES, VITOR MANFRINATO, ORHAN CELIKER, Massachusetts Institute of Technology, PIETER KRUIT, TU Delft, KARL BERGGREN, Massachusetts Institute of Technology — We propose the design and theoretical analysis of a quantum electron microscope (QEM), which utilizes interaction-free quantum measurement with electrons for nanoscale imaging. The QEM can be used to image electron-irradiation-sensitive materials, such as biological samples, with a high resolution and low radiation damage. Our QEM scheme is an electron interferometer with a storage resonator. The incoming electron beam is asymmetrically split into a strong reference beam and a weak sample beam, both of which are stored in the resonator. Only the weak sample beam transmits through the sample for multiple times. We propose to build the QEM with free-space electron optics. We develop a scattering matrix method to theoretically analyze the contrast mechanism, radiation damage, and measurement accuracy. We propose an electron-mirror-based storage resonator and we have performed electron optics simulation of electron trajectories within the resonator. We also report experimental implementation and characterization of the electron beam-splitter to be used in the QEM. Thin crystals fabricated with focused ion beam and nano-gratings fabricated with electron-beam lithography are two candidate beam-splitters, both of which are characterized by electron diffraction.

1This work is funded by Gordon and Betty Moore Foundation

12:51PM G21.00009 Light localization properties of biological cells via confocal imaging1 . PEETYUSH SAHAY, HEMENDRA M. GHIMIRE, HUDA ALMABADI, PRABHAKAR PRADHAN, Univ of Memphis — Detection and characterization of the spatial refractive index fluctuations of very weakly disordered dielectric media has ample applications in various fields ranging from soft condensed matter to biological research. We report a study of the submicron scale degree of the structural disorder of heterogeneous weakly disordered optical dielectric media, such as biological cells, by quantifying their submicron scale light-localization properties. Confocal microscopy is used to construct disordered optical lattices of these dielectric media. Light-localization properties are studied by the statistical analysis of the inverse participation ratio (IPR) of the localized eigenfunctions of these optical lattices at the submicron scales. The method is described and its importance is highlighted. As one of the applications, we demonstrate that using this method, different types of normal and cancerous cells can be distinguished by quantifying the structural disorder inside the cells via their confocal micrographs. Other potential applications of the technique to characterize weakly disordered media, as well as biological cells, in particular cancer detection, are also discussed.

1NIH and University of Memphis
1:03PM G21.00010 Enhanced partial wave spectroscopy (EPWS) for nanoscale sensitive structural disorder measurement in weakly disordered media1, HUDA ALMABADI, PEEYUSH SAHAY, PRABHAKAR PRADHAN, Univ of Memphis — Based on mesoscopic physics approach, partial wave spectroscopy (PWS) technique was introduced earlier for the measurement of the nanoscale structural disorder in very weakly disordered optical media, such as biological cells. We describe a modification and further improvement of this technique, by introducing an enhanced back reflection system to further increase the measurement sensitivity of the PWS technique. As a result, a nanoscale level of fluctuation or nanoscale alteration in a disordered medium can be measured with even higher sensitivity and accuracy. In this enhanced-PWS (EPWS) technique, semi-transparent metallic thin films are used to create a cavity like structure that holds the sample; this leads to an increased back reflected light intensity, which eventually results in high sensitivity in the nanoscale structural disorder measurements. Reflection coefficients of the backscattered signal obtained from the simulated disordered media, within the cavity, with varying refractive index fluctuation values, were statistically analyzed using mesoscopic physics approach. The results, of a sample with and without metallic cavity inside the system show a significantly high back reflected intensity with the metallic cavity case. We also discuss the possible applications of the developed technique in ultra-sensitive detection of cancer by the characterization of nanoscale fluctuations in biological cells.

1 NIH and University of Memphis

1:15PM G21.00011 Quantitative ultrasonic bone assessment using backscatter measurements at 1 MHz, PHILIP SPINOLO, Rhodes College. Department of Physics, BRENT HOFFMEISTER, Rhodes College, SANG-ROK LEE, University of Memphis, Department of Health and Sport Sciences, JINSONG HUANG, University of Tennessee Health Science Center, College of Medicine — Osteoporosis is a complicated metabolic degenerative bone disease affecting millions of Americans. The current standard for diagnosis is an x-ray technique called DXA, but ultrasound may offer a cheaper, more portable diagnosis method that may also be sensitive to bone strength in ways DXA is not. Ultrasonic backscatter techniques in the 5 MHz range have been shown to be sensitive to changes in bone mineral density (BMD) associated with osteoporosis. These techniques measure the power ratio between an earlier and later part of the backscatter signal. These ratios (called nMBD or nBAR in the time domain) depend on ultrasonic attenuation in bone which is known to correlate with BMD. This study measured nMBD and nBAR using a 1 MHz transducer. Lower frequency transducers increase signal penetration into bone. Linear regression analysis was used to investigate correlations between nMBD and nBAR and the density and microstructural characteristics of bone such as the structural model index (SMI) and trabecular number (TbN). Good linear correlations were observed for nMBD and nBAR vs. BMD at r=0.75 and r=0.70, respectively, comparable to correlations obtained using a 5 MHz transducer. Correlations with SMI and TbN were within the r=0.65-0.75 range.

1:27PM G21.00012 Thermal (rf) and non-thermal mechanisms of nanoparticles induced/enhanced cancer cell apoptosis, JAREK WOSIK, University of Houston, DHIYA KETHARNATH, University of Missouri Kansas City, MATTJEW J. WARE, BIANA GODIN, The Methodist Hospital Research Institute, WANADA ZAGODZODN-WOSIK, University of Houston — It was demonstrated that the rf procedures can be non-invasive and cancer selective when combined with nanoparticles (NPs) that work as rf heating enhancers. However, there are disparities, between theory and experimental results, especially for non-magnetic NP. Therefore, it is necessary to elucidate the physical mechanisms that control the reported rf heating. We have constructed an apparatus for rf heating, which allows for applying either E_r or H_r fields in the kHz-MHz frequency range. Our results of specific absorption rate (SAR) measurements for both magnetic and nonmagnetic of NPs indicate that rf electric field also plays the role in heating of magnetic NPs and that in the nonmagnetic case only interface losses are responsible for the observed heating. In search for a more efficient and non-thermal method, we have explored a cancer cell death through mechanical stress imposed on the cell membrane. We have designed a special setup to apply either static or magnetic fields or gradients (up 300T/m) to cultured cancer cell lines with/without PNs added. The fields and gradients, and forces applied were simulated using HFSS/Maxwell software. Pancreatic adenocarcinoma cell line, AsPC-1 stained with DRAQ7 were studied. Very strong dependence of number of dead cells on applied field strength was observed. Discussion of the two mechanisms (rf and non-rf) of observed apoptosis will be presented.

1:39PM G21.00013 Precise control of DNA recapture in solid-state nanopore, YING HU, ZHI ZHOU, XINYAN SHAN, ZHI XU, XUEDONG BAI, XINGHUA LU, None — Solid-state nanopore is a novel experimental method in detecting and analyzing single biomolecules such as DNA, protein and virus. The dynamic behavior of such molecules in a microfluidic system can be investigated by the back-and-forth translocation control. Such motion control is made possible by fast changing of the polarity of the driving voltage, and the repeat measurement of a single molecule is expected to increase the signal-to-noise-ratio (SNR) significantly. However, due to the existence of membrane capacitance and electrolyte resistance, transient current spike arises as driving voltage changes. Such current spike saturates the data acquisition system and leads to difficulty in detecting fast returned molecules. Simulation shows that the electric field in electrolyte is proportional to the ionic current and increases dramatically during the transient charging period. This extra electric force pulls the molecule back to the pore faster than expected. Our study demonstrates that the transient current can be compensated by modifying the profile of the driving voltage. With such improvement, the observed distribution of recaptured translocation events matches perfectly with the prediction by drift-diffusion transport equation. This finding will help building precise control technique towards DNA sequencing in nanopore.

1 Supported by the National Basic Research Program of China under Grant No 2012CB933002 and the Strategic Priority Research Program (B) of the Chinese Academy of Sciences under Grant No XDB07030100.

1:51PM G21.00014 Assessing the performance of trans rectal ultrasound to measure prostate weight and its association with other diagnostic factors, IRENE B. HELENOWSKI, BORKO D. JOVANOVIC, ROBIN G. LEIKIN, MICHAEL J. GURLEY, CHRISTOPHER K. MITCHELL, TIMOTHY M. KUZEL, Northwestern University — Trans rectal ultrasound is fast becoming an important tool used in the prognosis of prostate cancer. But how does it compare to other measures, such as the actual weight of the prostate obtained after radical prostatectomy? Here, we assess the association of prostate weight obtained via trans rectal ultrasound and actual specimen weight obtained after radical prostatectomy with body mass index (BMI) using linear regression models adjusted for Gleason score, pre-operative PSA, and age applied to subsets of Euro-Americans (n = 242) and African Americans (n = 34). The roles of both prostate weight and BMI are themselves part of ongoing research focused on prostate cancer prognosis. Our preliminary results show a marginal relationship between BMI and specimen weight obtained after surgery in Euro-Americans but no relationship between BMI and ultrasound measured weight in either race subset. Therefore, further work pertaining to the performance of trans rectal ultrasound may be warranted. This work is supported by the Northwestern University SPORE in Prostate Cancer (NIH/NCI P50 CA 90386).
2:03PM G21.00015 How to get into that “room at the bottom” of DNA analysis1, DANIEL BERARD, FRANCOIS MICHAUD, SARA MAHSHID, JALAL MOHAMMED AHAMED, McGill University, PIERRE BERUBE, ROBERT SLADEK, Genome Quebec Innovation Centre, WALTER REISNER, SABRINA LESLIE, McGill University — Linearly extending long DNA molecules in sub-50 nm nanochannels for genomic analysis, while retaining their structural integrity, is a major technological challenge. We employ “Convex Lens-induced Confinement” (CLIC) microscopy to gently load DNA into nanogrooves from above, overcoming the limitations of side-loading techniques used in direct-bonded nanofluiddic devices. In the CLIC technique, the curved surface of a convex lens is used to deform a flexible coverslip above a glass substrate, creating a nanoscale gap that can be tuned during an experiment to load and confine molecules into nanoscale features embedded in the bottom substrate. Since DNA molecules are loaded into the embedded nanotopography from above, CLIC eliminates the need for the high pressures or electric fields required to load DNA into direct-bonded nanofluiddic devices. To demonstrate the versatility of CLIC, we confine DNA to a variety of nanostructures, demonstrating DNA nanochannel-based stretching and denaturation mapping. In particular, we have successfully extended DNA in 27 nm channels, achieving high stretching (90 percent) that is in good agreement with Odijk deflection theory, and we have mapped genomic features using denaturation analysis.

1NSERC, CIHR


11:15AM G22.00001 Entanglement entropy near Kondo-destruction quantum critical points1, KEVIN INGERSENT, University of Florida, JEDEDIAH PIXLEY, University of Maryland, CHRISTOPHER WAGNER, TATHAGATA CHOWDHURY, University of Califonia, MATTHEW MIECNIKOWSKI, University of Colorado Boulder — We study the impurity entanglement entropy S_e in quantum impurity models that feature a Kondo-destruction quantum critical point (QCP) arising from a pseudogap in the conduction-band density of states and/or from an additional coupling of the impurity to a bosonic bath. On the local-moment (Kondo-destroyed) side of the QCP, the entanglement entropy contains a critical component that can be related to the order parameter characterizing the phase transition. In Kondo models describing a spin-S impurity, S_e assumes its maximal value ln(2S + 1) at the QCP and throughout the Kondo phase, independent of particle-hole (a)symmetry and irrespective of whether the Kondo phase features exact, over-, or under-screening of the impurity spin. In Anderson models, by contrast, S_e takes a nonuniversal value at the QCP. At particle-hole symmetry, S_e rises monotonically on passage from the local-moment phase to the Kondo phase, while breaking this symmetry can lead to a cusp peak in S_e due to a divergent charge susceptibility at the QCP. Implications of these results for quantum-critical systems and quantum dots are discussed.

1Supported by the East-DeMarco Fellowship and NSF Grants DMR-1107814 and DMR-1156737

11:27AM G22.00002 Low temperature phases of the periodic Anderson model with electron-phonon correlation 1, ENZHI LI, Louisiana State University, PENG ZHANG, Carnegie Institution of Washington, SHUXIANG YANG, KA-MING TAM, JUANA MORENO, MARK JARRELL, Louisiana State University — We study the periodic Anderson model with the conduction electrons coupled to phonons. It has been shown by using the dynamical mean field theory that the model contains two disordered phases, the Kondo singlet phase for strong hybridization and the local moment phase for weak hybridization. In the hybridization-temperature plane, these two phases are separated by a first order phase transition line which terminates at a second order phase transition point. At low temperature the entropy in the Kondo singlet phase is quenched by the formation of a Fermi liquid, while the local moment phase will have residual entropy unless it is quenched by ordering. We calculate the lattice charge susceptibility to demonstrate that the conduction electrons form a charge density wave ordering below a critical temperature.

1The current work is funded by the NSF EPSCoR LA-SIGMA project under award #EPS-1003897.

11:39AM G22.00003 Kondo-Heisenberg Lattice: Majorana fermions Mean field approach, SAYED ALI AKBAR GHORASHI, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX — We study Kondo lattice model including direct antiferromagnetic Heisenberg exchange interaction using Majorana fermions representation at half filling. An O(3)-symmetric Mean field Hamiltonian is derived on bipartite lattice. Different kind of possible spin-spin correlations functions between conduction band spins, c-electrons, and localized spin, f-electron in both on site and different sublattices are calculated in translationally invariant solution of the mean field Theory. Finite temperature behavior of Majoranas pairs correlations are investigated for some special limit of some of the mean filed parameters.

11:51AM G22.00004 Magnetic Excitons in Heavy Fermion Semimetals, PETER RISEBOROUGH, Physics Dept. Temple University — A magnetic excitation is a precursor magnetic exciton, similar to an antiparamagnon in a metal, which exists in strongly correlated semiconductors. The magnetic exciton has a spectrum which resembles the broadened dispersion relation of an antiparamagnon for excitation energies greater than the semi-conducting gap, but becomes sharp for energies less than the semi-conducting gap. The narrowness of the spectral feature is due to the absence of decay channels into the continuum of electron-hole pairs. Such excitations have been observed by inelastic neutron scattering experiments on the heavy-fermion semiconductors SmB6 and YbB12. However, magnetic excitons have not been observed in cerium based heavy-fermion semiconductors nor has their occurrence been linked to the vicinity of a quantum critical point. Here we investigate this problem using a phenomenological model for both the “nematic” (i.e. tetragonal symmetry-broken) and superconducting phases. Based on recent field-angle-dependent heat capacity and thermal conductivity data, as well as Kerr effect measurements, we consider a chiral d + id superconducting state that also breaks time-reversal symmetry. We find that in the presence of an orthorhombic/nematic order parameter, the system displays two sequential superconducting transitions: in the first, at Tc, the system enters a superconducting phase whereas in the second, at T^* < Tc, time-reversal symmetry is broken. Near the second transition, a “soft” but damped collective mode related to gap amplitude fluctuations emerges, which could be manifested in Raman scattering data. Between these two transitions, we find an unusual \omega log(\omega) dependence of the low-energy density of states, and show how it impacts the properties of several thermodynamic quantities in the T^* < T < Tc regime.

1This work was supported by the Department of Energy under Award Number DE-SC0012336.
12:15PM G22.00006 Crossover from non-Fermi liquid to Fermi liquid behavior and the superconducting dome in heavy electron systems. PEDRO SCHLOTTMANN, Florida State University — A nested Fermi surface and the remaining interaction between the carriers after the heavy particles are formed give rise to itinerant antiferromagnetism. We consider an electron and a hole pocket, separated by a wave vector $Q$, and Fermi momenta $k_{F_1}$ and $k_{F_2}$, respectively. The order is gradually suppressed by increasing the mismatch of the two Fermi momenta and a QCP is obtained as $T_N \to 0$. For critical mismatch of the Fermi vectors (tuned QCP) the specific heat over $T$ increases as $-\ln(T)$ as $T$ is lowered. And the linewidth of the quasi-particles is linear in $T$ and $\omega$. With increasing nesting mismatch and decreasing temperature the specific heat and the linewidth display a crossover from non-Fermi liquid ($\sim T$) to Fermi liquid ($\sim T^2$) behavior. If in addition the vector $Q$ is commensurate with the lattice (Umklapp with $Q = G/2$), pairs of electrons can be transferred between the pockets. To avoid the QCP this process may lead to superconductivity and a superconducting dome above the quantum critical point. We investigate the conditions under which such a dome arises.

1Supported by the Department of Energy under Grant No. DE-FG02-98ER45707

12:27PM G22.00007 Temperature-dependent behavior of mixed-valent SmS: a DFT+DMFT study. CHANG-JONG KANG, HONG CHUL CHOI, KYOO KIM, B. I. MIN, Pohang University of Science and Technology (POSTECH) — We have investigated temperature-dependent behaviors of electronic structure and resistivity in a mixed-valent golden phase of SmS (g-SmS), based on the dynamical mean-field theory band structure calculations. Upon cooling, the coherent Sm 4f bands are formed to produce the hybridization-induced pseudo-gap near the Fermi level, and accordingly the topology of Fermi surface is changed. Also we have discussed the topological nature in g-SmS. From the analysis of anomalous resistivity behavior in SmS, we have identified universal energy scales, which characterize the Kondo/mixed-valent semimetallic systems.

1Presented

12:39PM G22.00008 The Ising-Anisotropic Kondo Lattice in a transverse field: EDMFT study and implications for the global phase diagram. EMILIAN MARIUS NICA, Department of Physics and Astronomy, Rice University, Houston, Texas 77005, KEVIN INGERSENT, Department of Physics, University of Florida, P.O. Box 118440, Gainesville, Florida 32611, QIMIAO SI, Department of Physics and Astronomy, Rice University, Houston, Texas 77005 — Heavy-fermion materials exhibit a rich variety of phase transitions. Of particular interest are quantum phase transitions and the associated breakdown of the Fermi liquid picture. A theoretical example of this is the Kondo destruction effect in the context of local quantum criticality [1]. To capture this effect and others, a zero-temperature global phase diagram for heavy-fermion systems is proposed [1]. It incorporates the competition between the Kondo effect (promoted by exchange coupling $J_K$) and the variable quantum fluctuations of the local-moment magnetism (parameterized by $G$). We investigate this competition in the Ising-anisotropic Kondo lattice with a transverse magnetic field, where the field serves to tune $G$. We determine a zero-temperature phase diagram of this model within the extended dynamical mean-field theory (EDMFT), and discuss the implications of our results for the global phase diagram of heavy-fermion systems.


12:51PM G22.00009 Super-Symplectic spin and heavy fermion systems. ALINE RAMIRES, PIERS COLE-MAN, Rutgers University — Heavy-fermion materials are systems in which the presence of local moments leads to new physics. The phase diagram of these systems is very rich, usually presenting an antiferromagnetic (AFM) phase, a heavy Fermi liquid regime (HFL), and non-Fermi-liquid behavior above the AFM quantum critical point (QCP). Our understanding of what happens to the local moments in different extremes of this phase diagram is based in two different representations for the spin: a Schwinger boson representation, appropriate for the description of AFM, and an Abrikosov fermion representation, suitable for the understanding of the HFL development. The theoretical approaches to this problem so far have been restricted to describe only extremes of this phase diagram, and are not reliable for the description of the more interesting region of the diagram, around the QCP. In this region the magnetic and Kondo energy scales interplay and can lead to dramatic changes in the character of the quantum phase transition. Here we use supersymmetric symplectic spins in order to investigate this intermediate regime.

1:03PM G22.00010 Enhanced Pairing Correlations near a Quantum Critical Point in Two Impurity Anderson Model with a Pseudogap. ANG CAI, Rice University, JEDEDIAH PIXLEY, University of Maryland, QIMIAO SI, Rice University — Significant progress has been made on the understanding of quantum critical heavy fermion metals. In addition to the spin density wave quantum critical point (QCP), a Kondo destruction QCP beyond the Landau framework has been discovered. However, its implications on the formation of unconventional superconductivity remain unclear. Motivated by a cluster-EDMFT approach [1], we address this question in simplified models for Kondo destruction QCP, as arising in the two impurity pseudogap Anderson model. We study the model using the continuous time quantum Monte-Carlo method, with either an Ising or Heisenberg inter-impurity RKKY interaction. For each case we have found a QCP distinct from both the Kondo destruction criticality of a single impurity pseudogap Anderson model and the quantum criticality of the conventional two impurity model. We observe critical local moment fluctuations with a power-law divergence in the staggered spin susceptibility, and show that the single-particle spectral function obeys power-law over temperature scaling. We find that the singlet pairing susceptibility is significantly enhanced near the QCP. Implications for unconventional superconductivity in quantum critical heavy fermion systems will be discussed. [1] J.H. Pixley, A. Cai, Q.-Si, arXiv:1409.1090

1:15PM G22.00011 Numerical study of the periodic Anderson model with a quarter-filled conduction band. SHUXIANG YANG, JUANA MORENO, MARK JARRELL, Louisiana State Univ - Baton Rouge — Using the dynamical cluster approximation with continuous-time quantum Monte Carlo as the cluster solver and the recently introduced dual-fermion method, we study the underlying physics of the periodic Anderson model where the conduction band is near quarter-filling while the f-band electron band is half filled. For these parameters, the RKKY coupling changes its nature from ferromagnetic to anti-ferromagnetic, yielding an interesting phase-diagram. Especially, we find the charge ordering of the conduction band is strongly enhanced, which could be due to the proximity to a quantum critical point.

1:27PM G22.00012 Unconventional Superconductivity in the Vicinity of the Local Quantum Critical Point. QIMIAO SI, Rice University, JEDEDIAH PIXLEY, Condensed Matter Theory Center, University of Maryland, LILIL DENG, KEVIN INGERSENT, University of Florida — Unconventional superconductivity and its relationship with quantum criticality remains a central question in strongly correlated electron systems. In the case of heavy fermion metals, the existence of antiferromagnetic quantum critical points (QCPs) is well established. Theoretical work has identified the existence of a local QCP where the Kondo effect is driven critical concomitant with the vanishing of the magnetic order parameter. Experiments on the heavy fermion compound CeRhIn$_5$ and other materials have provided strong evidence that such a QCP drives unconventional superconductivity. With this in mind we solve the periodic Anderson model using a cluster extended dynamical mean field theory. We show that the Kondo energy scale is continuously suppressed at the antiferromagnetic critical point, and we determine the scaling form of the order parameter susceptibility and find remarkable agreement with well-established experiments in the related heavy fermion system CeCu$_{2−x}$Au$_x$. Most importantly, we find that the singlet pairing susceptibility is strongly enhanced at the QCP, which points towards a new pairing mechanism associated with both magnetic and local critical fluctuations.
1:39PM G22.00013 Metamagnetism in CeCoIn$_5$ and the Single Energy Scale Model. A. THANIZHAVEL, N. SANGEETA, S. RAMAKRISHNAN, Tata Institute of Fundamental Research, B. WHITE, BRIAN MAPLE, University of California, San Diego, ULRICH WELP, Argonne National Labs, PRADEEP KUMAR, University of Florida, V. CELLI, BELLAVE SHIVARAM, University of Virginia — The anisotropic linear and nonlinear magnetic response of the non-ordering heavy electron compound CeCoIn$_5$ will be presented. Many heavy electron materials exhibit a peak in the linear susceptibility at a temperature $T_1$ which correlates with the metamagnetic critical field, $H_c$. There is also a peak in the nonlinear susceptibility $\chi_2$ at $T_2 = 0.5T_1$; in many materials and this feature has been explained recently with a single energy scale model. In CeCoIn$_5$, however, a plateau rather than a peak is observed in the linear susceptibility which evolves into a paramagnetic type divergence upon further cooling. This apparent violation of the “ideal” metamagnetic behavior is resolved here. The single energy scale model augmented with a paramagnetic contribution successfully accounts for the observed linear and nonlinear anisotropic magnetic response in CeCoIn$_5$.

1:51PM G22.00014 Quantum criticality driven by geometrical frustration. PHILIPP GEGENWART, Experimentalphysik VI, Augsburg University, Germany, Y. TOKIWA, Kyoto University, Japan, C. STINGL, Experimentalphysik VI, Augsburg University, Germany, T. TAKABATAKE, Hiroshima University, Japan — Geometrical frustration describes situations where interactions are incompatible with the lattice geometry and stabilizes exotic phases such as spin liquids which cannot be classified by conventional order parameter theory and display emergent excitations. Whether geometrical frustration of magnetic moments in metals can induce unconventional quantum critical points is an active area of research. We focus on the heavy-fermion metal CeRhSn with two-dimensional triangular configuration of the Kondo ion. Low-temperature thermodynamic experiments prove zero-field quantum criticality. A striking anisotropy of the linear thermal expansion, displaying critical and non-critical behavior along and perpendicular to the basal plane, respectively, is ascribed to the effect of strong geometrical frustration. We further find evidence of fluctuating local 4f moments, implying a novel quantum critical spin liquid state with fractionalized quasiparticles.

2:03PM G22.00015 Many-body instabilities and mass generation in slow Dirac materials. CHRISTOPHER TRIOLA, William & Mary Coll, JIANXIN ZHU, Center for Integrated Nano Technology, Los Alamos National Laboratory, ALBERT MIGLIORI, Seaborg Institute, Los Alamos National Laboratory, ALEXANDER BALATSKY, Institute for Materials Science, Los Alamos National Laboratory — Some Kondo insulators are expected to possess topologically protected surface states with linear Dirac spectrum, the topological Kondo insulators. Because the bulk states of these systems typically have heavy effective electron masses, the surface states may exhibit extraordinarily small Fermi velocities that could force the effective fine structure constant of the surface states into the strong coupling regime. Using a tight-binding model we study the many-body instabilities of these systems and identify regions of parameter space for which antiferromagnetic, ferromagnetic and charge density wave instabilities occur.

1Work Supported by USDOE BES E304.


11:15AM G23.00001 Challenges for large scale ab initio Quantum Monte Carlo. PAUL KENT, Oak Ridge National Lab — Ab initio Quantum Monte Carlo is an electronic structure method that is highly accurate, well suited to large scale computation, and potentially systematically improvable in accuracy. Due to increases in computer power, the method has been applied to systems where established electronic structure methods have difficulty reaching the accuracies desired to inform experiment without empiricism, a necessary step in the design of materials and a helpful step in the improvement of cheaper and less accurate methods. Recent applications include accurate phase diagrams of simple materials through to phenomena in transition metal oxides. Nevertheless there remain significant challenges to achieving a methodology that is robust and systematically improvable in practice, as well as capable of exploiting the latest generation of high-performance computers. In this talk I will describe the current state of the art, recent applications, and several significant challenges for continued improvement.

1Supported through the Predictive Theory and Modeling for Materials and Chemical Science program by the Office of Basic Energy Sciences (BES), Department of Energy (DOE).

11:51AM G23.00002 SILK QMC, sign-learning simulations of molecular systems. XIAOYAO MA, Department of Physics and Astronomy, Louisiana State University, FRANK LOFFLER, Center for Computation and Technology, Louisiana State University, KAROL KOWALSKI, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, RANDALL HALL, Department of Natural Sciences and Mathematics, Dominican University of California, JUANA MORENO, MARK JARRELL, Department of Physics and Astronomy, Louisiana State University — The Sign Learning Kink (SILK) based Quantum Monte Carlo (QMC) is used to calculate the ground state energies for H$_2$O, N$_2$ and F$_2$ molecules. This method is based on Feynman’s path integral formalism and has two stages. The first, learning stage, reduces the minus sign problem by optimizing the Slater states which are used in the second, QMC stage. We test our method using different vector spaces and compare our results with other Quantum Chemical methods. We also perform exact diagonalization in those vector spaces as a benchmark. In each vector space and for each molecule, we perform SILK QMC for different bond lengths demonstrating that the SILK method is accurate for equilibrium and non-equilibrium geometries.

1Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA)

12:03PM G23.00003 Development and Use of Quantum Chemistry Methods on Intel Many-Integrated Core Units. EDOARDO APRA, Pacific Northwest National Laboratory — We will describe the approach we have taken in porting quantum chemistry algorithms based on local basis functions to the Intel MIC hardware. The implementation completed in the NWChem code shows the feasibility of effectively combining the processing power of traditional CPU architecture and coprocessor hardware on Petascale class computers. Benchmarks of scientific applications will be presented to illustrate the performances of large scale calculations.

3This work was conducted in the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), a national scientific user facility sponsored by DOE’s Office of Biological and Environmental Research and located at PNNL
12:15PM G23.00004 A scalable sparse eigensolver for petascale applications, MURAT KECELİ, Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, Illinois 60439, HONG ZHANG, PETER ZAPOL, Mathematics and Computational Science Division, Argonne National Laboratory, Lemont, Illinois 60439, DAVID DIXON, Department of Chemistry, The University of Alabama, Tuscaloosa, Alabama 35487, ALBERT WAGNER, Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, Illinois 60439 — Exploiting locality of chemical interactions and therefore sparsity is necessary to push the limits of quantum simulations beyond petascale. However, sparse numerical algorithms are known to have poor strong scaling. Here, we show that shift-and-invert parallel spectral transformations (SIPs) method can scale up to two-hundred thousand cores for density functional based tight-binding (DFTB), or semi-empirical molecular orbital (SEMO) applications. We demonstrated the robustness and scalability of the SIPs method on various kinds of systems including metallic carbon nanotubes, diamond crystals and water clusters. We analyzed how sparsity patterns and eigenvalue spectrum of these different type of applications affect the computational performance of the SIPs. The SIPs method enable us to perform simulations with more than five hundred thousands of basis functions utilizing more than hundreds of thousands of cores. SIPs has a better scaling for memory and computational time in contrast to dense eigensolvers, and it does not require fast interconnects.

12:27PM G23.00005 Simulation of high-Tc superconductors using the DCA+ algorithm, PETER STAAR, IBM Research Zurich — For over three decades, the high Tc-cuprates have been a gigantic challenge for condensed matter theory. Even the simplest representation of these materials, i.e. the single band Hubbard model, is hard to solve quantitatively and its phase-diagram is therefore elusive. In this talk, we present the recent algorithmic and implementation advances [1,2] to the Dynamical Cluster Approximation (DCA+). The algorithmic advances allow us to determine self-consistently a continuous self-energy in momentum space, which in turn reduces the cluster-shape dependency of the superconducting transition temperature and thus accelerates the convergence of the latter versus cluster-size. Furthermore, the introduction of the smooth self-energy suppresses artificial correlations and thus reduces the fermionic sign-problem, allowing us to simulate larger clusters at much lower temperatures. By combining these algorithmic improvements with a very efficient GPU accelerated QMC-solver [3], we are now able to determine the superconducting transition temperature accurately and show that the Cooper-pairs have indeed a d-wave structure, as was predicted by Zhang and Rice.


1:03PM G23.00006 A New Class of $J_{eff}=1/2$ Mott Insulators, TURAN BIROL, KRISTJAN HAULE, Rutgers, The State University of New Jersey — We predict a novel class of Jeff=1/2 Mott insulators in a family of Ir and Rh fluoride compounds with the K$_2$GeF$_6$ crystal structure that are previously synthesized, but not characterized extensively. First principles calculations in the level of all electron Density Functional Theory + Dynamical Mean Field Theory (DFT+DMFT) indicate that these compounds have large Mott gaps and some of them exhibit unprecedented proximity to the ideal, SU(2) symmetric Jeff=1/2 limit.

1:15PM G23.00007 Petascale electronic structure code with a new parallel eigensolver, EMIL BRIGGS, WENCHANG LU, MIROSŁAW HODAK, YAN LI, CT KELLEY, JERZY BERNHOLC, NCSU — We describe recent developments within the Real Space Multigrid (RMG) electronic structure code. RMG uses tetrahedron basis sets, and subspace diagonalization to solve the Kohn-Sham equations. It is designed for use on massively parallel computers and has shown excellent scalability and performance, reaching 6.5 PFLOPS on 18k Cray compute nodes with 28k CPU cores and 18k GPUs. For large problems, the diagonalization becomes computationally dominant and a novel, highly parallel eigensolver was developed that makes efficient use of a large number of nodes. Test results for a range of problem sizes are presented, which execute up to 3.5 times faster than standard eigensolvers such as Scalapack. RMG is now an open source code, running on Linux, Windows and Macintosh systems. It may be downloaded at:

1:27PM G23.00008 Full potential KKR approach to the calculation of Hellmann-Feynman force and total energy1, YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, G.M. STOCKS, Oak Ridge National Laboratory — The Korringa-Kohn-Rostoker (KKR) method is an ab initio electronic structure calculation method based on multiple scattering theory. Unlike the traditional approach, the full-potential KKR method, as well as its linear scaling approach, namely the full-potential LSMS method, does not make a spherical geometry assumption for the LDA potential and the charge density, i.e., the muffin-tin approximation. Consequently, these full-potential methods allow to calculate the Hellmann-Feynman force acting on each ion in the unit cell. In this presentation, we show an implementation of the full-potential KKR and LSMS methods, discuss the force and total energy calculation in the framework of multiple scattering theory, and finally discuss our approach to overcoming the major computational bottleneck in a full-potential calculation by employing GPGPU acceleration technique.

1:39PM G23.00009 Linear-scaling density-functional theory with wavelets: challenges and opportunities for petascale and beyond, LAURA RATCLIFF, Leadership Computing Facility, Argonne National Laboratory, LUIGI GENOVESE, STEPHAN MOHR, THIERRY DEUTSCH, CEA, INAC-SP2M, LSim, Grenoble, France — Density-functional theory (DFT) has been used to study a wide range of materials in simulations with a moderate level of parallelism. A common approach divides the electronic orbitals between MPI tasks, however this limits the number of tasks that can be used for a given system. The most straightforward path to exploiting petascale machines is therefore to increase the size of the system being studied. However, standard implementations of DFT scale cubically with the number of atoms so that the time rapidly increases for large systems. Algorithms must therefore be designed with reduced scaling, such as the linear-scaling approach in BigDFT, which uses an adaptive localized basis set that is itself represented in an underlying wavelet basis set. It thus retains all the benefits of wavelets, such as systematic convergence, while also presenting some new advantages, e.g. the definition of a fragment approach. Nonetheless, as we move towards the exascale, there remain a number of challenges associated both with increasing parallelism and the treatment of large systems. We will outline the algorithms and parallelization used in BigDFT and present some recent results which have been facilitated by this approach, as well as discussing some of the future challenges.

1:51PM G23.00010 Functional derivatives for multi-scale modeling, SAMUEL REEVE, ALEJANDRO STRACHAN, Purdue Univ — As we look beyond petascale computing and towards the exascale, effectively utilizing computational resources by using multi-fidelity and multi-scale materials simulations becomes increasingly important. Determining when and where to run high-fidelity simulations in order to have the most effect on a given quantity of interest (QoI) is a difficult problem. This work utilizes functional uncertainty quantification (UQ) for this task. While most UQ focuses on uncertainty in output from uncertainty in input parameters, we focus on uncertainty from the function itself (e.g. from using a specific functional form for an interatomic potential or constitutive law). In the case of a multi-scale simulation with a given constitutive law, calculating the functional derivative of the QoI with respect to that constitutive law can determine where a fine-scale model evaluation will maximize the increase in accuracy of the predicted QoI. Additionally, for a given computational budget the optimal set of coarse and fine-scale simulations can be determined. Numerical calculation of the functional derivative has been developed and methods of including this work within existing multi-fidelity and multi-scale orchestrators are explored.
2:03PM G23.00011 DMRG study of Many-Body Localization . XIONGJIE YU, BRYAN CLARK, University of Illinois, Urbana-Champaign, DAVID PEKKER, University of Pittsburgh — Numerical studies on many-body localization (MBL) problems have heavily relied on exact diagonalization (ED) techniques so far which has severely limited the system size that can be studied. Here we report a density matrix renormalization group (DMRG) based method for simulations in the many-body localized phase allowing us to reach size systems inaccessible to ED. We describe our techniques and report on our results applying DMRG to larger systems.

Tuesday, March 3, 2015 11:15AM - 2:15PM — Session G24 DCOMP: Electronic Structure Methods II 203AB - James Chelikowski, University of Texas at Austin

11:15AM G24.00001 Improved forces and nonlocal operators using high-order integration1 . GRADY SCHOFIELD, N. SCOTT BOBBITT, CHARLES LENA, JAMES R. CHELIKOWSKY, University of Texas at Austin — We present a new high-order modification to the finite-difference based real space pseudopotential density functional theory method. By giving a high-order treatment to the nonlocal pseudopotential terms in the Hamiltonian, as well as all quantities of interest obtained by post-processing the wavefunctions, we improve the accuracy of total energy, interatomic forces, vibrational modes, and anharmonic effects. We demonstrate the power of this new technique by computing vibrational modes for a few common molecules containing atoms that are more difficult for high-accuracy force calculations, such as oxygen and nitrogen, due to the depth of the pseudopotential. The reduction in numerical noise as atoms move over the grid allows using a larger grid spacing than would be required with a conventional finite difference based discretization. Savings in both memory and computational time, due to a smaller spectral radius, will be discussed.

1This work was supported by the DOE through the SciDAC program funded by ASCR and BES under award number DE-SC0008877. Computations were performed on machines at TACC.

11:27AM G24.00002 Electronic correlation contributions to structural energies1 . ROGER HAYDOCK, University of Oregon — The recursion method is used to calculate electronic excitation spectra including electron-electron interactions within the Hubbard model. The effects of correlation on structural energies are then obtained from these spectra and applied to stacking faults. http://arxiv.org/abs/1405.2288

1Supported by the Richmond F. Snyder Fund and Gifts

11:39AM G24.00003 Optimization algorithm for the generation of ONCV pseudopotentials1 . MARTIN SCHLIPF, FRANCOIS GYGI, Univ of California - Davis — We present an optimization algorithm to construct pseudopotentials and use it to generate a set of Optimized Norm-Conserving Vanderbilt (ONCV) pseudopotentials[1] for elements up to Z=83 (Bi) (excluding Lanthanides). We introduce a quality function that assesses the agreement of a pseudopotential calculation with all-electron FLAPW results, and the necessary plane-wave energy cutoff. This quality function allows us to use a Nelder-Mead optimization algorithm on a training set of materials to optimize the input parameters of the pseudopotential construction for most of the periodic table. We control the resulting pseudopotentials on a test set of materials independent of the training set. We find that the automatically constructed pseudopotentials provide a good agreement with the all-electron results obtained using the FLEUR code [2] with a plane-wave energy cutoff of approximately 60 Ry.

1Supported by DOE/BES grant DE-SC0008938

11:51AM G24.00004 MBTS Boundary Conditions in Continuous Systems . G. A. BENESH, Department of Physics, Baylor University, ROGER HAYDOCK, Department of Physics, University of Oregon — Boundary conditions imposed on a local system that is joined to a larger substrate system often introduce unphysical reflections that affect eigenstate energies, densities of states, and charge densities. These problems are common in both atomic cluster and surface slab calculations. Solutions of the Schrodinger equation for the physical system do not possess such reflections; these wave functions carry current smoothly across the (artificial) boundary between the local system and the underlying medium. Previously, Haydock and Nex derived a non-reflecting boundary condition for discrete systems [Phys. Rev. B 75, 205121 (2006)]. Solutions satisfying this maximal breaking of time-reversal symmetry (MBTS) boundary condition carry current away from the boundary at a maximal rate—in much the same way as the exact wave functions for the physical system. The MBTS boundary condition has proved useful in discrete systems for constructing densities of states and other distributions from moments or continued fractions. The MBTS approach has now been extended to studies employing continuous spatial wave functions, including surface slab calculations and model systems. Results are compared with free slab calculations, embedding calculations, and experiment.

12:03PM G24.00005 Quantal Density Functional Theory (QDFT): Further understandings . VIRAJT SAHNI, The Graduate Center, CUNY, XIAO-YIN PAN, TAO YANG, Ningbo University — We consider electrons in the following external fields: (a) \( A (\mathbf{r}, t) = - \nabla v(\mathbf{r}) \), (b) \( B (\mathbf{r}) = \nabla \times A (\mathbf{r}) \), and (c) \( E (\mathbf{r}) = - \nabla v(\mathbf{r}) \). The basic variables for these systems are for (a) the density \( \rho (\mathbf{r}, t) \) and physical current density \( j(\mathbf{r}, t) \), (b) the \( \mathbf{r} \) and (paramagnetic) \( j(\mathbf{r}, t) \), (c) \( \rho (\mathbf{r}) \) and \( j(\mathbf{r}) \), and (d) \( \rho (\mathbf{r}) \). In QDFT, the local potential of the model fermions is the work done in a conservative effective field. In each of the above cases the effective field is representative of the same correlations, viz. due to the Pauli exclusion principle, Coulomb repulsion and Correlation-Kinetic effects.

12:15PM G24.00006 Sum frequency generation spectroscopy from first principles1 . QUAN WAN, GIULIA GALLI, Univ of Chicago — Sum frequency generation (SFG) spectroscopy is widely used to study the structural and dynamical properties of surfaces and interfaces. Within the dipole approximation, SFG signals are solely determined by the surface, and bulk contributions vanish. However, the bulk portion of a material may contribute to SFG spectra through higher multipole excitations, e.g. quadrupole, which usually are difficult to separate in the measured spectra. Here we present a first principles theoretical framework, to compute SFG spectra of molecular solids and fluids. Within the dipole approximation, we computed the dipole and polarizability using maximally localized Wannier functions (MLWF) and density functional perturbation theory [1]. We then extended our method to include quadrupole contributions, and we computed quadrupole moments and their derivatives using MLWF and a real-space correction scheme [2], and an electric enthalpy functional. We applied our approach to investigate the ice Ih surface and we present results obtained by both finite differences and ab initio molecular dynamics [3] simulations. [1] Wan et al. J. Chem. Theory Comput. 9, 4124 (2013) [2] Stengal et al. Phys. Rev. B 73, 075121 (2006) [3] Qbox Code http://eslab.ucdavis.edu/software/qbox

1This work was supported by grant DOE-BES DE-SC0008938
A first principles method for simulating phonons in strongly disordered materials. TOM BERLLIN, OLIVIER DELAIRE, BEN LARSON, Oak Ridge National Laboratory — At the microscopic level the flow of vibrational heat is encoded not only in the energies of phonons but also in their lifetimes. In many functional materials these phonon lifetimes are controlled by strong disorder. Such systems are difficult to understand from conventional perturbation theories or mean field treatments. Here we will present an affordable and accurate first principles method for simulating phonons in strongly disordered materials. The method will be illustrated with applications ranging from thermoelectrics to nuclear fuels. TB was supported as a Wigner Fellow at the Oak Ridge National Laboratory, OD was supported by the US DOE-BES, Materials Science and Engineering Division, and BL was supported by the CMSNF Energy Frontier Research Center.

Real-Space Multiple-Scattering X-ray Absorption Spectroscopy Calculations of $d$- and $f$-state Materials using a Hubbard Model. CHRISTIAN VORWERK, KEVIN JORISSEN, JOHN REHR, Department of Physics, University of Washington, Seattle, Washington 98195 USA, AHMED TOWFIQ, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545 USA — We present calculations of the electronic structure and x-ray spectra of materials with correlated $d$- and $f$-electron states treated with the Hubbard model in a real-space multiple scattering (RSMS) formalism, and using a rotationally invariant local density approximation (LDA+$U$). Values of the Hubbard parameter $U$ are calculated ab initio using the constrained random-phase approximation (cRPA). The real-space Green’s function approach with Hubbard model corrections is an efficient way to describe localized electron states in strongly correlated systems, and their effect on core-level x-ray spectra. The method is shown to give the correct density states of $s$ and $x$-ray absorption spectra for Transition Metal- and Lanthanide-oxides such as Ce2O3 and NIO, where the traditional RSMS calculations fail.

Partial Rayleigh-Ritz procedure for quasi-minimal basis sets. VINCENT MICHAUD-RIOLUX, HONG GUO, McGill University — Recent Kohn-Sham DFT solver implementations [1-3] concentrate on building a subspace spanned by the occupied Kohn-Sham orbitals via Chebyshev filtering [1]. The Rayleigh-Ritz procedure is generally performed to populate the Kohn-Sham orbitals correctly and constitutes a bottleneck in large electronic structure simulations. We found that the full diagonalization of the projected Hamiltonian can be avoided; only the partly occupied subspace is the eigenvalue problem. The occupied subspace can be obtained from the orthogonal complement of the former. For quasi-minimal basis sets, the size of the eigenvalue problem can be reduced significantly at the cost of constructing an orthogonal supplement. The method can also be used with nonminimal basis sets such as atomic orbitals by preforming a second projection of the Kohn-Sham Hamiltonian. The partial Rayleigh-Ritz procedure was implemented in our real space electronic structure calculator, which we used to conduct a performance comparison of the state-of-the-art Rayleigh-Ritz procedure against the partial Rayleigh-Ritz procedure. [1] Zhou, et al., Phys. Rev. E 74, 066704 (2006). [2] Motamarri, et al., Journal of Computational Physics 253, 308 (2013). [3] Levitt, A. and Torrent, M., Computer Physics Communications, In Press (2014)

Spectral function from Reduced Density Matrix Functional Theory. PINA ROMANIELLO, STEFANO DI SABATINO, LPT, CNRS, IRSAMC, University Toulouse III - Paul Sabatier, France and European Theoretical Spectroscopy Facility, JAN A. BERGER, LCPQ, IRSAMC, University Toulouse III - Paul Sabatier. CNRS, France and European Theoretical Spectroscopy Facility, LUCIA REINING, LSI, Ecole Polytechnique, CNRS, CEA-DSM, France and European Theoretical Spectroscopy Facility — In this work we focus on the calculation of the spectral function, which determines, for example, photoemission spectra, from reduced density matrix functional theory. Starting from its definition in terms of the one-body Green’s function we derive an expression for the spectral function that depends on the occupied electronic state of the actual occupation numbers and on an effective energy [1] which accounts for all the charged excitations. This effective energy depends on both the two-body as well as higher-order density matrices. Various approximations to this expression are explored by using the exactly solvable Hubbard chains [2].

Kohn-Sham Band Structure Benchmark Including Spin-Orbit Coupling for 2D and 3D Solids. WILLIAM HUHN, Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC, USA, VOLKER BLOM, Department of Mechanical Engineering and Material Science, Duke University, Durham, NC, USA — Accurate electronic band structures serve as a primary indicator of the suitability of a material for a given application, e.g., as electronic or catalytic materials. Computed band structures, however, are subject to a host of approximations, some of which are more obvious (e.g., the treatment of the exchange-correlation of self-energy) and others less obvious (e.g., the treatment of core, valence electrons, or valence electrons, handling of relativistic effects, or the accuracy of the underlying basis set used). We here provide a set of accurate Kohn-Sham band structure benchmarks, using the numeric atom-centered all-electron electronic structure code FHI-aims combined with the "traditional" PBE functional and the hybrid HSE functional, to calculate core, valence, and low-lying conduction bands of a set of 2D and 3D materials. Benchmarks are provided with and without effects of spin-orbit coupling, using quasi-degenerate perturbation theory to predict spin-orbit splittings.

Self diffusion of water molecules simulated by model inter-atomic potentials determined by a combination of first-principles calculation and multi-canonical ensembles: exchange-correlation functional dependence. YOSHIHIKIDE YOSHIMOTO, Dept. of Computer Science, Graduate School of Information Science and Technology, The University of Tokyo — Water is an ubiquitous substance and is both scientifically and technologically important. In this study, the self diffusion of water molecules are simulated using Kumagai-Kawamura-Yokokawa type inter-atomic potentials [1] whose parameters are determined by a combination of first-principles calculation and multi-canonical ensembles [2,3]. Because of the property of multi-canonical ensemble, the determined potentials keep the thermodynamics of the reference first-principles simulations to a maximum extent. The author used PBE, PBE0, B3LYP, and B3LYP with DFT-D3 exchange-correlation potentials for the reference first-principles calculations to determine the model parameters. The obtained diffusion coefficients significantly depend on the choice of the exchange correlation functionals and the combination of B3LYP and DFT-D3 [4] produced the best agreement with the experimental one.

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3Supported by Fritz-Haber-Institut der Max-Planck-Gesellschaft

4This work is funded by Fritz-Haber-Institut der Max-Plank-Gesellschaft
Quantum pressure in molecules and solids: Influence of magnetic fields and spin-orbit coupling on electron localization

This work was supported by NSF, USAF, and DOE.

First-principles study of two-dimensional electrile: Yttrium carbide. CHANDANI NANDADASA, SUNGHO KIM, SEONG-GON KIM, Mississippi State University, Starkville, MS 39762, USA, YOUNG LEE, SUNG KIM, Center for Integrated Nanostructure Physics (CINAP), Institute for Basic Science (IBS), Department of Energy Science, Sungkyunkwan University, Korea — Electrides are an exclusive class of ionic compounds in which electrons serve as anions. We have performed first-principles density functional theory (DFT) calculations to investigate the structural, electronic and magnetic properties of two-dimensional layered-structure yttrium carbide (Y2C). Generalized gradient approximation (GGA) with Projector Augmented Potentials (PAW) was used to obtain optimized lattice parameters, energy band structure, charge density and density of states (DOS) plots for Y2C. The theoretically predicted structure of Y2C is in good agreement with the experimental results. The band crossing the Fermi energy level proved that Y2C has metallic properties. Additionally projected electronic density of states profiles were obtained to identify the electronic contribution from Y, C and non-atomic orbital located in interstitial site. The results of these calculations indicate that the presence of trapped electrons within the Y2C layers. Furthermore, surface energies of Y-Y and Y-C were calculated and charge densities were plotted with these surfaces. Magnetization density plots were used to obtain magnetic properties.

Topological Pair-Density-Wave Superconducting States

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Accessing topological superconductivity via a combined STM and renormalization group analysis

The search for topological superconductors (SC) has recently become a key issue in condensed matter physics, because of their possible relevance to Majorana states, non-Abelian statistics and fault-tolerant quantum computing. A new scheme is proposed here, which links as directly as possible the experimental search to a material-based microscopic theory. To this, the scanning tunneling microscopy (STM), which typically uses a phenomenological Ansatz for the SC gap functions is elevated to a theory, where a multi-orbital functional RG (IRG) analysis allows for an unbiased microscopic determination of the material-dependent pairing potentials. The conductance spectra are predicted for a normal metal-insulator-topological superconductor (N-I-S) junction, which imitates the STM setup and, therefore, is directly accessible to spectroscopic experiments. The strength of the combined approach is demonstrated for hexagonal systems, i.e. doped graphene and water-intercalated sodium cobaltates, where the lattice symmetry and electronic correlations can lead to a time-reversal symmetry breaking (chiral) topological SC state.

Low-Temperature Thermal Transport at the Interface of a Topological Insulator and a d-Wave Superconductor

We consider the low-temperature thermal transport properties of the 2D proximity-induced superconducting state formed at the interface between a topological insulator (TI) and a d-wave superconductor (dSC). This system is a playground for studying massless Dirac fermions, as they enter both as quasiparticles of the dSC and as surface states of the TI. For TI surface states with a single Dirac point, the four nodes in the interface-state quasiparticle excitation spectrum coalesce into a single node in the presence of an Ising spin symmetry. This topological PDW order parameter here is a Majorana zero mode (MZM) at an open boundary and at a junction with a uniform one-dimensional state emergent in extended Heisenberg-Hubbard models in two-leg ladders is topological in the presence of an Ising spin symmetry. This topological PDW order parameter is a charge-one can obtain a single Majorana fermion regardless of the sweep velocity.
12:03PM G25.00005 Interface effects and electronic transport in superconducting heterostructures with spin-orbit coupling\textsuperscript{1}, NAYANA SHAH, University of Cincinnati, KUEI SUN, The University of Texas at Dallas. Study on electronic transport in superconducting heterostructures with spin-orbit coupling (SOC) has become an active field for exploring spintronic properties or topological states of matter. For example, recently observed zero-bias conductance peaks in one-dimensional superconductor-semiconductor heterostructures in the presence of SOC and magnetic field are of interest for realizing Majorana fermions. However, most study considers SOC only in bulk materials, while the interface effects, which can significantly alter the physics in spin-active systems, have not been fully analyzed for systems with SOC. Here we construct a general model to describe interfaces in a superconductor-normal metal junction with bulk SOC. We also systematically investigate the trend of conductance as the system parameters vary. Our results are of interest for understanding a variety of transport behaviors in the presence of SOC and are of relevance also for characterizing interfaces in experimental systems.

\textsuperscript{1}Supported by University of Cincinnati

12:15PM G25.00006 Point defects and Majorana doublets in 3D time-reversal invariant topological superconductors and superfluids, MENGXING YE, University of Michigan, ZHENG-CHENG GU, Perimeter Institute for Theoretical Physics, KAI SUN, University of Michigan — In this talk, we study topological point defects in 3D time-reversal invariant topological superconductors and superfluids, focusing on the Majorana zero modes hosted at these defects. We will address the exotic properties of these Majorana modes especially the nontrivial exchange group and its connection to fermion parity. In contrast to 2D chiral topological superconductors, in which the braiding of Majorana zero modes has been studied extensively and well understood, the time-reversal invariant topological superconductors allow richer structures at topological defects and thus result in more sophisticated response as we exchange these defects.

12:27PM G25.00007 Nonmagnetic impurity effects in a superconducting topological insulator, YUKI NAGAI, YUKIHIRO OTA, MASAHIKO MACHIDA, CSSE, Japan Atomic Energy Agency — Unconventional features in superconductivity are revealed by responses to impurity scattering. We study nonmagnetic impurity effects in a superconducting topological insulator, focusing on an effective model of Cu-doped topological insulator Bi\textsubscript{2}Se\textsubscript{3}. Typically, this superconducting compound is considered to be dirty owing to the copper intercalated process. Using a self-consistent T-matrix approach for impurity scattering, we examine in-gap states in density of states. It is well known that the unconventional superconductors such as p-wave diminish via non-magnetic impurity scattering, different from the robustness of an s-wave state (Anderson’s theorem). We show that the impurity effects are well characterized by a simple material variable, which measures relativistic effects in the Dirac Hamiltonian. We find that the topological superconductor has two aspects, p- and s-wave features, depending on the weight of relativistic effects. The topological superconductors can not be simply regarded as one of the conventional unconventional superconductors.

12:39PM G25.00008 Sensitivity of a 3D fully-gapped topological superconductor to nonmagnetic impurities, YUKIHIRO OTA, YUKI NAGAI, MASAHIKO MACHIDA, Japan Atomic Energy Agency — Topological superconductors (TSC) are notable materials, owing to the mathematical curiosity and the application potential. The bulk TSC can emerge by copper intercalation into topological insulator Bi\textsubscript{2}Se\textsubscript{3}. In this paper, we theoretically study the non-magnetic impurity effects in the mean-field model of Cu\textsubscript{x}Bi\textsubscript{2}Se\textsubscript{3}, focusing on the odd-parity fully-gapped superconducting state. Calculating the density of states with a self-consistent T-matrix approach, we test the presence of mid-gap states, leading to pair-breaking effects. Remarkably, the sensitivity to non-magnetic impurities strongly depend on a normal-state dispersion character, i.e., either non-relativistic or relativistic dispersion relations. We show unification picture for understanding this intriguing result, deriving a low-energy effective superconducting theory.

12:51PM G25.00009 Crossed surface flat bands in superconducting Weyl semimetals, KEIJI YADA, BO LU, MASATOSHI SATO, YUKIO TANAKA, Nagoya University — Weyl semimetal is a new phase of matter where topological magnetic monopoles emerge in momentum space at so-called Weyl points.[1] Owing to the presence of the Weyl points, zero energy flat band called Fermi arc appears as a surface bound state between the Weyl points projected to the surface Brillouin Zone.[2] In this talk, we will show that the superconducting state with point nodes in doped Weyl semimetal may have more exotic surface bound states, i.e. “crossed flat bands”. [3] With the help of the crossed flat bands, the divergent behavior of the normalized conductance at zero bias voltage appears. This divergent behavior has never been seen in other superconducting system with point nodes. We found three conditions for the realization of the crossed flat bands mentioned below. i) a uniform pairing such as BCS s-wave pairing, ii) broken time reversal symmetry iii) magnetic mirror reflection symmetry. [1] S. Murakami, New J. Phys. 9, 356 (2007) [2] G. Xu et al., Phys. Rev. Lett. 107, 186806 (2011) [3] B. Lu, K. Yada, M. Sato and Y. Tanaka, arXiv:1406.3804

1:03PM G25.00010 Generating Giant Spin Currents by Majorana Flat Bands in Nodal Topological Superconductors, NOAH FANQI YUAN, YAO LU, JAMES JUN HE, KAM TUEN LAW, The Hong Kong University of Science and Technology — When a normal lead is coupled to a single Majorana fermion, electrons with certain spin polarization can undergo equal spin Andreev reflections, in which the reflected holes have the same spin as the incoming electrons. Moreover, electrons with opposite spin are all normally reflected. This process is called Majorana fermion induced selective equal spin Andreev reflections (SESARs) [1]. As a result of SESARs, spin polarized currents can be generated at the normal lead. Nevertheless, in this case, the maximum conductance of the normal lead/superconductor junction is 2e\textsuperscript{2}/h [2]. In this work, we show that Majorana fermions associated with Majorana flat bands in nodal topological superconductors can also induce SESARs. Importantly, due to the large number of Majorana fermions, the conductance at the normal lead/nodal topological superconductor junction is enormous. As a result, giant spin currents can be generated in the normal lead. Particularly, we point out that U$\uparrow$\textsubscript{3} can be the candidate to induce giant spin currents.


1:15PM G25.00011 Detecting Majorana Fermions in Ferromagnetic Atomic Chains in Proximity to Spin-orbit Coupled s-wave Superconductor, TONG ZHOU, NOAH FANQI YUAN, JAMES JUN HE, YAO LU, VIC KAM TUEN LAW, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China, PATRICK LEE, Department of Physics, Massachusetts Institute of Technology, Cambridge MA 02139, USA — Recently, it was proposed that Majorana bound states could be observed experimentally in ferromagnetic atomic chains on the surface of two-dimensional superconducting lead (Pb). Using the scanning tunneling microscope (STM), the experimental group obtained the spatially resolved density of states and observed zero bias peaks at the end of the chains. In this work, we study the topological phases of the proposed system. With realistic parameters, we study the transport properties at different positions along the chains. At zero temperature, resonant zero bias peaks emerge at the ends of the chains in the topological regimes, thus confirming the existence of Majorana bound states in the system. However, our transport calculation shows that at finite temperature, conductance peaks at zero bias also arise in the trivial regime due to the presence of low-energy fermionic end states in the system. Therefore, this would suggest that the experimentally observed zero bias peaks can have alternative theoretical explanations.
1:27PM G25.00012 Tunneling spectroscopy and Majorana modes emergent from topological gapless phases in high-$T_c$ cuprate superconductors\(^1\) CHUNG-YU MOU, JUN-TING KAO, Department of Physics, National Tsing Hua University, Taiwan, SHIN-MING HUANG, Graphene Research Centre and Department of Physics, National University of Singapore, Singapore, CHANG C. TSUEI, IBM Thomas J. Watson Research Center, Yorktown Heights, NY 10598, U.S.A. — We explore possible signatures for observing Majorana Fermions in the tunneling spectroscopy of high-$T_c$ cuprate superconductors. We find that as long as the Rashba spin orbit interaction is in presence either through the proximity effect due to an electrode made by heavy metal or by the intrinsic nature of cuprates, in addition to the Heisenberg spin exchange interaction, the Dzyaloshinskii-Moriya and spin dipole-dipole interactions are induced. As a result, $p$-wave superconductivity is induced with the gap function $\Delta$-vector being not aligned with the internal magnetic field of the spin-orbit interaction. Most importantly, the ground state goes through transitions into gapless phases with split nodal points. The split nodal structure always results in Majorana modes for any interfaces that are not exactly in (100) or (010) directions. Hence for general interfaces, existence of Majorana bound states is a robust feature. Our results indicate that these Majorana modes would result in a small plateau in tunneling spectrum near zero bias peak and in $4\pi$ periodicity in typical SIS$^2$ junctions. As a result, it is easy for a $\pi$-ring in tricrystal experiments to hold Majorana Fermions and exhibit periods of two flux quanta in external magnetic fields.

\(^1\)We acknowledge support from Ministry of Science and Technology of Taiwan.

1:39PM G25.00013 Time-Reversal-Invariant Topological Superconductivity in n-type Doped BiH, FAN YANG, CHENG-CHENG LIU, Beijing Institute of Technology, YU-ZHONG ZHANG, Tongji University, YUGUI YAO, Beijing Institute of Technology, DUNG-HAI LEE, University of California, Berkeley — Intrinsic and symmetry protected topological states have attracted lots of interest in condensed matter physics recently. In particular, time reversal symmetry protected fermion topological insulators have been theoretically predicted and experimentally verified. However despite considerable experimental and theoretical works, definitive evidence for time reversal invariant topological superconductivity is still lacking. Here we propose that upon electron doping the hydrogenated single bilayer Bi, namely BiH, will exhibit time reversal invariant topological superconductivity. If confirmed experimentally this material will constitute the first example of TIR topological superconductor.

1:51PM G25.00014 Vanishing edge currents and orbital angular momentum in non-$p$-wave topological chiral superconductors\(^1\) WEN HUANG, EDWARD TAYLOR, McMaster University, CATHERINE KALLIN, McMaster University, and Canadian Institute for Advanced Studies — The edge currents of two dimensional topological chiral superconductors with nonzero Cooper pair angular momentum--e.g., chiral $p$-, $d$-, and $f$-wave superconductivity--are studied. Bogoliubov-de Gennes and Ginzburg-Landau calculations are used to show that in the continuum limit, only chiral $p$-wave states have a nonzero edge current and orbital angular momentum. Outside this limit, when lattice effects become important, edge currents in non-$p$-wave superconductors are comparatively smaller, but can be nonzero. Using Ginzburg-Landau theory, a simple criterion is derived for when edge currents vanish for non-$p$-wave chiral superconductors on a lattice. The implications of our results for putative chiral superconductors such as Sr$_2$RuO$_4$ and UPt$_3$ are discussed.

\(^1\)Work supported by NSERC, CIFAR, Canada Council Killam programs (CK) and the National Science Foundation (CK)

2:03PM G25.00015 Non-topological nature of the edge current in a chiral $p$-wave superconductor\(^1\), EDWARD TAYLOR, University of Toronto, WEN HUANG, McMaster University, SAMUEL LEDERER, Stanford University, CATHERINE KALLIN, McMaster University — The edges of time reversal symmetry breaking topological superconductors support chiral Majorana bound states as well as spontaneous charge currents. The Majorana modes are a robust, topological property, but the charge currents are non-topological—and therefore sensitive to microscopic details—even if we neglect Meissner screening. We give insight into the non-topological nature of edge currents in chiral $p$-wave superconductors using a variety of theoretical techniques, including lattice Bogoliubov-de Gennes equations, the quasiclassical approximation, and the gradient expansion, and describe those special cases where edge currents do have a topological character. While edge currents are not quantized, they are generally large, but can be substantially reduced for a sufficiently anisotropic gap function, a scenario of possible relevance for the putative chiral $p$-wave superconductor Sr$_2$RuO$_4$.

\(^1\)Supported by NSERC and CIFAR at McMaster and by the Canada Research Chair and Canada Council Killam programs and NSF Grant No. NSF PHY11-25915 (CK). SL is supported by the DOE Office of Basic Energy Sciences, contract DEAC02-76SF00515


11:15AM G26.00001 The Non-Adiabatic dynamics of Singlet Fission in Polyacenes\(^1\), STEPHEN BRADFORTH, Univ of Southern California — Singlet fission involves the splitting of a single excitation into two coupled triplet excitations and is manifested in an increasing range of aromatic crystals and amorphous thin films. If the energy of the lowest triplet state is one half (or less) of the first singlet excited state, as it is for tetracene or pentacene and their derivatives, singlet fission may occur between two adjacent chromophores. Since there is no change in the overall spin state of the system, singlet fission can be exceptionally fast, occurring on the fs – ps range. If the triplets can diffuse away from the fission site they are available to the efficiency and speed of this process.

\(^1\)Work supported as part of the Center for Energy Nanoscience, an Energy Frontier Research Center funded by the U.S. Department of Energy (DE-SC0001013)

11:51AM G26.00002 Extracting Molecular Dynamics from Ion Imaging Experiments of Carboxyl Sulfide, WEI WEI, COLIN WALLACE, SIMON NORTH, Texas A&M Univ — Photodissociation of carboxyl sulfide at 215nm are studied in details with sliced ion imaging experiments. Energy partitioning as well as vector correlations between carboxyl sulfide transition dipole moments, CO recoil velocity vector and angular momentum will be revealed. They can provide valuable information about symmetry of excited states which are involved in photodissociation process. These results can reveal information about non-adiabatic dynamics in carboxyl sulfide excited states. The results will be compared with both computational chemistry study conducted by G. McBane and coworkers. The result will also be compared with previous study on dynamics from carboxyl sulfide photodissociation at longer wavelength by Bersohn and coworkers.
12:03PM G26.00003 Vibronic interactions in multi-chromophores. LYUDMILA SLIPCHENKO, Purdue University — Understanding and control of excitation energy transfer and electron-phonon interactions is quintessential for advances in solar energy utilization. Recently, we developed a vibronic model that is capable of predicting vibronic spectra in complex multi-chromophore systems. Parameters to the model are obtained from electronic structure calculations on monomer units of a multi-chromophore. This model can account for multiple vibrational modes, asymmetric wave functions, and inter-chromophore vibrations. Using this model, we explored vibronic spectra in a series of flexible bichromophores with available high-resolution experimental spectra. One of the goals of this work was to understand the effects of asymmetry in monomer units on vibronic interactions in bichromophores. Detailed investigation of diphenylmethane, partially deuterated diphenylmethane, and diphenylethane resulted in intriguing observation that asymmetry leads to a partial localization of one of the exciton states but leaves the other one delocalized. Extension of the developed methodology to modeling spectroscopy and dynamics in synthetic and biological multi-chromophore systems such as photosynthetic proteins will be also discussed.

12:39PM G26.00004 Non-Adiabatic Dynamics in the UV Photodissociation of Alkyl Radicals, JINGSONG ZHANG, Department of Chemistry and Air Pollution Research Center University of California, Riverside — This presentation focuses on the ultraviolet (UV) photodissociation dynamics of a series of prototypical alkyl radicals (ethyl, propyl, and butyl) using the high-n Rydberg atom time-of-flight (HRTOF) technique. Upon excitation to the 3s state at 246-nm, ethyl dissociates into H atom and ethylene. Bimodal profile in the product translational energy distribution and energy-dependent product angular distribution indicate two different dissociation pathways that are influenced by conical intersection. A slow and isotropic component corresponding to unimolecular dissociation of the hot radical after internal conversion from the 3s state to the ground state. A fast and anisotropic component corresponds to a direct, rapid H-atom scission via a nonclassical H-bridged transition state from the 3s state to yield H + C2H4. Upon excitation to the 3p state at 237 nm, i- and n-propyl radical dissociate into H atom and propene products. The product translational energy release of both n- and i-propyl radicals also have bimodal distributions. The H-atom product angular distribution in n-propyl is anisotropic, while that in i-propyl is isotropic. The bimodal translational energy distributions indicate two dissociation pathways: (i) a unimolecular dissociation pathway from the ground-state propyl after internal conversion from the 3p state, and (ii) a repulsive pathway directly connected with the excited state of the propyl radical. The UV photodissociation dynamics of the n- and i-propyl radicals are also investigated. The photodissociation mechanisms and the possible role of conical intersections will be discussed.

1:15PM G26.00005 Ultraviolet photodissociation dynamics of the cyclohexyl radical, MICHAEL LUCAS, YANLIN LIU, JINGSONG ZHANG. Univ of California - Riverside — Cycloalkanes are important components in conventional fuels and oil shale derived fuels and the combustion of cyclohexane fuels leads to the production of benzene, a pollutant precursor. One of the pathways from cyclohexane to benzene is through sequential hydrogen loss, including the cyclohexyl radical as an intermediate. The ultraviolet (UV) photodissociation dynamics of the cyclohexyl (c-C6H11) radical was studied for the first time using the high-n Rydberg atom time-of-flight (HRTOF) technique in the range of 232-262 nm. The translational energy distributions of the H-atom loss product channel, P(Ef)^i, show a large translational energy release and a large fraction of average translational energy in the total excess energy, ⟨Ef⟩, from 232-262 nm. The H-atom product angular distribution is anisotropic with a positive β parameter. The most likely H-atom loss pathway is an axial H ejection from the i-C-carbon in cyclohexyl to form cyclohexene + H, which along with the positive β parameter, indicates that the transition dipole moment, μ, is perpendicular to the ring. The P(Ef) and anisotropy of the H-atom loss product channel are significantly larger than those expected for a statistical unimolecular dissociation of a hot radical, indicating a non-statistical dissociation mechanism. The dissociation mechanism is consistent with direct dissociation on a repulsive excited state surface or on the repulsive part of the ground state surface to produce cyclohexene + H, possibly mediated by a conical intersection. Cyclohexyl is the largest radical so far showing a direct dissociation mechanism.

1:27PM G26.00006 Photoisomerization dynamics of a rhodopsin-based molecule (potential molecular switch) with high quantum yields. ROLAND ALLEN, Texas A&M University, CHEN-WEI JIANG, Xi’an Jiaotong University, XIU-XING ZHANG, Weinan Normal University, AI-PING FANG, HONG-RONG LI, RUI-HUA XIE, FU-LI LI, Xi’an Jiaotong University — It is worthwhile to explore the detailed reaction dynamics of various candidates for molecular switches, in order to understand, e.g., the differences in quantum yields and switching times. Here we report density-functional-based simulations for the rhodopsin-based molecule 4-[4-Methylbenzylidene]-5-p-tolyl-3,4-dihydro-2H-pyrrrole (MDP), synthesized by Sampredo et al. We find that the photoisomerization quantum yields are remarkably high: 82% for cis-to-trans, and 68% for trans-to-cis. The lifetimes of the S1 excited state in cis-MDP in our calculations are in the range of 900-1800 fs, with a mean value of 1270 fs, while the range of times required for full cis-to-trans isomerization is 1100-2000 fs, with a mean value of 1530 fs. In trans-MDP, the calculated S1 excited state lifetimes are 860-2140 fs, with a mean value of 1330 fs, and with the full trans-to-cis isomerization completed about 200 fs later. In both cases, the dominant reaction mechanism is rotation around the central C==C bond (connected to the pyrrole ring), and de-excitation occurs at an avoided crossing between the ground state and the lowest singlet state, near the midpoint of the rotational pathway.

Tuesday, March 3, 2015 11:15AM - 2:03PM

Session G27 DCP: Focus Session: Chemical Physics of Clusters: Bridging from Angstrom-scale Clusters to Micron-scale Aerosol Particles II
11:15AM G27.00001 Low temperature thermodynamics of water clusters studied by nanocalorimetry , BERND VON ISSENDORFF, Physikalisches Institut, Universität Freiburg — Water exhibits many unusual properties, which mirror the complexity of its hydrogen network structure. It is therefore not surprising that water clusters and nanoparticles are special in many aspects as well. We have recently shown that negatively charged water clusters exhibit a melting-like transition at surprisingly low temperatures (at about 120 K for H$_2$O$_{14}$) [1]. Further studies have shown that this behavior depends only weakly on the charge state of the cluster or on the type of impurity incorporated [2]. Furthermore the size dependence indicates that the transition does not extrapolate to the melting transition of normal ice, but rather to the glass transition of amorphous ice, which occurs at about 136 K. This can be rationalized by the fact that water clusters with few hundred molecules do not form a crystalline network like bulk ice, but exhibit structures much closer to that of the amorphous forms of solid water.


11:51AM G27.00002 Melting behavior of metallic clusters: An order parameter by instantaneous normal modes , TEN-MING WU, Institute of Physics, National Chiao-Tung University — In this paper, we investigated the melting behaviors of Ag$_{17}$Cu$_2$ and Ag$_{14}$ metallic clusters, which were generated by isothermal Brownian-type molecular dynamics simulation with the empirical many-body Gupta potentials, from low to high temperatures. For the two clusters, the temperature variation in the specific heat exhibited a maximum at a temperature, which was defined as the cluster melting temperature. However, an additional prepeak at a lower temperature was found in the specific heat variation of Ag$_{14}$ but no prepeak was found in that of Ag$_{17}$Cu$_2$. The instantaneous normal mode (INM) analysis was used to dissect dynamics of the two clusters. A new order parameter associated with a cluster was proposed to describe the melting behaviors of the cluster; the order parameter can be defined using either the INM vibrational density of states or three orthogonal eigenvectors describing the rotational motions of the cluster by considering it as a rigid body. For the two metallic clusters studied, our results showed the mutual agreement for the order parameter defined by the two methods. The interpretation by the order parameter for the melting transition of a cluster was consistent with the temperature variation in the specific heat of the cluster. Furthermore, the new order parameter provided a connection between the melting of clusters and the concept of broken symmetry, which was successfully applied for understanding the melting transition of bulk systems.

12:03PM G27.00003 Structural determination of metal nanoparticles from their vibrational (phonon) density of states$^1$ , IGNACIO GARZON, Universidad Nacional Autonoma de Mexico, HUZIEL SAUCEDA, Universidad Nacional Autonoma de Mexico — The vibrational (phonon) density of states of metal nanoparticles with size between 2-6 nm can be measured using nuclear resonant inelastic x-ray or plasmon resonance Raman scattering. In this work, we present atomistic calculations, based on a semiempirical tight-binding many-body Gupta potential, of the vibrational density of states (VDOS) for FCC, decahedral, and icosahedral (ICO) gold and silver nanoparticles with sizes ~4 nm (~2000 atoms). The calculated VDOS are compared with experimental data, recently published for gold and silver nanoparticles of similar size, obtained through plasmon resonance Raman scattering. The best agreement between the calculated and measured VDOS’s is obtained for the ICO morphology for both metal nanoparticles. These results indicate that most of the nanoparticles in the experimental samples should have icosahedral structures. The present study also shows that, as in the case of molecular systems and small clusters, vibrational spectroscopy of metal nanoparticles with few nanometers in size, together with theoretical calculations, are powerful tools for their structure determination. with your abstract body.

$^1$Work supported by CONACYT-Mexico under Project 177981.

12:15PM G27.00004 Simulation studies of glassy nanoclusters , RICHARD BOWLES, Dept. Chemistry, University of Saskatchewan — Glassy materials are amorphous solids usually formed by rapidly cooling a liquid below its equilibrium freezing temperature, trapping the particles in a liquid-like structure at the glass transition temperature. While appearing throughout nature and industry, these systems continue to challenge the way we think about the dynamics and thermodynamics of condensed matter and a fundamental understanding of the glass state remains elusive. This talk describes molecular simulation studies of glassy behaviour in binary Lennard–Jones nanoclusters. We show that the relaxation dynamics of the clusters is nonuniform and the core of the cluster goes through a glass transition at higher temperatures than at the surface. As the nanoclusters are cooled, they also exhibit a fragile–strong crossover in their dynamics and we explore how this phenomena is linked to the potential energy landscape of the clusters. Finally, we compare the properties of nanoclusters formed through vapour condensation, directly to the glassy state, with those of glassy clusters formed through traditional annealing. Nanoclusters exhibit some unique glassy features, while also offering potential insights into the development of supercooled liquids.

12:51PM G27.00005 Effects of Thermal Annealing and X-ray Exposure on Local Structures Surrounding Co in Y-Codoped CeO$_2$ Nanocrystals , TAI-SING WU, HORNG-TAY JENG, National Tsing Hua University, Taiwan, SHIH-LIN CHANG, National Synchrotron Radiation Research Center, Taiwan, YUN-LIANG SOO, National Tsing Hua University, Taiwan — Codoping of Y and Co in CeO$_2$ has been found to incur an unconventional bandgap narrowing effect in the host nanocrystal material. The dormant bandgap-tuning ability of Y appears to be turned on by the Co codopant in the oxygen-vacancy-rich CeO$_2$ host. The physical mechanism underlying such effect has also been revealed by DFT calculations. Synchrotron-Radiation-based X-ray absorption analysis has further demonstrated that the Co codopant atoms can be located in either of two different local bonding environments in the CeO$_2$ host. Thermal annealing is capable of driving Co atoms from one bonding environment to the other. On the other hand, when exposed to x-rays of sufficient photon energy, Co can resume the original local structure as in the as-made sample. A simple model is proposed to explain such intriguing interplay between the effects of annealing and x-ray exposure in these codoped nanoceria systems.

1:03PM G27.00006 The correspondence between the infrared vibrational spectra and the underlying hydrogen bonding network in aqueous clusters: caveats and tactics$^1$ , SOTIRIS XANTHEAS, Pacific Northwest National Laboratory — The structural – spectral correspondence relates the observed infrared (IR) vibrational spectra to the underlying molecular structure. In the case of hydrogen bonded clusters the IR ”fingerprint” region in the 3,000 – 4,000 cm$^{-1}$ spectral range provides a direct probe of the connectivity and dynamics of the cluster’s hydrogen bonding network. For medium size (~20) aqueous neutral and ionic clusters, the presence of several closely lying isomers that differ substantially in the oxygen atom network complicates both the sampling of the respective potential energy surfaces as well as the accurate determination of their energy order. Traditionally, a hierarchical procedure based on initial sampling with classical potentials and subsequent refinement with electronic structure methods has been used. We will highlight representative examples for the (H$_2$O)$_{20}$, (H$_2$O)$_{25}$ and H$_2$O$^+$/(H$_2$O)$_{20}$ clusters [1-3] where sampling with classical potentials fails to produce the most stable minima and outline approaches and strategies that are based on a combination of enhanced sampling of configurations in conjunction with electronic structure theory to obtain realistic cluster configurations that are consistent with the measured IR spectra.


1Work supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences & Biosciences. Pacific Northwest National Laboratory (PNNL) is a multi-program national laboratory operated for DOE by Battelle.
Strong phonons and their distorted lineshapes

Lattice. We are studying single crystals of the spin ice Dy

A rare-earth pyrochlore magnets are realization of spin ice which have macroscopically degenerate ground states. The elementary excitation of classical

The intensity arises from changes in the transition moment for the HOH bend as the low-frequency librations form

11:15AM G28.00001 Thermal and Magnetic Responses of Spin Ice via SQUID Magnetometry

The field direction dependence of \( \kappa \) is consistent with monopole excitations. However, the temperature dependence indicates that the energy gap is at most 0.2 K, which is much smaller than \( \Delta \sim 4 \) K. This reduction of gap suggests the band formation of monopole excitations, giving rise to coherent heat conduction of “quantum” monopoles. Unlike diffusive monopoles in classical spin ice, the mean free path of these quantum monopoles is extremely long \( \sim 100 \) nm.

12:15PM G28.00004 Phase transitions and charge ordering in a square spin ice model with conserved monopole density

These monopole dimers are charge neutral, and the interactions between them have also been investigated using our algorithm. In the cases of high monopole densities, we have argued that artificial spin ice can be arranged in extended lattices. Tailoring the geometry and the magnetic material of these lattices, the magnetic interactions and magnetization reversal energy barriers can be tuned [1,2]. This enables interesting interaction schemes to be examined on adjustable length and energy scales. As a result such nano-magnetic systems represent an ideal playground for the study of physical model systems, being facilitated by direct magnetic imaging techniques [3]. One particularly interesting case is that of systems exhibiting frustration, where competing interactions cannot be simultaneously satisfied. This results in a degeneracy of the ground state and intricate thermodynamic properties [1-4]. An archetypical frustrated physical system is water ice. Similar physics can be mirrored in nano-magnetic arrays, by tuning the arrangement of neighboring magnetic islands, referred to as artificial spin ice. Thermal excitations in such systems resemble magnetic monopoles [4]. In this presentation key concepts related to nano-magnetism and artificial spin ice will be introduced and discussed, along with recent experimental and theoretical developments. [1] V. Kapaklis et al., New J. Phys. 14, 035009 (2012). [2] U. B. Arnolds et al., Appl. Phys. Lett. 105, 042409 (2014). [3] A. Farhan et al., Nature Physics 9, 375 (2013). [4] V. Kapaklis et al., Nature Nanotech 9, 514 (2014).

11:15AM G28.00003 Ordering, thermal excitations and phase transitions in dipolar coupled mono-domain magnet arrays

The rare-earth pyrochlore magnets are realization of spin ice which have macroscopically degenerate ground states. The elementary excitation of classical

1 Work supported by the National Science Foundation under grant DMR-1341793

11:39AM G28.00003 Ordering, thermal excitations and phase transitions in dipolar coupled mono-domain magnet arrays

Yoshi Tokuwa, Daiki Terazawa, Yusuke Shimoyma, K. W. Schlax, J. A. Moyer, A. Thaler, K. Sendzikoski, G. J. MacDougall, P. Schiffer, J. D. Van Harlingen, University of Illinois at Urbana-Champaign — The spin ice pyrochlore class of frustrated magnets exhibits quasiparticle excitations that behave like Dirac monopoles on the pyrochlore lattice. We are studying single crystals of the spin ice Dy2Ti2O7 using dc SQUID magnetometry to look for thermal fluctuations in the monopole density. Specifically, we are seeking to observe a local excess of monopole magnetic charge induced by the simultaneous application of a temperature gradient, which should create a gradient in the monopole density, and a parallel field, which drives the flow and counterflow of oppositely-charged monopoles. This configuration should allow us to investigate the distribution, dynamics, and relaxation of the monopole-like excitations in spin ice pyrochlores.

1 Work supported by the National Science Foundation under grant DMR-1341793

Tuesday, March 3, 2015 11:15AM - 2:15PM

Session G28 GMAG DMP: Focus Session: Spin Ice 205 - Claudio Castelnovo, Cambridge University

11:15AM G28.00001 Thermal and Magnetic Responses of Spin Ice via SQUID Magnetometry

The role of phonons is to ensure that the vibrations we observe are consistent with the size of the particle, and to cause some degree of distortion in the spectral lineshape.

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The role of phonons is to ensure that the vibrations we observe are consistent with the size of the particle, and to cause some degree of distortion in the spectral lineshape.
12:27PM G28.00005 What is the quantum ground state of dipolar spin ice? , PAUL MCLCARTY, ISIS Neutron and Muon Source, STFC, OLGA SOKORA, NTU, RODERICH MOESSNER, MPIPKS, KARLO PENC, Institute for Solid State Physics and Optics, Budapest, FRANK POLLACK, MPIPKS, NIC SHANNON, Okinawa Institute of Science and Technology — Recent work on Dy2Ti2O7 spin ice has revealed a partial loss of residual entropy deep within the spin ice state [1]. It has been known for some time that the spin ice materials should have either magnetically ordered [2] or quantum spin liquid [3] ground states and this latest work hints at the possibility of determining them experimentally. We study a natural model for the dipolar spin ice materials and map out the entire ground state phase diagram in the presence of quantum tunneling between the ice states [4]. In the classical case, we show that the ground state of our 3D long-range interacting model can be determined from those of a short-range interacting 2D model and, remarkably, in the quantum case, only a very small tunneling coupling compared to the dipolar coupling is necessary to enter the quantum spin liquid state.


12:39PM G28.00006 Demagnetization Effects in Dipolar Systems , PATRIK HENELIUS, MIKAEL TWENGSTROM, 2 Department of Theoretical Physics, The Royal Institute of Technology, Sweden, LAURA BOVO, 2 London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, UK, MICHEL J. P. GINGRAS, Department of Physics and Astronomy, University of Waterloo, Canada & Canadian Institute for Advanced Research, Canada, STEVEN T. BRAMWELL, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, UK — The internal magnetic field of a uniformly magnetized body depends in general on the shape of the object. The calculation of this field, and the associated demagnetization factors, is a classical subject in the study of magnetism. Here we revisit the relationship between the demagnetization factor obtained through fluxmetric, magnetometric and bulk susceptibility techniques. Apart from simple uniaxial systems we also consider more complicated systems, such as the dipolar spin ice model on a pyrochlore lattice, where we compare our results to experimental bulk susceptibility measurements performed on a variety of sample shapes.

1 Theoretical modeling
2 Measurements

12:51PM G28.00007 Magnetic Susceptibility of Spin Ice , MIKAEL TWENGSTROM, 2 Department of Theoretical Physics, KTH, Sweden, LAURA BOVO, 2 London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, UK, TOM FENNELL, 2 Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, Switzerland, STEVEN T. BRAMWELL, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, UK, OLEG A. PETRENKO, University of Warwick, Department of Physics, UK, MICHEL J. P. GINGRAS, Department of Physics and Astronomy, University of Waterloo, Canada. Canadian Institute for Advanced Research, Canada, PATRIK HENELIUS, Department of Theoretical Physics, KTH, Sweden — The magnetic susceptibility of a spin ice material is a sensitive probe of the relevant physics in different temperature ranges. At high temperatures, where crystal field excitations dominate the susceptibility, the spin ice picture is not applicable. However, at temperatures below 10 K, the Ising anisotropy is well developed and the dipolar spin ice model (DSIM) can be employed. In this study we present experimental susceptibility data between 0.4 K and 10 K and revisit the DSIM in order to theoretically model this data. We find that the DSIM provides a good semi-quantitative description of both the temperature dependence of the uniform bulk susceptibility and the Q-dependent susceptibility measured by neutron scattering.

1 Simulations
2 Bulk measurements
3 Neutron scattering

1:03PM G28.00008 Pseudo-spin model and neutron scattering studies of hydrogen disorder in D2O , DAVID JONATHAN P. MORRIS, Xavier University, Cincinnati, OH, USA, KONRAD SIEMENSMYER, BASTIAN KLEEMKE, JENS-UWE HOFFMANN, ILLA GLAVATSKYI, KLAUS SEIFERT, Helmholtz-Zentrum Berlin for Materials and Energy, Berlin, Germany, SERGEI ISAKOV, ETH Zurich, Switzerland, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, ALAN TENNANT, Oak Ridge National Laboratory, Oak Ridge, TN, USA — The crystal structure of water is made up of a regular lattice of oxygen atoms connected by hydrogen bonds with an intermediate hydrogen atom. The hydrogen atom is displaced from the midpoint between nearest neighbor oxygen-oxygen atoms. Therefore the H-bond between neighboring hydrogen and oxygen can either be short or long. These H-bonds are known to obey the famous "ice rules" where each oxygen has two neighboring hydrogen sitting on the close site and two neighboring hydrogen sitting on the further site. The ice rules do not specify which hydrogen bonds will be short and which will be long for any particular oxygen, i.e. they do not describe long-range order, merely that there will be two short and two long bonds for a particular oxygen atom allowing for disorder. Here we will present a pseudo-spin model of water ice and diffuse neutron scattering measurements from D2O. The displacements of hydrogen away from the midpoint between neighboring oxygen-oxygen are treated as interacting Ising spins (σ = ±1). The diffuse neutron scattering measurements allow us to test the resulting theoretical predictions.

1:15PM G28.00009 Critical dynamics and finite-time scaling in spin ice systems , CLAUDIO CASTELNOVO, JAMES HAMP, University of Cambridge, ANUSHYA CHANDRAN, Perimeter Institute, RODERICH MOESSNER, MPIPKS — Spin ice materials such as Dy2Ti2O7 and Ho2Ti2O7 provide a rare instance of emergent gauge symmetry and fractionalisation in three dimensions. Magnetic frustration leads to highly degenerate yet locally constrained ground states. Their elementary excitations carry a fraction of the magnetic moment of the microscopic spin degrees of freedom and can be thought of as magnetic monopoles. One of the distinguishing manifestations of this emergent "Coulomb phase" is a liquid-gas phase diagram that appears in an applied magnetic field—a feature that is expected in itinerant charge liquids but unprecedented in localised spin systems. Monopoles act as facilitators to the spin dynamics. At low temperatures they are sparse and dynamics becomes slow, leading to an interplay between emergent topological properties and lattice response and equilibration properties. In this work, we investigate the dynamics in spin ice close to the critical end point of the liquid gas phase diagram. Critically divergent length scales give rise to finite time scaling properties that reflect the universal scaling exponents at the critical point. We use our results to explain these exponents by tuning the approach direction in the field-temperature plane.

1:27PM G28.00010 A Measure of Monopole Inertia in the Quantum Spin Ice Yb2Ti2O7 , LIDONG PAN, N. J. LAURITA, Institute for Quantum Matter, Department of Physics and Astronomy, Johns Hopkins University, KATE A. ROSS, Institute for Quantum Matter, Department of Physics and Astronomy, Johns Hopkins University; NIST Center for Neutron Research, EDWIN KERMARREC, Department of Physics and Astronomy, McMaster University, BRUCE D. GAULIN, Department of Physics and Astronomy; and Brockhouse Institute for Materials Research, McMaster University; Canadian Institute for Advanced Research, N. PETER ARMITAGE, Institute for Quantum Matter, Department of Physics and Astronomy, Johns Hopkins University. — We report a time domain terahertz spectroscopy study of quantum spin ice material Yb2Ti2O7. We measure the complex dynamic susceptibility of Yb2Ti2O7 in the temperature range between 1.4K and 20K. The data are consistent with a picture where the emergent magnetic monopoles are the principle degrees of freedom. Among other measures, we observe a zero crossing in the real part of the frequency dependent susceptibility. Such a feature is not possible without introducing inertial effects e.g. a mass dependent term to the equations of motion. Through a comparison of the magnetic spectral weight with numerical data that estimates the low temperature monopole density, we derive a value for the magnetic monopole mass.
Real time imaging of magnetic excitations in the spin ice Ho$_2$Ti$_3$O$_7$. LYA SOCHNIKOV, Stanford University — Theoretically, a special form of spin frustration in classical spin ices results in emergence of excitations that are directly mapped to magnetic monopoles. Experimentally, many aspects of the energetics of the magnetic excitations in spin ices are still not well understood, in part, because of scarcity of experimental tools that can explicitly and directly test for monopole dynamics. Using scanning Superconducting QUantum Interference Device (SQUID) microscopy we obtain real time images of spontaneous magnetic field fluctuations in the spin ice Ho$_2$Ti$_3$O$_7$. We determine a distribution of activation energies of spontaneous magnetic excitations from the temperature and frequency dependence of the observed field fluctuations. We discuss an agreement of the extracted energy distributions with the expected ones for monopole excitations. This study opens new horizons for studies of real space and real time magnetic fluctuations and their relations to emergent phenomena in a variety of frustrated magnets.

Tuesday, March 3, 2015 11:15AM - 2:15PM –
Session G29 GMAG: Cooperative Phenomena in Magnetism I
206A - Yang Zhao, National Institute of Standards and Technology

A minimal tight-binding model for ferromagnetic canted bilayer manganites. CHRISTOPHER LANE, Northeastern Univ., M. BAUBLITZ, Boston U., H. LIN, NUS, H. HAFIZ, R.S. MARKIEWICZ, B. BARBIELLINI, Northeastern U., Z. SUN, D.S. DESSAU, UC Boulder, A. BANSIL, Northeastern U. — Half-metallicity in materials has been a subject of extensive research due to its potential for applications in spintronics. Ferromagnetic manganites have been seen as a good candidate, and aside from a small minority-spin pocket observed in La$_{2-x}$Sr$_{1.2}$Mn$_2$O$_7$ ($x = 0.38$), transport measurements show that ferromagnetic manganites essentially behave like half metals. Here we develop robust tight-binding models to describe the electronic band structure of the majority as well as minority spin states of ferromagnetic, spin-canted antiferromagnetic, and fully antiferromagnetic bilayer manganites. Both the bilayer coupling between the Mn$_2$O$_7$ planes and the mixing of the $|x^2 - y^2 >$ and $|3z^2 - r^2 >$ Mn 3d orbitals play an important role in the subtle behavior of the bilayer splitting. Effects of $k_z$ dispersion are included.

High Pressure Transport Studies of NdIn$_3$. KENNETH PURCELL, Univ of Southern Indiana, DAVID GRAF, National High Magnetic Field Laboratory, TAKAO EBIHARA, Shizuoka University — NdIn$_3$ is a cubic antiferromagnetic metal that orders with a Neel temperature of 5.9 K and belongs to a family of rare earth intermetallic compounds RIn$_3$ that have a cubic AuCu$_3$-type crystal structure. At 0.5 K and the magnetic field applied in 100 direction, NdIn$_3$ exhibits metamagnetic transitions at 7.8 T and 8.9 T before entering a field induced paramagnetic state at 11.1 T. We report high pressure transport studies of single crystal NdIn$_3$ and the effect that pressure has on the Neel temperature, critical field, and metamagnetic transitions observed in the magnetoresistance. Comparisons to the behavior of the pressure induced superconductor CeIn$_3$ will be discussed.

Giant proximity effect and critical opalescence in EuS. TIMOTHY CHARLTON, Rutherford Appleton Laboratory, Science and Technology Facilities Council, United Kingdom., SILVIA RAMOS, JORGE QUINTANILLA, School of Physical Sciences, University of Kent, Canterbury, Kent, United Kingdom., ANDREAS SUTER, Paul Sherrer Institut, Switzerland, JAGADEESH MOODERA, Francis Bitter Magnet Laboratory, Massachusetts Institute of Technology, Cambridge, MA, United States. — The proximity effect is a type of wetting phenomenon where an ordered state, usually magnetism or superconductivity, “leaks” from one material into an adjacent one over some finite distance. For superconductors, the characteristic range is of the order of the coherence length, usually hundreds of nm. Nevertheless much longer, “giant” proximity effects have been observed in cuprate perovskite junctions. Such giant proximity effects can be understood by taking into account the divergence of the pairing susceptibility in the non-superconducting material when it is itself close to a superconducting instability: a superconducting version of critical opalescence. Since critical opalescence occurs in all second order phase transitions, giant proximity effects are expected to be general, therefor there must be a giant ferromagnetic proximity effect. Compared to its superconducting counterpart, the giant ferromagnetic proximity effect has the advantage that the order parameter (magnetization) can be observed directly. We have fabricated Co/EuS thin films and measured the magnetization profiles as a function of temperature using the complementary techniques of low energy muon relaxation and polarized neutron reflectivity. Details of the proximity effect near $T_c^{EuS}$ will be presented.

1:39PM G28.00011 Real time imaging of magnetic excitations in the spin ice Ho$_2$Ti$_3$O$_7$. LYA SOCHNIKOV, Stanford University — Theoretically, a special form of spin frustration in classical spin ices results in emergence of excitations that are directly mapped to magnetic monopoles. Experimentally, many aspects of the energetics of the magnetic excitations in spin ices are still not well understood, in part, because of scarcity of experimental tools that can explicitly and directly test for monopole dynamics. Using scanning Superconducting QUantum Interference Device (SQUID) microscopy we obtain real time images of spontaneous magnetic field fluctuations in the spin ice Ho$_2$Ti$_3$O$_7$. We determine a distribution of activation energies of spontaneous magnetic excitations from the temperature and frequency dependence of the observed field fluctuations. We discuss an agreement of the extracted energy distributions with the expected ones for monopole excitations. This study opens new horizons for studies of real space and real time magnetic fluctuations and their relations to emergent phenomena in a variety of frustrated magnets.

11:39AM G29.00003 $1/(N - 1)$ expansion, NRG, NCA, and exact $T \to \infty$ limit for the Green’s function of an SU($N$) Anderson impurity. AKIRA OGURI, Department of Physics, Osaka City University, RUI SAKANO, ISSP, University of Tokyo — We study the Green’s function of the $N$-orbital Anderson impurity in a wide range of the Coulomb interaction $U$, frequency $\omega$, and temperature $T$, carrying out the calculations with the $1/(N - 1)$ expansion [1], the numerical renormalization group (NRG), the non-crossing approximation (NCA), and the exact expression that is available at high temperatures or the high-bias limit of a nonequilibrium steady state [2]. Comparisons of these approaches are made, specifically, for the $N = 4$ particle-hole symmetric case. The $1/(N - 1)$ expansion is a new large $N$ approach based on the perturbation theory in $U [1]$, and is complementary to the NCA which uses the power series expansion in the hybridization matrix element $\gamma$. The calculations with this approach are carried out up to order $1/(N - 1)^2$, which reasonably capture the fluctuations beyond the random phase approximation (RPA) especially at low energies. We also discuss the $N$ dependence for $N > 4$. [1] A.O., R. Sakano, and T. Fuji, PRB 84, 113301 (2011).

11:51AM G29.00004 High Pressure Transport Studies of NdIn$_3$. KENNETH PURCELL, Univ of Southern Indiana, DAVID GRAF, National High Magnetic Field Laboratory, TAKAO EBIHARA, Shizuoka University — NdIn$_3$ is a cubic antiferromagnetic metal that orders with a Neel temperature of 5.9 K and belongs to a family of rare earth intermetallic compounds RIn$_3$ that have a cubic AuCu$_3$-type crystal structure. At 0.5 K and the magnetic field applied in 100 direction, NdIn$_3$ exhibits metamagnetic transitions at 7.8 T and 8.9 T before entering a field induced paramagnetic state at 11.1 T. We report high pressure transport studies of single crystal NdIn$_3$ and the effect that pressure has on the Neel temperature, critical field, and metamagnetic transitions observed in the magnetoresistance. Comparisons to the behavior of the pressure induced superconductor CeIn$_3$ will be discussed.

12:03PM G29.00005 Giant proximity effect and critical opalescence in EuS. TIMOTHY CHARLTON, Rutherford Appleton Laboratory, Science and Technology Facilities Council, United Kingdom., SILVIA RAMOS, JORGE QUINTANILLA, School of Physical Sciences, University of Kent, Canterbury, Kent, United Kingdom., ANDREAS SUTER, Paul Sherrer Institut, Switzerland, JAGADEESH MOODERA, Francis Bitter Magnet Laboratory, Massachusetts Institute of Technology, Cambridge, MA, United States. — The proximity effect is a type of wetting phenomenon where an ordered state, usually magnetism or superconductivity, “leaks” from one material into an adjacent one over some finite distance. For superconductors, the characteristic range is of the order of the coherence length, usually hundreds of nm. Nevertheless much longer, “giant” proximity effects have been observed in cuprate perovskite junctions. Such giant proximity effects can be understood by taking into account the divergence of the pairing susceptibility in the non-superconducting material when it is itself close to a superconducting instability: a superconducting version of critical opalescence. Since critical opalescence occurs in all second order phase transitions, giant proximity effects are expected to be general, therefor there must be a giant ferromagnetic proximity effect. Compared to its superconducting counterpart, the giant ferromagnetic proximity effect has the advantage that the order parameter (magnetization) can be observed directly. We have fabricated Co/EuS thin films and measured the magnetization profiles as a function of temperature using the complementary techniques of low energy muon relaxation and polarized neutron reflectivity. Details of the proximity effect near $T_c^{EuS}$ will be presented.

12:15PM G29.00006 Hole Properties In and Out of Magnetization Plateaus in 2-d Antiferromagnet. IMAM MAKHUFUDZ, PIERRE PUJOL, Laboratoire de Physique Théorique–IRSAMC, CNRS and Université de Toulouse, UPS, France — We study the signatures of magnetization plateaus and the presence or absence of Goldstone modes in terms of their effects on the physics of holes in hole-doped two-dimensional antiferromagnet defined on square lattice. Holes with quadratic dispersion around Fermi point existing at infinitesimally small doping and linear dispersion around nearly circular Fermi surface at finite but low doping are investigated. They are coupled to an effective gauge field, generated by the spin sector, which subsequently mediates interaction between the holes. We find that out-of-plateaus case leads to algebraically decaying long-range interaction between fermionic holes with both Coulombic and dipolar forms, whereas in-plateaus case leads to short-range (local) interaction. We show that the spectral peak is significantly broadened in the out-of-plateaus case, while the spectral weight is still sharply-peaked in the in-plateau case. This conclusion holds in both infinitesimally small doping limit and in the more realistic finite doping case. We also extend the result obtained for 1-D system where finite hole doping gives rise to a shift in the magnetization value of the plateaus. Reference: arXiv:1411.1713

IM is supported by grant No. ANR-10-LABX-0037 of the Programme des Investissements d’Avenir of France
12:27PM G29.00007 Emergence of New Magnetic Plateaus in Sheets of Magnetic Dimers, S. HARAVIFARD, UChicago/Argonne National Lab, D. GRAF, National High Magnetic Field Lab, A. FEIGUIN, Northeastern Univ, C.D. BATISTA, Los Alamos National Lab, J.C. LANG, Argonne National Lab, D. SILEVITCH, UChicago, G. SRAJER, Argonne National Lab, H.A. DABKOWSKA, B.D. GAULIN, McMaster Univ, S.W. TOZER, National High Magnetic Field Lab, T.F. ROSENBAUM, UChicago — SrCu2(BO3)2 has corner-sharing Cu2+ spin 1/2 dimers lying on a square lattice, corresponding to the two-dimensional Shastry-Sutherland model. At low temperatures and fields exceeding 20 T, there is a Bose-Einstein condensation of triplet excitations of the dimers. At higher magnetic fields, plateaus have been observed in the magnetization, which have been interpreted in terms of preferred filling of the singlet ground state with increasing densities of triplet roton states. We apply hydrostatic pressures up to 9 GPa to study the movement and suppression of the quantized magnetic plateaus identified at ambient pressure as well as the emergence of new superstructure configurations.

12:39PM G29.00008 Magnetism in RFe2Ge2 (R = Y, Lu, Tb) as seen by 57Fe Mössbauer spectroscopy1, SERGEY L. BURKOV, Ames Lab/ISU, MARCOS A. AVILA, UFABC, XIAOMING MA, Landzhou U. and Ames Lab/ISU, SHENG RAN, HYUNSOO KIM, PAUL C. CANFIELD, Ames Lab/ISU — Magnetic properties of RFe2Ge2 (R = Y, Lu, Tb) were studied using neutron scattering dependent (4.6 - 300 K) Mössbauer spectroscopy and specific heat capacity. In the paramagnetic state all three compounds have similar evolution of the isomer shift and quadrupolar splitting. Magnetic phase transitions can be detected both in LuFe2Ge2 and TbFe2Ge2, with an indication of very small iron magnetic moment in the ordered state for LuFe2Ge2. The Debye temperature evaluated from the temperature-dependent isomer shift for these three compounds is significantly higher that inferred from specific heat capacity measurements, that might indicate presence of magnetic correlations. The results will be compared with the bulk measurements.

1Supported by US DOE, BES under Contract No. DE-AC02-07CH11358 and China Scholarship Council.

12:51PM G29.00009 Quadrupolar order triggered by magnetic order in GdB4, HOYOUNG JANG, SSRL, SLAC National Accelerator Laboratory, B.Y. KANG, B.K. CHO, School of Materials Science and Engineering, Gwangju Institute of Science and Technology (GIST), J.-S. LEE, SSRL, SLAC National Accelerator Laboratory — Various electronic and magnetic properties and phase transition of Gd and Gd compounds have been measured. For example, 4f delocalization of Gd metal was revealed by resonant inelastic x-ray scattering study with high pressure condition [1]. Meanwhile, extremely large magnetic susceptibility in GdB4 was reported [2] – which is unexpected in the general Gd configuration. We investigated GdB4 by resonant soft x-ray scattering (RSXS) experiment at GTEM edge. In (100) reflection, huge RSXS signal was observed, which corresponds to the reported antiferromagnetic (AFM) order by neutron scattering measurement [3]. Besides, unexpected RSXS signal was also detected in different photon polarization, which cannot be explained by the reported AFM structure. The energy dependence of the unexpected signal might to 2 spin-coupling the different origin with the AFM order. We deduce that the unexpected signal comes from Gd quadrupolar order, which is triggered by magnetostriiction through the AFM order.


1:03PM G29.00010 Condensation of collective charge ordering in Chromium, A. SINGER, M. MARSH, S. DIETZE, Department of Physics, University of California-San Diego, V.V. UHLMIR, Center for Magnetic Recording Research, University of California-San Diego, Y. LI, D.A. WALKO, E.M. DUFRESNE, G. SRAJER, Advanced Photon Source, Argonne National Laboratory, M.P. COSGRIFF, P.G. EVANS, Department of Materials Science and Engineering, University of Wisconsin Madison, E.E. FULLERTON, Center for Magnetic Recording Research, University of California-San Diego, O.G. SHPYRKO, Department of Physics, University of California-San Diego — Here we report on the dynamics of the structural order parameter in a chromium film using synchrotron radiation in response to photo-induced ultra-fast excitations. Following transient optical excitations the effective lattice temperature of the film rises close to the Neel temperature and the charge density wave (CDW) amplitude is reduced. Although we expect the electron charge ordering to vanish shortly after the excitation we observe that the CDW is never completely disrupted, which is revealed by its unmodified period at elevated temperatures. We attribute the persistence of the CDW to the long-lived periodic lattice displacement in chromium. The long-term evolution shows that the CDW revives to its initial strength within 1 ns, which appears to behave in accordance with the temperature dependence in equilibrium. This study highlights the fundamental role of the lattice distortion in charge ordered systems and its impact on the re-condensation dynamics of the charge ordered state in strongly correlated materials.

1:15PM G29.00011 Direct probe of Fermi surface evolution at a pressure-induced quantum phase transition, D.M. SILEVITCH, University of Chicago, YEJUN FENG, Argonne National Laboratory, A. PALMER, YISHU WANG, T.F. ROSENBAUM, University of Chicago — The nature of a material's Fermi surface is crucial to understanding its electronic, magnetic, optical, and thermal characteristics. Traditional measurements such as angle resolved photoemission spectroscopy and de Haas-van Alphen quantum oscillations can be difficult to perform in the vicinity of a pressure-driven quantum phase transition. We demonstrate here that magnetic x-ray diffraction in combination with Hall effect characteristics. Traditional measurements such as angle resolved photoemission spectroscopy and de Haas-van Alphen quantum oscillations can be difficult to perform in the vicinity of a pressure-driven quantum phase transition. We demonstrate here that magnetic x-ray diffraction in combination with Hall effect measurements in a diamond anvil cell can provide valuable insight into the Fermi surface evolution in spin- and charge-density-wave systems near quantum phase transitions. In particular, we delineate the critical pressure and absence of Fermi surface reconstruction at the spin-flip transition in elemental chromium.

1:27PM G29.00012 Factors influencing achievement of chemical order in tetragonal FeNi, NINA BORDEAUX, ANA MARIA MONTES-ARANGO, Northeastern University, JIAXING LIU, KATAYUN BARMAK, Columbia University, LAURA HENDERSON LEWIS, Northeastern University — Chemically ordered ferromagnetic compounds with the L10 structure have attracted wide interest for rare-earth-free permanent magnets applications. In particular, L10-structured FeNi is a promising candidate due to the abundance and low cost of the constituent elements and high theoretical maximum energy product (BH)max = 42 MGOe [1]. Synthesis of L10 FeNi has been hindered by extremely sluggish kinetics below the equilibrium order-disorder temperature TOD = 320 °C and the phase is known to form in meteorites over millions of years. In this work, the thermodynamic stability of the L10 phase and kinetics of the L10 → fcc magnetostructural phase transformation are quantitatively determined via magnetic and thermal measurements of bulk L10 FeNi extracted from meteorites. Influences on phase transformation kinetics, including effects of magnetism, will be discussed. [1] L. H. Lewis, et al., IEEE Mag Lett 5 (2014) 550104.

1:39PM G29.00013 Phase Transitions on Random Lattices: How Random is Topological Disorder?1, HATEM BARGHATHI, THOMAS VOJTA, Missouri Univ of Sci & Tech — We study the effects of topological (connectivity) disorder on phase transitions. We identify a broad class of random lattices whose disorder fluctuations decay much faster with increasing length scale than those of generic random systems, yielding a wandering exponent of ν > 2 rather than the usual Harris criterion ν = 2, making topological disorder less relevant than generic randomness. The Imry-Ma criterion is also modified for first-order transitions to survive in all dimensions d > 1. These results explain a host of puzzling violations of the original criteria for equilibrium and nonequilibrium phase transitions on random lattices. We discuss applications, and we illustrate our theory by computer simulations of random Voronoi and other lattices.

1This work was supported by the NSF under Grant Nos. DMR-1205803 and PHYS-1066293. We acknowledge the hospitality of the Aspen Center for Physics.
1:51PM G29.00014 Pressure Dependence of Magnetism in KCuF$_3$

BRIAN NGUYEN, ALEXANDER THALER, Univ of Illinois - Urbana, CLARINA DELA CRUZ, Oak Ridge National Lab, GREGORY MACDOUGALL, Univ of Illinois - Urbana — The perovskite KCuF$_3$ is a prototypical compound for studying both orbital ordering and 1-D Heisenberg antiferromagnetism. In the conventional Kugel-Khomskii picture, this material undergoes a Jahn-Teller distortion at T$_{JT}=800$ K causing long-range ordering of 3d Cu$^{2+}$ orbitals, effectively driving the spin interactions 1-D. A second magnetic transition to 3-D antiferromagnetism is observed at the Néel temperature, T$_N=39$ K. Recent data by Lee et al. suggests a new interpretation where Cu$^{2+}$ orbitals do not order until a glassy structural transition at T$_s=50$ K, and this transition is a necessary precursor to 3-D ordering of spins. It was later shown that the glassy transition can be suppressed to zero temperature with pressures as low as P=$7$ kbar, implying that spin order should follow suit. Contrary to this prediction, single crystal neutron scattering measurements by our group demonstrated a moderate increase in T$_N$ with pressure, opposite of predictions. However, some evidence for uniaxial strain complicated interpretation. In an attempt to resolve this issue, we performed neutron powder diffraction measurements in helium gas and clamp pressure cells. We will present these data and discuss them in the context of the Lee et al. model.

2:03PM G29.00015 Neutron Study of the Magnetic Structures and Phase Transitions in RCuAs$_2$ (R=Pr, Nd, Tb, Dy, Ho, Yb), YANG ZHAO, Department of Materials Science and Engineering, University of Maryland, College Park, Maryland 20742, USA, J. W. LYNN, NIST Center for Neutron Research, Gaithersburg, Maryland, 20899, USA, GOHIL S. THAKUR, ZEBA HAQUE, L.C. GUPTA, A-K. GANGULI, Department of Chemistry, Indian Institute of Technology Delhi, India — Neutron diffraction and inelastic scattering studies have been carried out on polycrystalline samples of the above titled materials as a function of temperature and applied magnetic field to determine the magnetic structures, order parameters, and overall spin dynamics. The space group of this compound is P4/nmm with typical (tetragonal) lattice parameters a $\sim$ 3.9 Å and c $\sim$ 10.0 Å. PrCuAs$_2$ develops commensurate magnetic order at T$_N=6.4$ K with an ordered moment of 1.24 $\mu_B$ oriented along the c-axis. The ordering wave vector is (0.0,1/2), with a $\Gamma_7$ representation. NdCuAs$_2$ orders at T$_N=3.54$ K with the same ordering wave vector (with the $\Gamma_7$ or $\Gamma^0_9$ representations), but with the moment direction in the a-b plane along [110] of magnitude 3.5 $\mu_B$. TbCuAs$_2$ and HoCuAs$_2$ exhibit incommensurate order at T$_N=9.1$ and 4.0 K, respectively. The results for the inelastic scattering will be discussed.

Tuesday, March 3, 2015 11:15AM - 2:15PM
Session G30 GMAG DMP FIAP: Focus Session: Skyrmions III

11:15AM G30.00001 Tailoring magnetic skyrmions at transition-metal interfaces, BERTRAND DUPÉ, MARKUS HOFFMAN, CHARLES PAILLARD, STEFAN HEINZE, Christian Albrechts University of Kiel — Skyrmions in magnetic materials offer attractive perspectives for future spintronic applications [1] since they are localized, topologically stabilized spin structures which can be manipulated at electric current densities which are by orders of magnitude lower than those required for moving domain walls. Recently, it has been discovered that due to the broken inversion symmetry at surfaces magnetic skyrmions can also occur in ultra-thin transition metal films at surfaces [2,3]. Here, we use first-principles electronic structure theory to show how transition-metal interfaces can be modified such that they exhibit skyrmion phases and to explain the observation of individual skyrmions in an ultra-thin film composed of Pd and Fe on the Ir(111) surface [3,4]. We determine the magnetic interactions in this system using density functional theory and explain the occurrence of skyrmion phases in an external magnetic field using Monte-Carlo simulations. Our work paves the way to tailor the properties of skyrmions at transition-metal interfaces.


11:27AM G30.00002 Oxygen-enable control of Dzyaloshinskii-Moriya Interaction in Fe/Ir(001) bilayers, ABDERREZAK BELABBES, King Abdullah Univ, GUSTAV BIHLMAYER, STEFAN BLÜGEL, Peter Grünberg Institut and Institute for Advanced Simulation, D-59225 Jülich, Germany, AURELIEN MANCHON, King Abdullah Univ — Using relativistic first principles calculations, we demonstrate that the magnitude and sign of the Dzyaloshinskii-Moriya interaction (DMI) of Fe/Ir(001) interface can be controlled by tuning the coverage of the oxygen capping layer, which changes the spin-wave length and the depth of the energy minimum. In addition, we explain how the magnetic interactions [Exchange interaction, DMI, and the magnetocrystalline anisotropy (MAE)] at such transition metal interface are modified in the presence of Oxygen, which might prevent any stable magnetic order due to the small energy scale. We observe a change sign of the DMI when the coverage exceeds 50%. In particular, we found that due to the C4 breaking symmetry and the large spin-orbit interaction of the Ir substrate the DMI exceeds a critical strength and competes with the exchange interaction and causes homochiral magnetic structures. This study reveals that in realistic systems capped by an oxide, such as HM/F/MOx (HM is a heavy metal, F a ferromagnet an MOx=MgOx, CoOx, TaOx etc., the DMI can be tuned by changing the oxidation conditions of the capping layer, offering a convenient way to control it. Therefore, understanding of the these phenomena may have impact in the context of facilitating applications in spintronics.

11:39AM G30.00003 Imprinting topological domain structure in epitaxial Ni/Fe/Co/Cu(001), ALI TAN, JIA LI, ZI QIANG QU, University of California Berkeley, ELKE ARENHOLZ, ANDREAS SCHOLL, Lawrence Berkeley National Laboratory, CHANYONG HWANG, Korea Research Institute of Standards and Science — A vortex state can be stabilized in magnetic thin films by reducing the lateral dimension of the thin film such that the shape anisotropy imposes flux-closure on the magnetic domains. In the language of skyrmions, a vortex state has a topological skyrmion charge $Q = \pm 1/2$, with vorticity $w = \pm 1$ and helicity $\gamma = \pm \pi/2$. By tuning the interlayer coupling strength, various domain structures can be imprinted on the adjacent ferromagnetic layer. We investigated domain imprinting by cobalt (Co) vortices on nickel (Ni) layer through a face-centered-cubic (fcc) iron (Fe) interlayer in a Ni/Fe(wedge)/Co/disks/Cu(001) trilayer system. Using element-specific X-ray Magnetic Circular Dichroism, we observed a strong antiferromagnetic IEC for 5 ML thick Fe interlayer. From the domain images of each elements obtained using Photoemission Electron Microscopy (PEEM), we observed that the relative strength of the bilinear and biquadratic exchange coupling changes as a function of Fe interlayer thickness, leading to non-collinear coupling between Ni and Co around 5.5 ML of Fe. The resulting Ni domain structures have topological skyrmion charge $Q = \pm 1/2$, with vorticity $w = \pm 1$ but varying helicity $\gamma$. 

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under award number DE-FG02-07ER46453.
11:51AM G30.00004 Biskyrmion bubble lattice in Fe/Gd alloy thin films, JAMES LEE, Lawrence Berkeley National Laboratory and University of Oregon, Eugene, XIAOWEN SHI, JORDAN CHESS, University of Oregon, Eugene, SERGIO MONTOTOYA, Center for Magnetic Recording Research, University of California, San Diego, SHRAWAN MISHRA, Lawrence Berkeley National Laboratory, LEV SAKHAROV, University of Oregon, Eugene, DANIEL PARKS, Lawrence Berkeley National Laboratory, BEN MCMORRAN, University of Oregon, Eugene, STEVEN KEVAN, Lawrence Berkeley National Laboratory and University of Oregon, Eugene, ERIC FULLERTON, Center for Magnetic Recording Research, University of California, San Diego, SUJOY ROY, Lawrence Berkeley National Laboratory — Magnetic bubbles with topologically non-trivial twists, called “skyrmion bubbles,” exhibit particle-like properties and novel magnetic interactions with each other. They are seen in non-centrosymmetric crystals, such as MnSi, and monolayers of Fe on Ir(111) substrates. Our study considers whether skyrmion bubbles can also form in soft ferromagnetic alloys with perpendicular anisotropy. Using resonant X-ray scattering at the Fe L3 and Gd M2 transition edges, we show that triangular lattices of skyrmion bubbles form in Fe/Gd thin films in a limited temperature and magnetic field range. Uniaxial anisotropy in the resonant scattering pattern indicates the lattice unit cell contains two skyrmions. Lorentz TEM images reveal that the repeating unit is a bound pair of bubbles called biskyrmions. Adjusting the composition of the films can shift the temperature range of the biskyrmion lattice by 100 K, allowing the lattice to form at room temperature. Fe/Gd thin films may prove a promising material for spintronics.

12:03PM G30.00005 Investigation of the Stripe-Bubble Phase in La2-2xSr1+2xMn2O7(x=0.32) by Magnetic Force Microscopy, JUYOUNG JEONG, JINHO YANG, CALDES, Institute for Basic Science and Department of Physics, Pohang Univ of Sci & Tech, JUAN HERNANDO, JABEEL KIM, CALDES, Institute for Basic Science, ILKYU YANG, Department of Physics, Pohang Univ of Sci & Tech, JIANSHI ZHOU, Texas Material Institute, the University of Texas at Austin, NELIZA LEON, ROMAN MOVSHEVICH, Los Alamos National Laboratory, ALEX DE LOZANNE, Department of Physics, the University of Texas at Austin, H.W. YEOM, CALDES, Institute for Basic Science and Department of Physics, Pohang Univ of Sci & Tech, J.B. GOODENOUGH, Texas Material Institute, the University of Texas at Austin, NESTOR HABERKORN, Centro Atomico Bariloche, JEEHOON KIM, CALDES, Institute for Basic Science and Department of Physics, Pohang Univ of Sci & Tech — We constructed a home-built low temperature magnetic force microscope (LTMFM) with the fiber interferometer detection scheme: The base temperature is 4 K and magnetic field range is up to 6 T. The MFM system is applied to investigate unconventional magnetism of La2-2xSr1+2xMn2O7(x=0.32) in a wide span of temperature and magnetic field. We imaged spin reorientation transition and found two types of bubble domains. The behavior of bubble domains shows the same upon field cycle, indicating a reversible magnetization property reported previously in the bulk magnetization measurement. The origin of the two types of the bubble domains will be discussed by comparing MFM and bulk magnetization data.

12:15PM G30.00006 Metastable multi-domain state in ultrathin films with Dzyaloshinskii-Moriya Interaction, PARNIKA AGRAWAL, SEONHOON WOO, GEOFFREY BEACH, MIT — Helical spin structures such as skyrmions and chiral domain walls are stabilized in magnetic films with strong Dzyaloshinskii-Moriya interaction (DMI) [1,2]. The chiral spin state is the ground state when the ratio of the effective DMI field to anisotropy field is greater than 2/p [3]. However, even when the DMI is too weak to generate a chiral ground state, such states can be metastable if the uniform state is appropriately perturbed [1,4]. Here, we show that an in-plane applied field reduces the energy barrier for domain wall formation, and provides a simple technique to generate a multistate domain uniform in magnetic films. Further, we identify that the threshold between the stable single-domain state and the metastable multidomain state can be controlled by two parameters—magnetizing energy and geometrical confinement. We use these parameters to create isolated geometrically confined magnetic bubbles in patterned disks of Pt/Cr/GdOx multilayers. These bubbles may provide insight into the mechanism of creation of skyrmions in magnetic thin films with strong DMI.

12:27PM G30.00007 Tailoring the topology of an artificial magnetic skyrmion, JIA LI, University of California, Berkeley — A skyrmion is a topological twist of a continuous field that was first proposed by Skyrme to describe discrete nucleons. In condensed-matter physics, skyrmions emerge as topological invariant spin textures in two dimensional Heisenberg spin lattice. Evidence of skyrmions in condensed matter physics appeared after the discovery of the Quantum Hall Effect in which the lowest energy charged excitations can be mapped onto two-dimensional magnetic skyrmion states. Despite theoretical predictions, it remains an experimental challenge to realize an artificial magnetic skyrmion whose topology can be well controlled and tailored so that its topological effect can be revealed explicitly in a deformation of the spin textures. Here we report epitaxial magnetic thin films in which an artificial skyrmion is created by embedding a magnetic vortex into an out-of-plane aligned spin environment. By changing the relative orientation of the central vortex core polarity and the surrounding out-of-plane spins, we are able to control and tailor the system between two skyrmion topological states. An in-plane magnetic field is used to annihilate the skyrmion core by converting the central vortex state into a single domain state. Our result shows distinct annihilation behaviour of the skyrmion core for the two different skyrmion states, suggesting a topological effect of the magnetic skyrmions in the core annihilation process.

1:03PM G30.00008 Interlayer Exchange Coupling: A route to stabilize skyrmions in magnetic multilayers, ASHIS KUMAR NANDY, NIKOLAI S. KISELEV, STEFAN BLÜGEL, IAS-1, PGI-1, Forschungszentrum Jülich and JARA, Jülich, Germany — Magnetic skyrmion is a topologically nontrivial spin texture with particle like properties, which may emerge under an appropriate applied magnetic field in any magnetic thin layer or multilayer with surface or interface induced Dzyaloshinski-Moriya interaction. However, magnetic fields required to stabilize skyrmions can be extremely large. We present an approach, which allows the stabilization of skyrmions in such magnetic multilayers even at zero magnetic field. It is based on fine-tuning the interplay between internal and interfaces induced interactions by adjusting the thicknesses and interface compositions of multilayers. Our multiscale approach is based on DFT calculations and atomistic spin dynamic simulations, which predicts the existence of a skyrmion lattice and isolated skyrmions in a thin film of a transition-metal monolayer grown on a heavy metal substrate. The simulated skyrmions exhibit high stability in an applied magnetic field and temperature. We provide a description for the complex phases occurring in such systems and present a magnetic phase diagram for a prototype example of Mn/W(001).

1:15PM G30.00009 Novel rare-earth free magnetic nanostructures1, BHASKAR DAS, BALAMURUGAN BALASUBRAMANIAN, PINAKI MUKHERJEE, PRIYANKA MANCHANDA, RALPH SKOMSKI, University of Nebraska, Lincoln, NE 68588, GEORGE HADJIPANAYIS, University of Delaware, Newark, DE 19716, DAVID SELLMYER, University of Nebraska, Lincoln, NE 68588 — Magnetic nanostructuring including stabilization of novel structures without critical elements, easy-axis alignment, and self-assembly are important for creating new magnetic materials. We use a single-step evaporation of a cluster-deposited nanoparticle array to fabricate large area magnetic nanostructures from magnetic materials with potential for high-energy magnet or spintronics applications.1 For example, MnSi nanoclusters of diameter about 8 nm form hexagonal D8h structure and show strong ferromagnetic properties with a high Tc = 590 K, an appreciable K1 = 12 Mergs/cm3, and a high J=1.25 kG. This result is in a sharp contrast to the antiferromagnetic ordering observed in bulk MnSi with T= 100 K, and is supported by DFT calculations. On the other hand, MnSi nanoclusters form B20-type cubic crystal structure and are ferromagnetically below T = 25 K. Skyrmion-type spin textures have been observed in MnSi thin films and evidence for such structures in nanoclusters will be discussed.

1 This research is supported by U.S. DOE-BES-DMSE (DE-FG02-04ER46152) and NCMN.

1:27PM G30.00010 Growth and Properties of Skyrmionic MnSi Nanowires and Thin Film on Silicon . ZHENG GAI, Oak Ridge National Laboratory, Oak Ridge, TN, JIEYU YI, SIWEI TANG, University of Tennessee, Knoxville, TN, IVANJ. KRAVCHENKO, GUIXIN CAO, Oak Ridge National Laboratory, Oak Ridge, TN, DAVID MANDRUS, University of Tennessee, Knoxville, TN, OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TN COLLABORATION, UNIVERSITY OF TENNESSEE, KNOXVILLE, TN COLLABORATION — Magnetic skyrmion lattice, a vortex-like spin texture recently observed in chiral magnets, is of great interest to future spin-electronic data storage and other information technology applications. The skyrmion lattice in MnSi appears in a small region (known as the A phase) of the H-T phase diagram in bulk samples, but in 2D samples like thin films the skyrmion phase is much more robust. If skyrmion ordering can persist in one-dimensional MnSi nanowires and 2D films, then these systems may be very promising for spintronics applications as the magnetic domains and individual skyrmions could be manipulated with small currents. We have systematically explored the synthesis of single crystal MnSi nanowires via controlled oxide-assisted chemical vapor deposition and observed a characteristic signature of skyrmion magnetic ordering in MnSi nanowires. The SiO2 layer plays a key role for the high yield, correct stoichiometric and crystalline growth of the B20 MnSi nanowires. A growth phase diagram was constructed. For the thin films, an unique growth receipt was developed for the growth of high quality of thin films. The structure and magnetic properties of the films at different thickness were studied.

1:39PM G30.00011 Manipulating Topological States by Imprinting Non Collinear Spin Textures . PETER FISCHER, Lawrence Berkeley Natl Lab, ROBERT STREUBEL, LUYANG HAN, Institute for Integrative Nanosciences IFW Dresden, MI-YOUNG IM, Lawrence Berkeley Natl Lab, FLORIAN KRONAST, Helmholtz-Zentrum Berlin fuer Materialien und Energie GmbH, ULRICH K. ROESSLER, Institute for Theoretical Solid State Physics IFW Dresden, FLORIN RADU, ABRUDAN, Helmholtz-Zentrum Berlin fuer Materialien und Energie GmbH, GUNGUN LIN, OLIVER G. SCHMIDT, DENYS MAKAROV, Institute for Integrative Nanosciences IFW Dresden — Topological magnetic states, such as chiral skyrmions, are of great scientific interest and show huge potential for novel spintronics applications, provided their topological charges can be fully controlled. So far skyrmionic systems have been observed in noncentrosymmetric crystalline materials with low symmetry and at low temperatures. We propose theoretically and demonstrate experimentally the design of spin textures with topological charge densities that can be tailored at ambient temperatures. Tuning the interlayer coupling in vertically stacked nanopatterned magnetic heterostructures, such as a model system of a Co/Pd multilayer coupled to Permalloy, the in-plane non-collinear spin texture of one layer can be imprinted into the out-of-plane magnetised material. We observe distinct spin textures, e.g. vortices, magnetic swirls with tunable opening angle, donut states and skyrmion systems of Dn symmetry. We show that applying a small magnetic field, a reliable switching between topologically distinct textures can be achieved at remanence.

1:51PM G30.00012 Dzyaloshinkii-Moriya interaction mediated by combined exchange and Rasha bands . ANIRBAN KUNDU, SHUFENG ZHANG, Univ of Arizona — Domain wall structure determined by the competition among exchange, anisotropy, and magnetostatics does not have a preferred wall chirality, i.e., the clockwise and anti-clockwise spin rotations of the domain wall are equally probable. Dzyaloshinskii-Moriya interaction (DMI) has been identified as the dominant mechanism for the observed chiral domain walls in ultrathin ferromagnetic CoNi films. We show that the DMI arises from the interplay between the ferromagnetic exchange coupling and the interface Rashba spin-orbit coupling; these two couplings generally exists for ultrathin films with perpendicular magnetic anisotropy. The DMI displays an oscillatory dependence on the distance of two magnetic ions. In the limit that the Rashba coupling is much smaller than the exchange coupling, the strength of the DMI is linear with respect to the Rashba coupling. In the opposite limit, the DMI depends on the quadratic Rashba coupling. We apply our results to study the chiral dependence of the domain walls. In particular, we quantitatively relate the Rashba coupling strength to the wall structure and map out the preferred Neel or Bloch walls with definite chirality. The results agree with the experiment.

This work was supported by NSF-ECCS.


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2:03PM G30.00013 Observation of Skyrmions in Mn-Pt-Sn based Heusler material. AJAYA KUMAR NAYAK, ROSHNEE SAHOO, Max Planck Institute for Chemical Physics of Solids, JOHANNES WILD, Faculty of the Institute of Experimental and Applied Physics, Regensburg, Germany, DANIEL EBKE, Max Planck Institute for Chemical Physics of Solids, JOSEF ZWECK, Faculty of the Institute of Experimental and Applied Physics, Regensburg, Germany, STUART PARKIN, Max Planck Institute of Microstructure Physics, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids — Mn2YZ based Heusler materials often exhibit collinear spin alignment. However, in a recent work we found Mn2RhSn displays a non-collinear magnetic structure. The presence of noncollinear spin alignment with lack of inversion symmetry sets up a perfect condition for skyrmions in Mn2RhSn. However, experimentally it is still to be verified. To find skyrmions in Heusler system we search for materials with large spin-orbit coupling and lack of inversion symmetry. Here we present the experimental evidence of skyrmions in Mn-Pt-Sn Heusler compound. This sample shows an order-disorder transition around 400 K, followed by a spin-reorientation transition at low temperature. Our magnetization and ac-susceptibility measurements display a similar type of behavior that generally found in the skyrmion system. We have performed high resolution Lorentz transmission electron microscopy measurements to get a direct evidence of skyrmions in Mn-Pt-Sn sample. Our results show evolution of skyrmions in particular fields and temperature intervals.


1This work was supported by FAPESP and CNPq.
11:27AM G31.00002 Effects of magnetic site disorder of the 1-D Ising spin chain compounds Ca₃(\text{Co,Mn})₂O₆ with dilute doping

11:27AM G31.00003 Neutron scattering studies of a bond-disordered $S = 1$ quantum spin liquid

11:39AM G31.00004 Quasi-one-dimensional spin nematic states and their excitations

12:27PM G31.00005 Competing orders of a magnetic impurity lattice in a one-dimensional Fermi gas

12:39PM G31.00006 Altering TCNQ-TCNQ interactions and a study of the spin-Peierls state including muon-fluorine entanglement

12:51PM G31.00007 Direct measurement of the spin gap in a quasi-one-dimensional clinopyroxene: NaTiSi₂O₆

1:03PM G31.00008 ABSTRACT WITHDRAWN

1:03PM G31.00009 ABSTRACT WITHDRAWN
1:15PM G31.00009 Z2 symmetry-protected topological phases in SU(3) AKLT model. TAKAHIRO MORIMOTO, HIROSHI UEDA, TSUTOMU MOMOI, AKIRA FURUSAKI, RIKEN — We study Z2 symmetry-protected topological (SPT) phases in one-dimensional systems with Z2 × Z2 symmetry. We construct MPS wavefunctions for Z2 SPT phases by using non-trivial cocycles of the group cohomology H2(Z2 × Z2, U(1)) = Z2. Their parent Hamiltonian turns out to be an SU(3) version of the AKLT model consisting of bilinear and biquadratic terms of su(3) operators in the Z representation. We apply iDMRG method to the SU(3) bilinear-biquadratic model of general coupling constants. We determine its phase diagram in which the nontrivial Z2 SPT phase is present for a parameter range including the point of vanishing biquadratic term as well as the SU(3) AKLT point. We find a continuous phase transition from the Z2 SPT phase to an SU(3) dimer phase, where we obtain a central charge c = 16/5 from a scaling of the entanglement entropy. We also discuss that an S = 1 spin chain with staggered quadrupole couplings reduces to the SU(3) AKLT model in the strong coupling limit.

1:27PM G31.00010 Symmetry fractionalization in SU(2n) antiferromagnetic Heisenberg chains, ANDREAS WEICHSELBAUM, Ludwig Maximilians University, THOMAS QUELLA, University of Cologne — We explore generalizations of the Affleck-Kennedy-Lieb-Tasaki (AKLT, 1987) model for spin-1 antiferromagnetic Heisenberg chains to higher-rank SU(2n) symmetries. In particular we show that by proper tuning of higher order spin interactions there also exist exact low-dimensional matrix-product ground states with fractionalized edge states, and that these states are adiabatically connected to the ground state of the plain SU(2n) Heisenberg model. The parameter space is explored using state of the art density matrix renormalization group (DMRG), explicitly utilizing SU(N) symmetry up to N=6 based on the QSpace tensor library.

1:39PM G31.00011 Unusual Magnetic Response of an S = 1 Antiferromagnetic Linear-Chain Material, J.S. XIA, M.W. MEISEL, Dept. of Physics and NHMFL, Univ. of Florida, A. OZAROWSKI, NHMFL, Florida State Univ., P.M. SPURGEON, A.G. GRAHAM, J.L. MANSON, Dept. of Chem. and Biochem., Eastern Washington Univ. — An S = 1 antiferromagnetic polymeric chain, [Ni(HF2)3(Cpy)]BF4 (py = pyridine), has been identified to have nearest-neighbor antiferromagnetic interaction J/kB = 4.86 K and single-ion anisotropy D/kB = 4.3 K, while avoiding long-range order down to 25 mK. With D/J = 0.88, this system is close to the D/J ≈ 1 gapless quantum critical point between the topologically distinct Haldane and Large-D phases. The magnetization was studied over a range of temperatures, 50 mK ≤ T ≤ 1 K, and magnetic fields, B ≤ 10 T. The results allow an upper bound of the critical field, Bc, which closes the Haldane gap, to be estimated. Specifically, Bc(4.2 K) < (35 ± 10) mT, which is close to the predicted 46 mT [1] when using the reported 12 values of J, D, and g. In low fields, the magnetic signal increases with decreasing T for 400 mK < T < 800 mK but is independent of T for 50 mK ≤ T < 400 mK. This observation is consistent with a significant increase in the specific heat arising from the accumulation of entropy in the vicinity of the quantum critical point.

1:51PM G31.00012 Evolution of Spinons with Magnetic Heavy Fermion Yb2Pt2Pb1, W.J. GANNON, L. WU, Stony Brook University, USA, I.A. ZALIZNYAK, Brookhaven National Laboratory, USA, F. DEMME, Rutherford Appleton Laboratory, UK, M.C. ARONSON, Stony Brook University and Brookhaven National Laboratory, USA — The antiferromagnetic (AF) metal Yb2Pt2Pb has a layered crystal structure, with Yb ions arranged in chains along the c-axis, while pairs of chains form orthogonal dimers in the tetragonal a-b plane, an in-plane structure that is topologically equivalent to the Shasyu-Sutherland lattice (SSL). In zero magnetic field, 70% of the magnetic spectral weight is static, consisting of AF Bragg peaks corresponding to moments that order at TN = 2.07 K, while fluctuations of the Yb moments, present even at T = 0, are responsible for the remaining 30%. The low energy magnetic excitation spectrum observed in neutron scattering experiments is unambiguously one-dimensional, consisting exclusively of gapped, Heisenberg-like spinons that disperse along the Yb chain direction, while remaining dispersionless in the SSL layers. As field is increased, the static magnetic order is suppressed and a rapidly evolving set of longitudinal modes with dispersions both parallel and perpendicular to the Yb chains is observed, until the Yb moments are fully polarized at fields above 2.3 T. This places Yb2Pt2Pb very near but on the ordered side of the quantum critical point that links quantum mechanical Heisenberg and classical Ising physics in one dimension.


11:15AM G32.00001 Strain driven anisotropic magnetoresistance in antiferromagnetic La0.4Sr0.6MnO3 thin films, T. ZAC WARD, Oak Ridge National Laboratory, A.T. WONG, University of Tennessee, YAYOI TAKAMURA, University of California, Davis, ANDREAS HERKLOTZ, Oak Ridge National Laboratory — Antiferromagnets (AFM) are a promising alternative to ferromagnets (FM) in spintronic applications. The reason stems from the fact that at high data storage densities stray fields could destroy FM set states while AFMs would be relatively insensitive to this data corruption. This work presents the first ever example of antiferromagnetic La0.4Sr0.6MnO3 thin films stabilized in different strain states. Strain is found to drive different types of AFM ordering, and these variations in ordering type are shown to have a profound impact on both the magnitude and character of the materials' resistive response to magnetic field direction, or anisotropic magnetoresistance (AMR) behavior (one standard of spintronic suitability). The compressively strained film shows the highest recorded AMR response in an ohmic AFM device of 63%, while the tensile strained film shows a typical AFM AMR of 0.6%. These findings demonstrate the necessity of understanding electron ordering in AFM spintronic applications and provide a new benchmark for AMR response.

This work was supported by the U. S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division.
11:27AM G32.00002 Magnetic anisotropy and anisotropic damping in LSMO/STO(001). HANKYU LEE, IGOR BARSKOV, LIU YANG, University of California, Irvine, ADRIAN SWARTZ, BONGJU KIM, HAROLD HWANG, Stanford University, ILYA KRIVOROTOV, University of California, Irvine — La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO) is a promising material for spintronics applications due to its half-metallic nature. To successively exploit LSMO, both the anisotropy (MA) and damping need to be well understood and, ultimately, controlled. Here, we study 30 nm epitaxial LSMO thin films grown by pulsed laser deposition on TiO$_2$ terminated (001)SrTiO$_3$. By means of angle- and frequency dependent ferromagnetic resonance (FMR) at room temperature, we separate various contributions to the in-plane MA: i) The four-fold magnetocrystalline anisotropy is present but negligibly small. ii) The strongest contribution $B_{uni} = 4.2$ mT is uniaxial with EA along [010]. While uniaxial MA in LSMO systems is commonly related to terrace formation from the substrate miscut, we find that the terrace direction and the MA symmetry axis do not correlate, indicating a different origin of the MA. By evaluating the FMR linewidth, three nonlinear magnetic damping channels due to the two-magnon scattering are found: j) The dominant four-fold contribution with maxima along $<100>$ axes emerges due to the crystalline defects. jj) A two-fold contribution with the maximum along [010] and jjj) a small two-fold contribution with maximum perpendicular to the terraces are identified.

11:39AM G32.00003 Anisotropic magnetotransport behavior in electronic phase-separated La$_{0.67}$Ca$_{0.33}$MnO$_3$ (LCMO) films under anisotropic strain$^1$. LONGQIAN HU, LIUQI YU, STEPHAN VON MOLNAR, PENG XIONG, Florida State University, LINGFEI WANG, WENBIN WU, University of Science and Technology of China — Anisotropic transport measurements have been performed on LCMO films grown on NdGaO$_3$ (001) substrates. Three samples from a film 48 nm thick were post-annealed for 1.5h, 5h and 20h to produce increasing degrees of anisotropic strain, which promotes electronic phase separation (PS). As demonstrated previously, the presence and growth of antiferromagnetic insulating (AFI) regions in the samples can be controlled by the strain, resulting in a state of coexisting ferromagnetic metallic (FMM) and AFI domains. To study the effects of the strain anisotropy on the PS and formation of the AFI states, we carried out simultaneous magnetotransport measurements along the two orthogonal in-plane directions using an L-bar geometry. Substantial anisotropy in the temperature and magnetic field dependent resistivity between the two directions was observed, implying the formation of the AFI states has an orientation preference under the anisotropic strain. These differences are dramatically enhanced with increasing strain. Furthermore, accompanying the emergence of the AFI states, a glass-like behavior signified by time relaxation was observed in the field-dependent resistivity, which provides new insight into the dynamics of the phase-separated AFI and FMM domains.

$^1$Work supported by NSF grant DMR-1308613

11:51AM G32.00004 Critical thickness for ferromagnetism in LaMnO$_3$ films. HANS HILGENKAMP, MESA+ Institute for Nanotechnology, University of Twente, The Netherlands — We studied LaMnO$_3$ (001) films, deposited by pulsed laser deposition, with thicknesses ranging from 1 unit cell to 24 unit cells. Using Scanning SQUID Magnetic Microscopy, the local magnetization was mapped for these films with micrometer resolution. We find that the magnetic ground state of the films switches sharply from antiferromagnetic to ferromagnetic state when the film thickness exceeds a critical value of 5 unit cells. The films remain electrically insulating. The magnetic transition at the critical thickness is qualitatively explained in terms of an internal electronic reconstruction in the polar LaMnO$_3$ thin films, driven by a polar catastrophe.


12:27PM G32.00005 Tunneling Anisotropic Magnetoresistance with Half-Metallic Electrodes. J .D. BURTON, EVGENY T. TSYPMBAL, University of Nebraska - Lincoln — Tunneling anisotropic magnetoresistance (TAMR) is the difference in resistance of a magnetic tunnel junction due to a change in direction of the magnetization of one or both of the magnetic electrodes with respect to the flow of current, i.e. tunnel magnetization in the plane differs from magnetization out of the plane. The origin of the effect is spin-orbit coupling (SOC). We will present results of first-principles density functional calculations of the TAMR effect in a half-metallic material, i.e., a metal that has free carriers only in one spin channel. In particular we explore the TAMR effect in magnetic tunnel junctions with La$_{0.75}$Sr$_{0.3}$MnO$_3$ (LSMO) electrodes and a SrTiO$_3$ (STO) tunneling barrier. We find ~ 500% difference in resistance between magnetization in the plane and out of the plane. This large TAMR effect originates from the half-metallic nature of LSMO: when magnetization is out-of-plane SOC contributions to the transmission comes only from spin-flip scattering, which is still inherently small due to the half-metallicity. For in-plane magnetization, however, there is a large non-spin-flip SOC contribution to the conductance. The spin-flip vs. non-spin-flip dichotomy along with the orbital character of the states on the Fermi surface of LSMO leads to the large TAMR effect. This effect should be a general feature of half-metallic or highly spin-polarized magnetic electrodes and could open the door to enhanced spintronic device functionalities.

12:39PM G32.00006 Metal-insulator transition at a surface of a ferromagnetic-metal La$_{0.75}$Ca$_{0.3}$MnO$_3$/SrTiO$_3$(100) thin film. ROYTA SHIMIZU, AIMAIR, Tohoku University, SHUNYA NAKAMURA, YASUNOBU ANDO, EMI MINAMITANI, Department of Materials Engineering, The University of Tokyo, KATSUYA IWAYA, RIKEN, AIMAIR in Tohoku University, TAKEO OHSAWA, NIMS, AIMAIR in Tohoku University, SATOSHI WATANABE, Department of Materials Engineering, The University of Tokyo, TAKAO OHSAWA, AIMAIR, Tohoku University, JST-PRESTO — We have performed low-temperature scanning tunneling microscopy/spectroscopy (STM/STS) measurements on a ferromagnetic-metal La$_{0.75}$Ca$_{0.3}$MnO$_3$/SrTiO$_3$(100) thin film surface. Our topographic images show two-domain zigzag patterns with $(\sqrt{2} \times \sqrt{2})$ periodicities in the perovskite structure. In addition, we measured an energy gap at the Fermi level in our STS spectra, in contrast to the ferromagnetic-metal properties obtained by ensemble measurements. First-principle calculations suggest that the topmost zigzag structure is caused by the structural relaxation based on the orthorhombic nature in bulk, suppressing the carrier itinerancy.

12:51PM G32.00007 Magneto-thermoelectric transport in ferromagnetic La$_{2/3}$Sr$_{1/3}$MnO$_3$ thin films$^1$. CONG TINH BUI, FRANCISCO RIVADULLA, University of Santiago de Compostela — La$_{2/3}$Sr$_{1/3}$MnO$_3$ (LSMO) thin films have been widely utilized in spintronics because of its nearly full spin-polarization and high Curie temperature. However, the spin-dependent thermoelectric effects in this material such as spin Seebeck effect (SSE), anomalous Nernst effect (ANE), planar Nernst effect (PNE), which might either interfere the performance of the spintronic devices or be utilized for other potential applications, have not been attended adequately. Herein, we present the observation of PNE and ANE in thin films of LSMO grown epitaxially on SrTiO$_3$ substrate. Through a careful control of the thermal gradients, the ANE can be suppressed and separated from the symmetric PNE response. The observation of sign change of ANE over the temperature, which can be understood in terms of Mott relation between anomalous Nernst and Hall coefficients, leads to the intrinsic scattering mechanism of anomalous Hall effect. We also observe a perfect correspondence between the magneto-thermal effects and their electrical counterparts. Finally, the absolutely comparable ANE and PNE signals using either Pt or Au exclude any contribution from SSE within our resolution limit.

$^1$This research was supported by the European Research Council (ERC StG-259082, 2DTHERMES) and Xunta de Galicia (2012-CP071).
1:03PM G32.00008 Bismuth Manganite Thin Film Characterization. DANIEL PAJEROWSKI, LISA KRAVER, BRUCE RAVEL, JULIE BORCHERS, National Institute of Standards and Technology, HYOUNG JEEN JEEN, Pusan National University, AMLAN BISWAS, University of Florida — We have performed detailed characterization of bismuth manganite (BMO) deposited via pulsed laser deposition onto crystalline strontium titanate. BMO is a ferromagnet that has a pseudo-perovskite structure. Actually, the structure deviates from perovskite depending upon growth conditions, and one important parameter is the oxygen content. Thin films of BMO are interesting because they can show ferroelectricity as well as ferromagnetism, but it is not entirely clear why. Another open question is why BMO films are reported to have much less magnetism than expected, based upon comparative measurements of BMO powders. Neutron reflectometry is useful to interrogate these issues because neutrons are sensitive to oxygen content and polarized neutrons can probe the depth dependence of magnetism. These neutron data are supported by high-resolution transmission electron microscopy, X-ray diffraction, and temperature dependent X-ray absorption studies. By considering these techniques in concert, a consistent model of the film is presented.

1:15PM G32.00009 Epitaxial growth of ultra thin films of electron doped manganites. SRIMANTA MIDDEY, M. KAREEV, D. MEYERS, X. LIU, Y. CAO, S. TRIPATHI, Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, USA, D. YAZICI, M.E. MAPLE, Department of Physics, University of California, San Diego, La Jolla, California 92093, USA, P.J. RYAN, J.W. FREELAND, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA, J. CHAKHALIAN, Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, USA — We report on the fabrication of ultra-thin films of the electron doped manganese in a layer-by-layer growth mode on SrTiO3 (001) substrates by pulsed laser interval deposition. A combination of RHEED (reflection high energy electron diffraction), synchrotron based x-ray diffraction and x-ray absorption spectroscopy measurement confirmed the excellent structural, chemical, and electronic quality. All grown films show a ferromagnetic ground state as revealed by both dc magnetization and x-ray magnetic circular dichroism (XMCD) measurements and remain insulating. The present study opens exciting possibilities of merging this electron doped material with the other hole doped systems to fabricate oxide based spintronic junction.

1:27PM G32.00010 Enhancement of Magnetic Anisotropy in Ultrathin Epitaxial La0.67Sr0.33MnO3 Thin Films via Nanostructure Engineering. ANIL RAJAPITAMAHUNI, LE ZHANG, JOHN BURTTON, VIJAY SINGH, EVGENY TSYMBAL, XIA HONG, University of Nebraska-Lincoln — We report a more than ten-fold enhancement of magnetic anisotropy in nanostructured La0.67Sr0.33MnO3 (LSMO) thin films grown epitaxially on (001) SrTiO3 substrates. We have etched periodic linear trenches in 6 nm LSMO films, and investigated magnetic anisotropy in these nanostructured thin films via the planar Hall effect (PHE). These trenches have depth of 2 nm and periodicities of 200 - 400 nm. The PHE resistance of the un-patterned LSMO films exhibits sinusoidal angular dependence in an in-plane magnetic field, and shows four-fold sharp resistance switching below a critical magnetic field of 400 Oe, corresponding to a biaxial magnetic anisotropy of > 10^5 erg/cm^3 along <110> directions. In the nanostructured samples, we observe an additional two-fold resistance switching feature, which persists in magnetic fields higher than 4000 Oe, corresponding to a uniaxial magnetic anisotropy > 1x10^6 erg/cm^3 along one of the biaxial magnetic easy axes. This significant enhancement of magnetic anisotropy cannot be accounted for by shape anisotropy or a uniform strain modulation. We also discuss the effects of the orientation and periodicity of the nano-trenches on the anisotropy enhancement.

1:39PM G32.00011 ABSTRACT WITHDRAWN —

1:51PM G32.00012 Control of the magnetic properties of LaMnO3 epitaxial thin films grown by Pulsed Laser Deposition1. BENJAMIN MARTINEZ, ICMAB - CSIC, JAUME ROQUETA, ICN2, Institut Catala de Nanociencia I Nanotecnologia, ALBERTO POMAR, LLUIS BALCELLS, CARLOS FRONTERA, ZORICA KONSTANTINOVIC, FELIP SANDIUMENG, ICMAB - CSIC, JOSE SANTISO. ICN2, Institut Catala de Nanociencia I Nanotecnologia, ADVANCED MATERIALS CHARACTERIZATION TEAM, THIN FILMS GROWTH TEAM — LaMnO3 (LMO), the parent compound of colossal magnetoresistance based manganites has gained renewed attention as a building block in heterostructures with unexpected properties. In its bulk phase, stoichiometric LMO is an A-type antiferromagnetic (AFM) insulator (T_N = 140K) with orthorhombic structure that easily accommodate an oxygen excess by generating cationic (La or Mn) vacancies. As a result, a fraction of Mn^{4+} changes to Mn^{4+} leading to a double-exchange mediated ferromagnetic (FM) behavior. In thin films the AFM phase has been elusive up to now and thin films with FM ordering are usually reported. In this work, we have systematically studied the growth process of LaMnO3 thin films by pulsed laser deposition on SrTiO3 (001) substrates under different oxygen partial pressures (PO2). A close correlation between the structure (explored by XRD) and the magnetic properties (SQUID measurements) of the films with PO2 has been identified. At high PO2 FM behavior is observed. In contrast, at very low PO2, the results obtained for unit cell volume (close to stoichiometric bulk values) and magnetic moment (0.2 µB/Mn) strongly indicate antiferromagnetic ordering.

1We acknowledge financial support from the Spanish MINECO (MAT2012-33207).

2:03PM G32.00013 Electrical transport and magnetic properties of epitaxial LSMO films grown on STO substrates1. WEI YUAN, YUELEI ZHAO, TANG SU, QI SONG, WEI HAN, Peking Univ., JING SHI, University of California, Riverside — La0.7Sr0.3MnO3 (LSMO) is a very attractive material for spintronics due to its half-metallic ferromagnetic properties. The LSMO films are epitaxially grown on STO (100) substrates using pulsed laser deposition. The effects of substrate temperature, laser power, oxygen pressure, and annealing on the LSMO growth are systematically investigated by the reflection high energy electron diffraction and atomic force microscopy. Under the optimized growth condition, we have achieved atomically flat LSMO thin films with a wide terrace width of more than 5 micro-meters. The electrical transport properties of LSMO films with various thicknesses ranging from 8 to 20 monolayers are studied by measuring the resistivity as a function of temperature. We find that the growth condition plays an important role in the critical film thickness for the metal-insulator transition and the Curie temperature.

1the Ministry of Science and Technology of China

Tuesday, March 3, 2015 11:15AM - 2:15PM
Session G33 DCMP: Metal Physics: Structural and Mechanical Properties including Alloys and Superalloys
208 - David Parker, Oak Ridge National Laboratory
11:15 AM G33.00001 Bulk Modulus of Spherical Palladium Nanoparticles by Chen-Mobius Lattice Inversion Method\textsuperscript{1}, ESAM ABDUL-HAFIDH, Yanbu University College — Palladium is a precious and rare element that belongs to the Platinum group metals (PGMS) with the lowest density and melting point. Numerous uses of Pd in dentistry, medicine and industrial applications attracted considerable investment. Preparation and characterization of palladium nanoparticles have been conducted by many researchers, but very little effort has taken place on the study of Pd physical properties, such as, mechanical, optical, and electrical. In this study, Chen-Mobius lattice inversion method is used to calculate the cohesive energy and modulus of palladium. The method was employed to calculate the cohesive energy by summing over all pairs of atoms within palladium spherical nanoparticles. The modulus is derived from the cohesive energy curve as a function of particles’ sizes. The cohesive energy has been calculated using the potential energy function proposed by (Rose et al., 1981). The results are found to be comparable with previous predictions of metallic nanoparticles.

\textsuperscript{1}This work is supported by the Royal commission at Yanbu- Saudi Arabia

11:27 AM G33.00002 Using magnetization measurements to detect small amounts of plutonium hydride formation in plutonium metal. C.H. MIELKE, Los Alamos Natl Lab, J.W. KIM, Rutgers Center for Emergent Materials, E-D. MUN, Simon Fraser University; J.P. BAIARDO, A.I. SMITH, S. RICHMOND, J. MITCHELL, D. SCHWARTZ, V.S. ZAPF, Los Alamos National Laboratory — We report the formation of plutonium hydride in 2 at.% Ga-stabilized $\delta$-Pu, with 1 atomic % H charging. We show that magnetization measurements are a sensitive, quantitative measure of ferromagnetic plutonium hydride against the nonmagnetic background of plutonium. It was previously shown that at low hydrogen concentrations, hydrogen forms super-abundant vacancy complexes with plutonium, resulting in a bulk lattice contraction. Here we use magnetization, X-ray and neutron diffraction measurements to show that in addition to forming vacancy complexes, at least 30% of the H atoms bond with Pu to precipitate PuH$_x$, largely on the surface of the sample with $x \sim 1.9$. We observe magnetic hysteresis loops below 40 K with magnetic remanence, consistent with precipitates of ferromagnetic PuH$_{1.9}$.

11:39 AM G33.00003 Influence of van der Waals corrected xc-functional on the anisotropic mechanical properties of coinage metals. JI-HWAN LEE, JONG-HUN PARK, YOUNG-KWANG JUNG, ALOYSIUS SOON, Global E3 Institute and the Department of Materials Science and Engineering, Yonsei University, Seoul 121-749, South Korea — Current materials-related calculations employ the density-functional theory (DFT), commonly using the (semi-)local-density approximations for the exchange-correlation (xc) functional. The accuracy to studying the electronic structure depends not only on the employed approximation to the xc potential but also upon the system which is being investigated. The difficulties in arriving at a reasonable description of van der Waals (vdW) interactions by DFT-based models, is to date a big challenge. This stems from the well-known fact that vDW interaction is a non-local correlation effect which is not captured in the deployed (semi-)local xc functionals. In this work, using various flavours of vdw-corrected DFT xc functionals, we study the lattice and mechanical properties (including the elastic constants and anisotropic stress-strain curves) of the coinage metals (copper, silver, and gold), and critically assess the reliability of the different vdW-corrected DFT methods in describing their anisotropic mechanical properties which are less reported on in the literature.

11:51 AM G33.00004 High-precision study of time- and temperature-dependence of the elastic properties of $^{239}$Pu. B. MAJOROV, B.J. RAMSHAW, Los Alamos National Laboratory, A. SHEKHTER, National High Magnetic Field Laboratory, J.B. BETTS, F. FREIBERT, A. MIGLIORI, Los Alamos National Laboratory — It is important to determine the origin of changes in elastic properties in $^{239}$Pu as a function of time. The measurement of mechanical resonance frequencies can be made with extreme precision and used to compute the elastic moduli without corrections giving important insight in this problem. The precision of these measurements enabled observation of changes in elastic properties of 1 part in 107 for measurements lasting hours up to several days. The most likely source of these changes include a) ingrowth of radioactive decay products such as He and U, b) the introduction of radiation damage, c) phase instabilities associated with transformations to the delta phase or to Pu$_2$Ga. Using Resonant Ultrasound Spectroscopy, measurements were made of the mechanical resonance frequencies of 300mg cylinders of fine-grained polycrystalline alpha-phase $^{239}$Pu with about 600PPM Ga. We present the surprising result that at temperatures below 60K, there is a strong dependence on temperature of the rate of change of elastic moduli with time. Older results showed that the sign of this rate of change reverses at higher temperature. Such studies of nascent state are key to exploring damage evolution and its impact on specific volume and elastic moduli. Future studies will continue these measurements to above ambient temperatures.

12:03 PM G33.00005 First-principles study of energy, structure and atomic solubility of twinning-associated boundaries in hexagonal metals. ANIL KUMAR, JIAN WANG, CARLOS TOME, Los Alamos National Laboratory — HCP metals are widely used as structural materials in many industries, ranging from transport and energy to biomedical applications due to their low density, high specific strength. Twining is one of the important plastic deformation modes in HCP metals. Understanding atomic structure and damage evolution and its impact on specific volume and elastic moduli. Future studies will continue these measurements to above ambient temperatures.

12:15 PM G33.00006 Ti$_{1-x}$Au$_x$ Alloys: Hard Biocompatible Metals and Their Possible Applications\textsuperscript{1}, ETERI SVANIDZE, Rice University, TIGLET BESARA, Florida State University, M. FEVIZI OZAYDIN, Texas A&M, YAN XIN, KE HAN, Florida State University, HONG LIANG, Texas A&M, THEO SIEGRIST, Florida State University, EMILIA MOROSAN, Rice University — The search for new hard materials is often challenging from both theoretical and experimental points of view. Furthermore, using materials for biomedical applications calls for alloys with high biocompatibility which are even more sparse. The Ti$_{1-x}$Au$_x$ (0.22 \leq x \leq 0.8) exhibit extreme hardness and strength values, elevated melting temperatures (compared to those of constituent elements), reduced density compared to Au, high malleability, bulk metallicity, high biocompatibility, low wear, reduced friction, potentially high radio opacity, as well as osseointegration. All these properties render the Ti$_{1-x}$Au$_x$ alloys particularly useful for orthopedic, dental, and prosthetic applications, where they could be used as both permanent and temporary components. Additionally, the ability of Ti$_{1-x}$Au$_x$ alloys to adhere to ceramic parts could reduce the weight and cost of these components.

\textsuperscript{1}The work at Rice was supported by NSF DMR 0847081 (E.M. and E.S.).
12:27PM G33.00007 Ab initio phase stability at high temperatures and pressures in the V-Cr system. ALEXANDER LANDA, PER SODERLING, LIN YANG, Lawrence Livermore National Laboratory — Vanadium metal has seen a surge in research, experimental and theoretical, driven mainly by its importance in applications but also because of its surprising destabilization of the body-centered cubic (bcc) ground-state phase close to 60 GPa. The phase stability of vanadium metal and vanadium-chromium alloys at high temperatures and pressures is explored by means of first-principles electronic-structure calculations. Utilizing the self-consistent ab initio lattice dynamics approach in conjunction with density-functional theory, we show that pressure-induced mechanical instability of body-centered cubic vanadium metal, which results in formation of a rhombohedral phase at around 60 GPa at room temperature, will prevail significant heating and compression. Further, employing the transition state theory at high stabilization of the body-centered cubic phase occurs at elevated pressure. Computing support for this work came from the LLNL Computing Grand Challenge program. This work performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344 and funded by the Laboratory Directed Research and Development Program at LLNL under project tracking code 11-ER-033.

12:39PM G33.00008 Structure and dynamics of bulk liquid iron near melting. A first principles study1. DAVID J. GONZALEZ, MIRIAM MARQUES, LUIS E. GONZALEZ, Dept. Fisica Teorica, Atomica y Optica, Facultad de Ciencias, Universidad de Valladolid, 47011 Valladolid — First principles molecular dynamics simulations, based on the density functional theory and the projector augmented wave technique, have been performed in order to study several static and dynamic properties of bulk liquid Fe at a thermodynamic state near melting. As for the static properties, the obtained results for the pair distribution function and the static structure factor show a good agreement with the available X-ray and neutron diffraction data. The calculated dynamical principle reveals collective density excitations with an associated dispersion relation which closely follows recent experimental data; moreover, its slope at the long-wavelength limit provides an estimate for the velocity of sound. The dynamical structure factors have been calculated and they are compared with their experimental counterparts, which have recently been measured by inelastic X-ray diffraction experiments. Finally, results are also reported for some transport coefficients.

1 We acknowledge support from the Spanish MSI (project FIS2012-33126) and JCyL (grant CIP13/03).

12:51PM G33.00009 Evidence for reentrant strain glass behavior in a ferroelastic-martensitic system Ti-Pd-V. XIAOMING ZHANG, GUIZHOU XU, ENKE LIU, WENHONG WANG, GUANGHENG WU, Institute of Physics, Chinese Academy of Sci (CAS), INSTITUTE OF PHYSICS TEAM — The concept of strain glass (SG) has recently received much attention because of its unique properties such as shape memory effect, superelasticity, and stress-tuned intelligent damping behavior. Recent in-situ TEM experiments have proved that, only local-symmetry change in the crystal structure has been observed during the SG transition, but the macroscopic symmetry of the structure is still not completely uncerntained. In this presentation, we report the discovery of reentrant-strain-glass (RSG) behavior in a ferroelastic-martensitic system Ti50Pd50-Vx (x is from 6 to 12). Unlike the SG, with decreasing of temperature, the RSG system first undergoes a macroscopic martensitic transition and then the martensite variants further transforms to a frustrated glassy state below a critical temperature. The X-ray diffraction and high resolution TEM results further indicate the RSG no longer remains the average structure of the high-temperature parent phase, but rather low-temperature martensitic phase. This new discovery may open a new research field and may lead to new insights into a range of possible applications of this unique class of materials.

0:03PM G33.00010 Studying the enhanced ductility in bimodal nanocrystalline metals using a model with tunable crystallinity and crystallite stiffness. GUO-JIE JASON GAO, Department of Mechanical Engineering, National Taiwan University, YUN-JIANG WANG, Institute of Mechanics, Chinese Academy of Sciences, SHIGENOBU OGATA, Department of Mechanical Science and Bioengineering, Osaka University — We propose a polycrystalline model composed of small and large particles, where crystallinity and stiffness of each crystallite can be separately tuned by varying the number ratio of small/large particles [H. Shiba et al., Phys. Rev. E. 81, 051501 (2010)], and implementing 2D molecular dynamics (MD) simulations to study the shear deformation of the model consist of stiff crystallites, soft crystallites, or stiff and soft crystallites. We find the flow stress increases monotonically with increasing crystallite stiffness, and it can be systematically adjusted via changing the ratio of soft/stiff crystallites. We address the application of our results to study the enhanced ductility found in bimodal nanocrystalline metals, where shear localization and propagation are presumably weakened due to crystallites of two properties.

1:15PM G33.00011 Magnetic and Structural Properties in Non-Stoichiometric Gallium Deficient Ni2MnGa1−x Heusler Alloys, IAN FERRALLI, ANTHONY RUFFINO, MICHAEL PIERCE, LINDA BARTON, Rochester Institute of Technology — Magnetic data show that off-stoichiometric gallium deficient Heusler alloys of the form Ni2MnGa1−x have martensite transition temperatures that increase strongly with x, while their ferromagnetic Curie temperatures remain nearly unchanged. The martensite transition approaches room temperature for x = 0.13. Within the tetragonal martensite phase, bulk magnetic properties depend strongly on stresses within the sample. These effects were investigated using neutron and X-ray diffraction and neutron scattering experiments. These treatments effect the bulk coercivity but do not move the transition temperatures. As the martensite forms, lattice elongations of >3% are observed using XRD. Domain properties are reported, for both structural grains and magnetic ones, within the martensite phase, from optical and MFM imaging.

1:27PM G33.00012 A search for new cobalt-based high temperature superalloys. CHANDRAMOULI NYSHADHAM, JACOB HANSEN, Brigham Young University, STEFANO CURTAROLO, Duke University - Center for Materials Genomics, GUS L.W. HART, Brigham Young University — The discovery of a high temperature Co0.5Al0.5W [1] superalloy has provided a promising avenue for further search of other Co-based superalloys. The L12 Co0.5Al0.5W system is found to have higher strength and melting temperature than common Ni-based alloys. The high strength of super alloys is generally attributed to the stable or metastable austenitic face-centered cubic crystal structure. We performed an extensive series of ab-initio calculations to search for stable or metastable Co-based ternary alloys of the form Co5Al5W5. A 32 atom cell special quasi random structure (SQS-32) is considered to mimic the properties of the alloy at high temperatures. The DFT calculations for over 780 different Co-based ternary systems and the potential candidates of the future high temperature super alloys is presented.


1:39PM G33.00013 Ab Initio Investigation of He Bubbles at the Y2Ti2O7-Fe Interface in Nanostructured Ferritic Alloys, CELINE HIN, THOMAS DANIELSON, Virginia Tech — Nanostructured ferritic alloys are promising materials candidates for the next generation of nuclear reactors due to their ability to withstand high temperatures and pressures, high neutron flux and especially, the presence of high concentrations of transmutation product helium. As helium diffuses through the matrix, large number densities of complex oxide nanoclusters act as trapping sites for individual helium atoms and helium clusters. Consequently, there is a significant decrease in the amount of helium that reaches grain boundaries, mitigating the threat of pressurized bubble formation and embrittlement. In order to understand the trapping phenomena of the oxides, the interface between the nanoclusters and the iron matrix must be modeled. We present results obtained using density functional theory on the structural and thermodynamic properties of the Y2Ti2O7-Fe interface containing helium. In addition, helium bubbles of varying sizes have been introduced in order to observe the effects of a growing helium bubble.
it is unclear how coverage efficiency competes with mechanical cost as thickness is decreased, and what wrapping shapes will emerge. We place a thin (hampered by the mechanical cost of bending the sheet. Thinner sheets deform more readily by forming small-scale wrinkles and stress-focussing patterns, but

D´EMERY, BENNY DAVIDOVITCH, CHRISTIAN SANTANGELO, THOMAS RUSSELL, NARAYANAN MENON, Univ of Mass - Amherst — A liquid drop using a thin enough sheet results in maximal coverage. gross shape, which neglects small-scale features, is correctly predicted by a simple geometric approach wherein the exposed area is minimized. Thus, simply

emerge: Oscillations, slowed relaxation and even the formation of wrinkles and extrusions. We characterize these phenomena and propose explanations. dynamics of such bubbles using high-speed video recordings. Peculiar dynamics intermediate between those of simple viscous fluid films and an elastic response

membranes (e.g. vesicles). Due to their layered phase structure, smectic liquid crystals can form stable, uniform and easy-to handle fluid films of immense aspect properties except surface tension are often neglected for simple fluid films (e.g. soap bubbles), whereas they govern the dynamics in systems with more complex membranes (e.g. vesicles). Due to their layered phase structure, smectic liquid crystals can form stable, uniform and easy-to handle fluid films of immense aspect ratios. Recently, freely floating bubbles detached from a support were prepared. We analyze the relaxation from strongly non-spherical shapes and the rupture dynamics of such bubbles using high-speed video recordings. Peculiar dynamics intermediate between those of simple viscous fluid films and an elastic response emerge: Oscillations, slowed relaxation and even the formation of wrinkles and extrusions. We characterize these phenomena and propose explanations.

1 Supported by the US DOE under Contract No. DEAC02-05CH11231 under the Materials Project Center grant (award no. EDCBEE).


RADHAKRISHNA T G, ANIL VIR, JASON PICARDO, PUSHPAVANAM SUBRAMANIAM, Indian Institute of Technology Madras — In this work, the effect of Marangoni flows on mass transfer is investigated for stratified flow of two immiscible liquids in a microchannel. Experiments involving reactive extraction of carboxylic acids from organic phase using aqueous sodium hydroxide are performed. Often in analysis, the liquid-liquid interface is assumed to be flat. However, a deforming interface was observed for certain flow rate ratios. The conditions under which the interface deforms are determined. The experiments are complemented with mathematical modeling and simulation. Navier-Stokes equation and transport equation are simplified using the lubrication approximation and an approximate solution is obtained. The interphase mass transfer and hydrodynamics are coupled through the shear stress boundary condition. In cases where the interface is flat, the transport equation is solved numerically using finite difference method. In cases where the interface deforms, the evolution of interface is captured using kinematic boundary condition and the transport equation is solved numerically.

1 This work is supported by China Scholarship Council (Grant No. 201306020117) and DOE-BES (Grant No. DEFG02-04ER46148).

11:27AM G34.00002 Radiation Pressure Induced Nonlinear Optofluidics in Liquid Droplets1, 2, PENG ZHANG, SUNGHWAN JUNG, Department of Biomedical Engineering and Mechanics, Virginia Tech, Blacksburg, VA 24060, YONG XU, ARAM LEE, Department of Electrical and Computer Engineering, Virginia Tech, Blacksburg, VA 24060 — In the present study, we analyze a nonlinear optofluidic process associated with a high quality (Q) factor whispering gallery mode (WGM) in liquid droplets. Optical radiation pressure induced droplet deformation can produce a frequency shift proportional to the WGM power. Droplet deformation will be obtained both theoretically and numerically by boundary element method. We will show that the nonlinear optofluidic effect is stronger than temperature-induced nonlinearity. Using liquid properties that are experimentally attainable (e.g., oil drop in water), we find that measurable WGM resonance shift may be generated by only a few photons. This technique may also lead to the possibility of fluid viscosity and interfacial tension measurement by non-destructive optical forces.

11:39AM G34.00003 From viscous to elastic sheets: Dynamics of smectic freely floating films1, 2, KIRSTEN HARTH, KATHRIN MAY, TORSTEN TRITTEL, RALF STANNARIUS, Otto von Guericke University Magdeburg — Oscillations and rupture of bubbles, composed of an inner fluid separated from an outer fluid by a membrane, represent an old but still immensely active field of research. Membrane properties except surface tension are often neglected for simple fluid films (e.g. soap bubbles), whereas they govern the dynamics in systems with more complex membranes (e.g. vesicles). Due to their layered phase structure, smectic liquid crystals can form stable, uniform and easy-to handle fluid films of immense aspect ratios. Recently, freely floating bubbles detached from a support were prepared. We analyze the relaxation from strongly non-spherical shapes and the rupture dynamics of such bubbles using high-speed video recordings. Peculiar dynamics intermediate between those of simple viscous fluid films and an elastic response emerge: Oscillations, slowed relaxation and even the formation of wrinkles and extrusions. We characterize these phenomena and propose explanations.

1 This research was partially supported by the National Science Foundation (CBET 1438112)

11:51AM G34.00004 Thin sheets achieve optimal wrapping of liquids 1, JOSEPH PAULSEN, VINCENT DÉMERY, BENNY DAVIDOVITCH, CHRISTIAN SANTANGELO, THOMAS RUSSELL, NARAYANAN MENON, Univ of Mass - Amherst — A liquid drop can wrap itself in a sheet using capillary forces [Py et al., PRL 98, 2007]. However, the efficiency of “capillary origami” at covering the surface of a drop is hampered by the mechanical cost of bending the sheet. Thinner sheets deform more readily by forming small-scale wrinkles and stress-focussing patterns, but it is unclear how coverage efficiency competes with mechanical cost as thickness is decreased, and what wrapping shapes will emerge. We place a thin (~ 100 nm) polymer film on a drop whose volume is gradually decreased so that the sheet covers an increasing fraction of its surface. The sheet exhibits a complex sequence of axisymmetric and polygonal partial, and fully- wrapped shapes. Remarkably, the progression appears independent of mechanical properties. The gross shape, which neglects small-scale features, is correctly predicted by a simple geometric approach wherein the exposed area is minimized. Thus, simply using a thin enough sheet results in maximal coverage.
12:15PM G34.00006 Simple analytical model of evapotranspiration in the presence of roots. CESARE CEJAS, Laboratoire Microfluidique, MEMS, Nanostuctures (MMN), ESPCI, Paris, JEAN-CHRISTOPHE CASTAIN, Solvay Research and Innovation Centre-Aubervilliers, LARRY HOUGH, CNRS Complex Assemblies of Soft Matter COMPASS (UM13254), CHRISTIAN FREITIGNY, CNRS Sciences et Ingenerie de la Matiere Mole (SIMM) UMR7615, REMI DREYFUS, CNRS Complex Assemblies of Soft Matter COMPASS (UM13254), COMPASS TEAM — Water is essential for plant growth. The loss of water via evaporation in soil remains to be an important limiting factor for root growth and consists of well-debated mechanisms. The presence of a plant also provides an additional pathway for water transport in the form of transpiration. Prediction of total evapotranspiration flux permits estimation of the remaining quantity of water in the soil. Using a controlled visual 2D model set-up, we perform evaporation experiments with real root systems under different relative humidity conditions. We use the results on mass loss and evaporation front positions to develop a simple model, based on basic principles of evaporation flux, which predicts the position of the evaporating front and the total mass of water that is lost from the evapotranspiration of water out of the granular medium. The model also helps predict the lifetime of the plant — an important application in agriculture.

12:27PM G34.00007 Growth and densification of frost around a circular cylinder under humid air on cross flow1. VICTOR MADRID, FAUSTO SANCHEZ, SIMON MARTINEZ, ARTURO MORALES, UNIVERSIDAD AUTONOMA DE NUEVO LEON, FIME — Formation, growth and densification of frost around a circular cylinder under humid air on cross flow at different Reynolds numbers has been numerically studied using the finite volume method. The frost formation phenomenon takes place when humidity goes through a desublimation phase change at a temperature lower than its solidification point. Continuity, momentum, energy and mass transport equations have been solved for a whole domain including both phases, gas and solid, and the two components in the gas phase, i.e. dry air and humidity. The mass of water that goes from the gas to the solid phase is used as a source term in the mass conservation equation for solid phase and as a sink for the gas phase, affecting source terms in all the other conservation equations (energy and momentum) also. A volume of fraction conservation equation for solid phase is used to obtain local fractions of ice droplets, considering formally as frost those fraction values greater than a critical value. Once those local fractions are known, local frost properties such as density and thermal conductivity can be calculated as functions of the phase fraction allowing to compute the evolution of growth and local properties of frost.

12:39PM G34.00008 Parallel magnetic resonance imaging of gas-liquid flows. CHRISTOPH MUELLER, Laboratory for Energy Science and Engineering, ETH Zurich, ALEXANDER PENN, Laboratory for Energy Science and Engineering, ETH Zurich and Institute for Biomedical Engineering, University and ETH Zurich, KLAAS P. PRUESSMANN, Institute for Biomedical Engineering, University and ETH Zurich — Gas-liquid flows are commonly encountered in nature and industry. Experimental measurements of gas-liquid flows are challenging since such systems can be visually opaque and highly dynamic. Here we report the implementation of advanced magnetic resonance imaging (MRI) strategies allowing us to probe the dynamics (voidage and velocity measurements) of gas-liquid flows with ultra-fast acquisition speeds. Specifically, parallel MRI which exploits the spatial encoding capabilities of multiple receiver coils was implemented. To this end a tailored, 16 channels MR receive array was constructed and employed in the MR acquisition. A magnetic susceptibility matched gas-liquid system was set-up and used to probe the motion, splitting and coalescence of bubbles. The temporal and spatial resolution of our acquired data was 5 ms and 3.5 mm x 3.5 mm, respectively. The total field of view was 200 mm x 200 mm. We will conclude with an outlook of future possible additional advances in MRI that have the potential to reduce substantially the acquisition time, providing flexible gains in temporal and spatial resolution.

12:51PM G34.00009 Air flows generated by an impacting drop. IRMGARD BISCHOFBERGER, Univ of Chicago, BAHNI RAY, TAEHUN LEE, JEFF MORRIS, CCNY, SIDNEY R. NAGEL, Univ of Chicago, UNIVERSITY OF CHICAGO COLLABORATION, CCNY COLLABORATION, — A drop impacting a solid surface with sufficient velocity will splash and emit many small droplets. Lowering the ambient air pressure suppresses splashing completely. This effect, robustly found for different liquid and substrate properties, raises the fundamental question of how air affects a spreading drop. We visualize the air induced capillary waves which sharpen a collision front. Computers with high-speed video imaging. Comparison with the air flow created by an impacting solid sphere allows us to decouple the vorticity components of the falling drop from that of the spreading liquid. Our studies reveal the emergence of vorticity on two length scales. On larger scales, the airflow induced in the drop’s wake leads to vortex structures due to interaction with the substrate. On smaller scales, the spreading of the drop generates a vortex ring above the outer edge of the spreading liquid. We show that this vorticity generation is governed by a balance between inertial and viscous forces.

1:03PM G34.00010 Flow reversing in the gas layer in droplet impact. ZHEN JIAN, PASCAL RAY, CHRISTOPHE JOSSENRAND, STEPHANE ZALESKI, Univ Pierre et Marie Curie — Recent numerical and experimental studies demonstrated the crucial role of surrounding gas in droplet impact. While the high pressure and high temperature gas effect in droplet splashing is still far from a crystal clear comprehension, Complicated dynamics occur in a small temporal and spatial scale before direct contact with the target surface, which are related to the origin of the splashing. Direct numerical simulations were executed with a code called Gerris for both droplet impact on a liquid surface and on a solid substrate. New dynamics in the gas layer between the droplet and the target surface were discovered. Unexpectedly, a “reversing” gas flow (towards the center) is observed as the droplet approaches the target surface. With further descending of the droplet, the flow is reversed and evacuates towards the outside. The reversing of the flow motion direction is followed by the pressure jump and the dimple formation which have been reported as some crucial gas dynamics in droplet splashing mechanism in our previous work. An aerodynamic mechanism is proposed for the flow reversing dynamics.

1:15PM G34.00011 Simulation of splashing of micro-scale droplets on a dry surface. ARNOUT BOELENS, ANDRZEJ LATKA, CACEY STEVENS, JUAN DE PABLO, University of Chicago — Results are presented for the simulation of micro-scale droplets splashing on a dry surface. The simulations are performed using a Volume Of Fluid approach and a Finite Volume technique. The contact line is described using a Generalized Navier Boundary Condition with a dynamic microscopic contact angle. Both the gas phase and the liquid phase are assumed to be incompressible. The results of these simulations show good agreement with experiments. Independent of the wetting properties of the surface, simulations reveal the formation of a liquid sheet with an apparent contact angle approaching 180 degrees. This liquid sheet breaks up into smaller droplets as the spreading progresses. When the pressure of the system is reduced, the droplet does not break up and splashing is suppressed. Depending on the velocity with which the contact line moves, different flow regimes are observed. One of these regimes involves air bubbles becoming entrained in the liquid phase, similar to what is observed during wetting failure in coating processes. Mesh resolution is critical to describe contact line behavior, liquid sheet formation, and to reproduce the effect of pressure. In this work, the resolution is of the order of 10 nm, and the droplets are several hundred microns large.
1:27PM G34.00012 Comparison of splashing of low- and high- viscosity liquids . CACEY STEVENS, ANDRZEJ LATKA, SIDNEY NAGEL. The James Franck Institute and Department of Physics, University of Chicago — The splash of a liquid drop on a dry surface was shown to be suppressed at low ambient air pressure [1-3]. However the mechanism by which air causes a drop to splash remains unresolved. This is further complicated by the finding that there are two distinct splashing regimes that depend on the viscosity of the liquid. Accordingly, we determine the evolution of splashing at both low and high viscosities. A high-viscosity drop splashes by emitting a thin sheet of liquid from the spreading drop long after it has first contacted the solid. This film subsequently breaks up into smaller droplets to form the splash. We have found that there is also a delay in the ejection of a thin sheet when a low-viscosity drop splashes. This suggests a common mechanism of delayed thin sheet ejection for splashing in both viscosity regimes. We also show how the ejection time of the thin sheet depends on liquid viscosity and ambient air pressure. [1] L. Xu, W. W. Zhang, and S. R. Nagel, Phys. Rev. Lett., 94(18), 184505 (2005). [2] L. Xu, Phys. Rev. E, 75(5), 056316 (2007). [3] A. Latka et. al., Phys. Rev. Lett., 109(5), 054501 (2012).

1:39PM G34.00013 Force response of actively deformed microdroplets: dependence on the solid/liquid boundary condition . JONAS HEPPPE, INM - Leibniz Institute for New Materials and Saarland University, Experimental Physics, D-66123, Saarbruecken, Germany, JOSHUA D. MCGRAW, Saarland University, Experimental Physics, D-66123, Saarbruecken, Germany, ROLAND BENNEWITZ, INM - Leibniz Institute for New Materials, D-66123, Saarbruecken, Germany, KARIN JACOBS, Saarland University, Experimental Physics and INM, D-66123, Saarbruecken, Germany — In fluid dynamics, the solid/liquid boundary condition can play a major role in the flow behavior of a liquid. For example, in the dewetting of identical polymer films on weak slip or strong slip substrates, large qualitative and quantitative differences are observed. Therefore, when applying an external load to a liquid resting on such substrates, the measured reaction forces and the ensuing flow should also depend on the boundary condition. We present atomic force microscopy measurements in which the reaction force of a cantilever is measured as the tip pierces liquid polymer micro sized droplets and films. These indentations are done on substrates with tuned slip. Accessing the size, depth and rate dependence of the resulting force distance curves, we show an influence of the slip condition on the dissipated energy and adhesion.

1:51PM G34.00014 Lyapunov Based Predictions of Droplet Shapes in Thermocapillary Driven Nanofilms , ZACHARY NICOLAOU, SANDRA TROAIN, California Institute of Technology, MC 128-95, Pasadena, CA — Previous work in our group has focused on the spontaneous formation of pillar arrays in nanoscale molten films subject to an extremely large transverse thermal gradient. The shape of these formations is influenced by the relative strength of thermocapillary to capillary forces which is strongly dependent on the system geometry, fluid properties, magnitude of the initial thermal gradient, and whether volume is conserved or not. Here we examine the parameter regime corresponding to steady state shapes resembling either isolated or extended sinusoidal-like waveforms. The stability of these one dimensional and axisymmetric shapes is investigated by a combination of Lyapunov analysis, asymptotic techniques and numerical simulations. Our findings indicate that radially symmetric arrays with small peak heights are linearly stable to perturbations. The existence of such stable states for parameter values accessible to experiment offers an intriguing route for non-contact fabrication of optical and photonic components.

2:03PM G34.00015 Improved Measurement of the 3D Dominant Mode Wavelength in NanoBénard Instability . KEVIN FIEDLER, SANDRA TROAIN, California Institute of Technology, MC 128-95, Pasadena, CA — Molten nanofilms exposed to an initial uniform and very large transverse thermal gradient ($10^5$ to $10^7$ C/cm) are prone to spontaneous formation and growth of nanopillars typically separated by tens of microns or less. Linear stability analysis of the corresponding interface equations suggest these formations result either from electrostatic attraction between the molten film and proximate substrate due to fluctuation induced surface image charge or fluctuation induced thermocapillary forces leading to 3D Bénard-like structures. In this talk, we discuss a number of improvements to our original experimental system including image analysis of structure formation at much earlier times. Our current measurements indicate even closer agreement with the thermocapillary mechanism proposed.

Tuesday, March 3, 2015 11:15AM - 2:03PM — Session G35 DAMOP: Dipolar Gases, Rydberg Atoms, Cold Molecules, and Few-body Systems 210B - Colin Parker, University of Chicago

11:15AM G35.00001 Roton phenomena and stability properties of dipolar condensates . ALEKSEY FEDOROV, Russian Quantum Center, IGOR KURBAKOV, YURIII LOZOVIK, Institute of Spectroscopy RAS — Experimental and theoretical studies of novel quantum phenomena in dipolar systems have a great impact for atomic physics. These systems provide an interface between physics of strongly and weakly correlated matter. Being typical for strongly correlated systems, the roton-maxon excitation spectrum, originally observed in superfluid helium, occurs to appear in a weakly interacting dipolar gas. Due to the contribution, two dipolar bosonic systems are under consideration: dipolar excitons in semiconductor layers of heterostructures and tilted dipolar particles in a quantum layer. In weak correlation regime, we predict a generation of the roton-maxon excitation spectrum for BEC of dipolar excitons in a semiconductor layer. We discuss observation of the roton-maxon spectrum for exciton BEC in GaAs heterostructures. We calculate the stability diagrams for 2D tilted bosonic dipolar particles in a quantum layer. Breaking of the rotational symmetry for a system of tilted dipoles leads to the appearance of optical and photonic components.

11:27AM G35.00002 Dipolar Quasi-2D Bosons with Non-zero Dipole Tilt Angle . PENGTAO SHEN, KHANDKER QUADER, Department of Physics, Kent State University, Kent, OH 44242 — We study properties of dipolar bosons in quasi-2D geometry, with dipoles oriented at an angle to the direction perpendicular to the confining 2D plane. Starting from time-dependent Gross-Pitaevskii equations, and the resulting Bogoliubov-de Gennes equations, we calculate the excitation spectrum of the Bose-Einstein condensate, and explore possible instabilities of the system as the tilt angle, system density and the relative strength of the dipole-dipole interaction are varied. We study how the depletion of the condensate varies with respect to these parameters. We also explore the effect of the anisotropic dipolar interaction on results in different momentum directions.

1A.K.F. is supported by the Dynasty Foundation fellowship
11:51AM G35.00004 Competing instabilities of a Dipolar Fermi Gas, AHMET KELES, George Mason University, University of Pittsburgh, ERHAI ZHAO, George Mason University — Recent experiments in the cold atom Fermi gas have explicitly shown the deformation of the Fermi surface in the presence of long range dipolar interactions. Motivated by this, we investigate the competing instabilities of a dipolar Fermi gas within the functional renormalization group approach. We analyze the flow of the effective action in the particle-particle as well as particle-hole channel, consider the self energy term, and discuss the interplay of different instabilities at low temperatures.

12:15PM G35.00006 Photonic Controlled-Phase Gate Based on Rydberg Interactions, MOHAMMADSADEGH KHAZALI, KHAMAT HESHAMI, CHRISTOPH SIMON, Institute for Quantum Science and Technology, University of Calgary — Photons are ideal carriers of information in quantum communication. Since they do not interact, the implementation of deterministic photonic quantum computation depends on the creation of a non-permanent strong interaction between single photons. The implementation of neutral Rydberg atom gates inspired the development of photonic gates, using the coherent reversible mapping of the quantum states of photons onto highly interacting Rydberg atoms. Here we propose an interaction-based two-qubit gate between photons stored in Rydberg levels of an atomic ensemble. We perform a detailed study of errors due to the many-body interaction between Rydberg spin-waves, and we propose a compensation scheme for these errors. Furthermore we completely separate interaction and propagation by eliminating the Rydberg level from the storage process. Our proposed controlled-phase gate can achieve 99% fidelity with current technology.

12:27PM G35.00007 Rydberg Impurity Probes in Ultracold Gases, MARK MITCHISON, Imperial College London, TOMI JOHNSON, National University of Singapore, University of Oxford, MARTIN PLENIO, Universität Ulm, Imperial College London, DIETER JAKSCH, University of Oxford, National University of Singapore — Impurities immersed in ultracold gases can act as highly sensitive, tunable and potentially non-destructive probes of their environment. In this setting, we propose the use of an atomic impurity in a Rydberg state to measure density fluctuations via Ramsey interferometry. The rapid collisional dynamics of the light Rydberg electron interacting with the heavy gas particles, combined with the capability to quickly change the state of the impurity with optical pulses, make such a probe ideal for measuring local properties of ultracold gases. Our proposed device promises angle-resolved density measurements with sub-micron spatial resolution, and with no need to integrate over the line of sight. We outline how Rydberg impurity probes could be applied to study various interesting quantum states of current experimental relevance. We also discuss the possibility of using multiple Rydberg atoms to extract the spatial pair distribution function \( g^{(2)}(r) \). Our work is placed in the context of other recently proposed impurity-based probes.

12:39PM G35.00008 Revealing the origin of super-Efimov states in the hyperspherical formalism, CHAO GAO, Institute for Advanced Study, Tsinghua University, Beijing 100084, China, JIA WANG, Department of Physics, University of Connecticut, STORRS, CONNECTICUT 06269 USA, ZHENHUA YU, Institute for Advanced Study, Tsinghua University, Beijing 100084, China — Quantum effects can give rise to exotic Borromean three-body bound states even when any two-body subsystems can not bind. An outstanding example is the Efimov states for certain three-body systems with resonant s-wave interactions in three dimensions. These Efimov states obey a universal exponential scaling that the ratio between the binding energies of successive Efimov states is a universal number. Recently a field-theoretic calculation predicted a new kind of universal three-body bound states for three identical fermions with resonant p-wave interactions in two dimensions. These states were called "super-Efimov" states due to their binding energies \( E_n \approx E_0 \exp(-2e^{\nu_0/n_0+\phi}) \) obeying an even more dramatic double exponential scaling. The scaling \( \phi_0 = 4/3 \) was found to be universal while \( E_0 \) and \( \theta \) are the three-body parameters. Here we use the hyperspherical formalism and show that the "super-Efimov" states originate from an emergent effective potential \(-1/4\rho^2-(\kappa_0+1/4)/\rho^2\ln^2(\rho)\) at large hyperradius \( \rho \). Moreover, our numerical calculation indicates that the three-body parameters \( E_0 \) and \( \theta \) are also universal for pairwise interparticle potentials with a van der Waals tail.

12:51PM G35.00009 Three-body scattering hypervolume for bosons with two-body repulsive Gaussian potentials, SHANGGUO ZHU, SHINA TAN, Georgia Inst of Tech — It has been known that the three-boson low energy effective interaction influences the dynamic and the static properties of many bosons, including the ground state energy of a dilute Bose-Einstein condensate. The three-body scattering hypervolume, which is a three-body analogue of the two-body scattering length, characterizes this effective interaction. For bosons with two-body repulsive Gaussian potentials, we determine the scattering hypervolume by solving the three-body Schrödinger equation numerically, and matching the solution with the asymptotic expansions for the wave function at large hyperradii.
or simply by the interfaces themselves, effects a splitting in the topological degeneracy which generally scales as $L^2$, where $L$ is the size of the system and $K$ is the Luttinger parameter. However, when the interfaces are sufficiently smooth, as in the case of a harmonic confining potential, the splitting becomes exponentially small in the system size. We also discuss the experimental implications of the novel ground state degeneracy, as manifest for example in the response to simple dipole modulations of the harmonic trap potential.

1:15PM G35.00011 Few Body Physics in Synthetic Dimensions with SU(N) Interactions\(^1\), SUDEEP K. GHOSH, UMESH K. YADAV, VIJAY B. SHENOY, Department of Physics, Indian Institute of Science — Cold atomic systems with SU(N) symmetric interactions have been of recent experimental and theoretical interest. Motivated by this, we study few body physics in such systems which also realize synthetic dimensions (Celi et al., PR Letters 112, 043001) within the cold atom setting by coupling the atomic hyperfine states via light. Choosing the light appropriately also provides ability to control magnetic flux in the plaquettes of the synthetic lattice. Using a combination of exact diagonalization and analytical methods, we uncover the novel physics that emerges in the interplay of non-local interactions in synthetic dimensions and the magnetic flux. Attractive SU(N) interactions, in absence of flux, obtains a sequence of many-particle “baryonic” bound states. We show how the presence of flux stabilizes a different sequence of baryonic states, presenting a detailed few body phase diagram. We also discuss consequences of our findings to the many body setting, pointing out the novel phases that can be realized in these systems. These results will be of interest to both experimentalists (suggesting systems with novel physics), as well as theorists for exploring the novel phases realized.

\(^1\)S.K.G. acknowledges support from CSIR, India via SRF grants. U.K.Y. acknowledges support from UGC, India via Dr. D.S. Kothari Post-doctoral Fellowship scheme. V.B.S. is grateful to DST, India and DAE, India (SRC grant) for generous support.

1:27PM G35.00012 A microwave trap for sympathetic cooling of polar molecules\(^1\), DEVIN DUNSEITH\(^2\), STEFAN TRUPPE, RICHARD HENDRICKS, BEN SAUER, EDWARD HINDS, MICHAEL TARBUTT, Imperial College, London — We have been developing techniques to cool molecules into the microkelvin regime. One method is to use sympathetic cooling, using ultracold atoms as a refrigerant to cool molecules. Previous work has suggested that atoms and molecules can be trapped in the antinode of a Fabry-Perot microwave cavity. We couple microwave power into this cavity from a rectangular waveguide via a small hole in one mirror. We have developed an analytical model that helps us understand this coupling, and gives us an idea of how the size of the hole affects the cavity's coupling and finesse. We carried out finite-difference time-domain simulations and performed experiments on a prototype cavity to verify this model. We have now designed and built this trap for operation under ultra high vacuum, with the ability to cool the mirrors to 77 K and couple in up to 2 kW of microwave power. This will allow us to trap molecules with a moderate dipole moment at temperatures of hundreds of millikelvin, as well as atoms at a few millikelvin. We will present our work in creating and understanding the microwave trap, as well as our first results demonstrating trapping of lithium atoms in the microwave trap.

\(^1\)The authors would like to thank EPSRC for supporting this work.

\(^2\)The first two authors contributed equally

1:39PM G35.00013 Hybrid Decelerator for Cold Molecular Beams, IGOR LYUKSYUTOV, Texas A&M University — We shall discuss design, simulation and operation of the hybrid decelerator to produce cold molecules. Hybrid decelerator is a combination of the counter rotating source of slow molecular beam with the single stage magnetic decelerator. We operate counter rotating source which provide intense beam of molecules/atoms with the speed smaller than 50 m/s. This beam can be a source for the single stage magnetic decelerator. For example, by decreasing the molecular oxygen speed with mechanical decelerator down to 50 m/s, one can use a single stage magnetic decelerator with a maximum current less than 360 A, to decrease the speed of oxygen molecules to about 2 m/s. Thus, the use of the magnetic stage in hybrid magneto-mechanical decelerator, can provide slow molecular beams with high intensity.

1:51PM G35.00014 Ultracold nonreactive molecules in an optical lattice, ANDRIS DOCAJ, Rice University, MICHAEL L. WALL, JILA, NIST, CU-Boulder, KADEN R.A. HAZZARD, Rice University — Nonreactive (NR) ultracold molecules in optical lattices are free from the two-body losses that occur in chemically reactive molecules, opening up new possibilities for quantum science. Despite the absence of chemical reactions, NR molecules scatter in extremely complex ways – not captured by a delta function pseudopotential – due to the enormous number of rotational and vibrational states. We calculate the bound state energies of two NR molecules confined to a single site of an optical lattice, as a first step towards deriving an effective lattice model that can describe many molecules in a lattice. To describe the short-range collisional properties, which are presently experimentally unknown, we employ random matrix theory. However, our formalism is capable of handling arbitrary short-range collisional physics.

Tuesday, March 3, 2015 11:15AM - 2:15PM
Session G36 DAMOP: Topological Phases and Majorana Fermions in Cold Atoms

11:15AM G36.00001 Topological States in a One-Dimensional Fermi Gas with Attractive Interactions, JONATHAN RUHMAN, EREZ BERG, EHUD ALTMAN, Weizmann institute of science — We show that a single one-dimensional Fermi gas with Rashba-like spin-orbit coupling, a Zeeman field and intrinsic attractive interactions exhibits a novel topological superfluid state, which forms in spite of total number conservation and the absence of a single particle gap. Topological ground state degeneracy is associated with interfaces between two distinct phases that naturally form in the harmonic confining potential due to the spatial variations of the chemical potential. We find that backscattering by impurities, or simply by the interfaces themselves, effects a splitting in the topological degeneracy which generally scales as $1/L^{K/2}$, where $L$ is the size of the system and $K$ is the Luttinger parameter. However, when the interfaces are sufficiently smooth, as in the case of a harmonic confining potential, the splitting becomes exponentially small in the system size. We also discuss the experimental implications of the novel ground state degeneracy, as manifest for example in the response to simple dipole modulations of the harmonic trap potential.

11:27AM G36.00002 One-dimensional topological chains in two-dimensional non-topological optical lattices\(^1\), LEI JIANG, CHUANWEI ZHANG, University of Texas at Dallas — Majorana fermions appear near the topological phase boundary. In 2D, Majorana fermions are found when vortices, which stand for topological defects, are formed in topological superfluids. Due to the complications to generate 2D topological superfluids in experiments, Majorana fermions are not easily achievable in 2D systems. In our work, we show, by imprinting 1D local potentials in a finite 2D system, we can realize a 1D topological chain on demand even in originally non-topological 2D systems. A pair of zero-energy Majorana fermions can be stable in this system and exist at the ends of the topological chain. We also demonstrate the possibility to arrange an array of Majorana fermions by separating topological chains with non-topological ones. Similar results can be obtained in 3D optical lattices. Compared with strictly 1D systems, quantum fluctuations are strongly suppressed in such high dimensional optical lattices. Because all requirements of our model are within the reach of current experiments, our proposed scheme may provide an experimental feasible platform for observing Majorana states in 2D ultra-cold atom optical lattices.

\(^1\)We acknowledge supports from ARO, AFOSR and NSF.
11:39AM G36.00003 Dynamical detection of a topological phase transition in one-dimensional spin-orbit-coupled Fermi gases1, F. SETIAWAN, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland, College Park, KRISHNENDU SENGUPTA, Indian Association for the Cultivation of Science, Kolkata, India, IAN SPIELMANN, Joint Quantum Institute, National Institute of Standards and Technology, and University of Maryland, College Park, JAY SAU, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland, College Park — We theoretically study the dynamics of topological phase transition in one-dimensional (1D) spin-orbit coupled (SOC) Fermi gases with attractive interaction as a means of detecting the phase transition. The transition from conventional (trivial) superfluid to topological superfluid phase happens as the intensity of the Raman lasers (Zeeman field) is ramped above the critical value. To minimize effect of heating, we propose to ramp from a conventional superfluid phase through the topological phase transition and back. We calculate the momentum distribution of the atoms after the ramp by solving the time-dependent Bogoliubov-de Gennes (BdG) equations self-consistently with the initial state of the Fermi gas being the thermal state. We show that the phase transition can be detected by measuring the signal of the momentum distribution with the ramp rate.

1This work is supported by NSF-JQI-PFC and ARO-Atomtronics-MURI

11:51AM G36.00004 Distribution functions and probes of far-from-equilibrium topological matter1, YUNXIANG LIAO, MATTIEH FOSTER, Rice University — We investigate radio-frequency (RF) spectroscopy and superconductor-normal metal tunneling as probes of out-of-equilibrium topological systems. As an example, we study a 2D p-i-p superfluid following an instantaneous quench of the coupling strength [Foster et prl 2013, PRL 2014]. The long-time asymptotic order parameter of this system can be constant or time-periodic. In both cases, the post-quench Cooper pairs each occupy a linear combination of two states, with coefficients determined by the distribution function. In strong quenches where the order parameter is periodic, the bases are two Floquet states with opposite quasi-energy. We derive expressions for the RF and tunneling spectra for these post-quench states, examining both average values and harmonics. While the distribution function strongly affects the RF signal, it disappears from the tunneling spectrum. We show that the bulk RF signal obtained by occupying the lower Floquet band is dramatically different from that of the post-quench states. This is intimately related to the difference between the topology of the state, which cannot change under closed evolution, versus the topology of the non-equilibrium excitation spectrum. We also look for signatures of Majorana edge states in systems with an edge. We compute the local RF signal, which depends upon the non-equilibrium excitation spectrum of bulk and edge states as well as their occupation.

1This research was supported by the Welch Foundation under Grant No. C-1809 and by an Alfred P. Sloan Research Fellowship (BR2014-035).

12:03PM G36.00005 Fractional Angular Momentum in Cold-Atom Systems, YUHE ZHANG, Pennsylvania State Univ, SREEJITH GANESH JAYA, NORDITA, Roslagstullsbacken 23, 10691 Stockholm, Sweden, NATHAN D GEMELKE, JAINENDRA K JAIN, Pennsylvania State Univ — The quantum statistics of bosons or fermions are manifest through the even or odd relative angular momentum of a pair. We show theoretically that, under certain conditions, a pair of certain test particles immersed in a fractional quantum Hall (FQH) state possesses, effectively, a fractional relative angular momentum, which can be interpreted in terms of fractional braid statistics. We propose that the fractionalization of the angular momentum can be detected directly by measuring the pair correlation function and rotating the sample. In a fractional quantum Hall state, the FQH state will also provide direct evidence for the effective magnetic field resulting from Berry phases arising from attached vortices, and of excitations with a fractional particle number, analogous to the fractional charge of the electron fractional quantum Hall state. We extend our work to investigate the quasiholes in 5/2 FQH state which are believed to obey non-Abelian statistics. We will study the effect of non-Abelian statistics for test particles binding quasiholes in a Moore-Read Pfaffian state, which is produced for bosons subject to a three-body contact interaction, and also for bosons with two-body contact interaction.

This work was supported by NSF-JQI-PFC and ARO-Atomtronics-MURI.

12:15PM G36.00006 Rotational properties of two-component Bose gases in the lowest Landau level1, MARIUS MEYER, Univ of Oslo, GANESH JAYA SREEJITH, PCS Max Planck Institute, SUSANNE VIEFERS, Univ of Oslo — We study the rotational (yrast) spectra of dilute two-component atomic Bose gases in the low angular momentum regime, assuming equal interspecies and intraspecies interaction. Our analysis employs the composite fermion (CF) approach including a pseudospin degree of freedom. While the CF approach is not a priori expected to work well in this angular momentum regime, we show that composite fermion diagonalization gives remarkably accurate approximations to low energy states in the spectra. For angular momenta 0 < \lambda < M (where N and M denote the numbers of particles of the two species, and M ≥ N), we find that the CF states span the full Hilbert space and provide a convenient set of basis states which, by construction, are eigenstates of the symmetries of the Hamiltonian. Within this CF basis, we identify a subset of the basis states with the lowest \lambda-level kinetic energy. Diagonalization within this significantly smaller subspace constitutes a major computational simplification and provides very close approximations to ground states and a number of low-lying states within each pseudospin and angular momentum channel.

1This work was financially supported by the Research Council of Norway and by NORDITA.

12:27PM G36.00007 Probing Fractional Quantum Hall Physics with Rotating Bose Gases, LOUIS JACOME, JIANSHI ZHAO, NATE GEMELKE, Pennsylvania State University — Rapidly rotating and repulsively interacting Bose gases are expected to exhibit character reminiscent of the fractional quantum Hall effect (FQH) in two-dimensional electron gases. Such states are expected to possess excitations with fractionalized braid statistics, although no convincing measurement of this behavior has yet been made in either system. In this talk, we describe progress toward realizing FQH physics using cold Rb-87 atoms confined to an optical lattice with rotating lattice sites. The inclusion of high resolution optical microscopy to perform occupancy-resolved detection expands on previous measurements, and promises new avenues to directly interrogate novel behavior including pair-correlation and braiding statistics as proposed recently [1]. Finally, we discuss new emergent phenomena in chains of tunnel-coupled FQH droplets, including the existence of a novel class of insulating and superfluid states which exhibit local fractional Hall character, and dissipationless transport phenomena governed by new topological invariants. [1]Fractional Angular Momentum in Cold-Atom Systems, Yuh Zhang, G. J. Sreejith, N. D. Gemelke, and J. K. Jain, PRL 113, 160404 (2014)

12:39PM G36.00008 Emergent Fermi Sea in A System of Interacting Bosons1, YINGHAI WU, Max Planck Institute of Quantum Optics, JAINENDRA JAIN, The Pennsylvania State University — An understanding of the possible ways in which interactions can produce fundamentally new emergent many-body states is a central problem of condensed matter physics. We ask if a Fermi sea can arise in a system of bosons subject to contact interaction. Based on exact diagonalization studies and variational wave functions, we predict that such a state is likely to occur when a system of two-component bosons in two dimensions, interacting via a species independent contact interaction, is exposed to a synthetic magnetic field of strength that corresponds to a filling factor of unity. The bosons each bind a single vortex as a result of the repulsive interaction, and these fermionic bound states, namely composite fermions, form a spin-singlet Fermi sea.

1financial support from the DOE under Grant No. DE-SC0005042
12:51PM G36.00009 Few-body treatment of the quantum Hall system\textsuperscript{1} , CHRIS GREENE, KEVIN DAILY, RACHEL WOOTEN, Purdue University — The quantum Hall system is perhaps the simplest real physical system to exhibit complicated, highly-correlated quantum behavior\textsuperscript{2}. Our initial theoretical exploration of this problem approaches it from a few-body perspective using the adiabatic hyperspherical representation developed originally for atomic systems. Such a 2D system with interacting charged particles that move in an external magnetic field can be simulated for cold atoms using artificial vector gauge potentials.

\textsuperscript{1}Supported by NSF


1:03PM G36.00010 Majorana modes in single channel cold atomic gases with short-ranged attractive interactions\textsuperscript{1} , JAY SAU, XIAOPENG LI, Condensed Matter Theory Center and Joint Quantum Institute at the University of Maryland — Majorana modes have been predicted to exist in topological superfluids that generated by a combination of spin-orbit coupling and short-ranged attractive interactions. One dimensional superfluids with intrinsic interactions, however, present a precarious competition between phase fluctuations and topological superfluidity. Previously, it has been argued that the Majorana nature survives with some modification in multi-channel and proximity-induced superfluidity systems of ultra-cold atoms. This discussion is more subtle in the single channel case because the universal properties of one dimensional fermions with attractive interactions are known to be described by a simple Luttinger liquid in the low-energy limit. In this talk, we will discuss the properties of Galilean invariant one dimensional fermi gases with attractive interactions and show how they display properties consistent with both being a topological (or non-topological) superfluid and a Luttinger liquid.

\textsuperscript{1}Condensed Matter Theory Center and Joint Quantum Institute at the University of Maryland

1:15PM G36.00011 Floquet FFLO superfluids and Majorana fermions in a shaken fermionic optical lattice , ZHEN ZHENG, The University of Texas at Dallas; University of Science and Technology of China, CHUNLEI QU, The University of Texas at Dallas, XUBO ZOU, University of Science and Technology of China, CHUANWEI ZHANG, The University of Texas at Dallas — Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) superfluids, Cooper pairings with finite momentum, and Majorana fermions (MFs), quasiparticles with non-Abelian exchange statistics, are two topics under intensive investigation in the past several decades, but unambiguous experimental evidences for them have not been found yet in any physical system. Here we show that the recent experimentally realized shaken optical lattice provides a new pathway to realize FFLO superfluids and MFs. By tuning the shaking frequency and amplitude, various coupling between the s- and p-orbitals of the lattice (denoted as the pseudo-spins) can be generated. We show that the combination of the inverted s- and p-band dispersions, the engineered pseudo-spin coupling, and the on-site attractive interaction, naturally allows the observation of FFLO superfluids as well as MFs in different parameter regions.

1:27PM G36.00012 Majorana edge modes in Kitaev model on honeycomb lattice\textsuperscript{1} , MANISHA THAKURATHI, Indian Institute of Science, Bengaluru, India, KRISHNENDU SENGUPTA, Indian Association for the Cultivation of Science, Kolkata, India, DIPTIMAN SEN, Indian Institute of Science, Bengaluru, India — We study the Majorana modes, both equilibrum and Floquet, which can appear at the edges of the Kitaev model on the honeycomb lattice. We first present the analytical solutions known for the equilibrium Majorana edge modes for both zigzag and armchair edges of a semi-infinite Kitaev model and chart the parameter regimes of the model in which they appear. We then examine how edge modes can be generated if the Kitaev coupling on the bonds perpendicular to the edge is varied periodically in time as periodic $\delta$-function kicks. We derive a general condition for the appearance and disappearance of the Floquet edge modes as a function of the drive frequency for a generic $d$-dimensional integrable system. We confirm this general condition for the Kitaev model with a finite width by mapping it to a one-dimensional model. Our numerical and analytical study of this problem shows that Floquet Majorana modes can appear on some edges in the kicked system even when the corresponding equilibrium Hamiltonian has no Majorana mode solutions on those edges. We support our analytical studies by numerics for finite sized system which show that periodic kicks can generate modes at the edges and the corners of the lattice.

\textsuperscript{1}We thank CSIR, India and DST, India for financial support.

1:39PM G36.00013 Fractionalized Majorana modes in ultracold bosonic systems\textsuperscript{1} , MOHAMMAD F. MAGHREBI, Joint Quantum Institute. University of Maryland College Park, SRIRAM GANESHAN, Condensed Matter Theory Center, University of Maryland College Park, DAVID CLARKE, Station Q, ALEXEY GÖRSHKOV, Joint Quantum Institute, and the National Institute of Standards and Technology, JAY DEEP SAU, Condensed Matter Theory Center and the Joint Quantum Institute at the University of Maryland College Park — Fractionalized Majorana fermions, also known as parafermions, are exotic topologically protected modes that go beyond the simplest non-Abelian anyons, Majorana fermions. They commute up to a nontrivial phase factor in contrast to the minus sign for fermions. These modes are proposed to emerge in devices fabricated from a fractional quantum Hall system and a superconductor. With recent advances towards the realization of fractional quantum Hall states of bosonic ultracold atoms, we propose a realization of parafermions in a system consisting of two Bose-Einstein-condensate trenches within a bosonic fractional quantum Hall state. We show that parafermionic zero modes emerge at the endpoints of the trench and give rise to a topologically protected degeneracy. We also discuss methods for preparing and detecting these modes.

\textsuperscript{1}University of Maryland for start-up support, and NSF PFC at the JQI

1:51PM G36.00014 Extracting Entanglement Entropy Via Non-Destructive Imaging of an Ultracold Atomic Gas , CRAIG PRICE, QI LIU, NATHAN GEMELKE, Pennsylvania State Univ — Entanglement plays an important role in determining the thermodynamic ground state of many many-body quantum systems, and recent theoretical studies have provided evidence that broad classes of quantum critical and topologically ordered states may be characterized by the scaling properties of their entanglement entropy (EE)\textsuperscript{1,2}. We describe how EE can be extracted in a QND imaging process, in which slicing of the beam provides information is transferred from one quantum gas to another using pairwise entangling schemes, and how the subsequent non-local thermal back-action of detection may be used to probe pre-existing entanglement in the sample. We discuss related applications of quantum collisional microscopy, including minimally destructive imaging of non-equilibrium quantum gases, and the algorithmic cooling of a Mott-insulator by non-destructive detection and removal of thermal defects.\textsuperscript{[1]} V. Vedral, M.B. Plenio, M.A. Rippin, P. L. Knight. Quantifying Entanglement. Phys. Rev. Lett. 78, 2275 (1997) \textsuperscript{[2]} G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev. Entanglement in quantum critical phenomena. Phys. Rev. Lett. 90, 227902 (2003)
2:03PM G36.00015 Two-dimensional topological order of kinetically constrained quantum particles. STEFANOS KOURTIS, TCM Group, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom — Motivated by recent experimental and theoretical work on driven optical lattices, we investigate how imposing kinetic restrictions on quantum particles that would otherwise hop freely on a two-dimensional lattice can lead to topologically ordered states. The kinetically constrained models introduced here are derived as an approximate generalization of strongly interacting particles hopping on Haldane and equivalent lattices and are pertinent to systems irradiated by circularly polarized light. After introducing a broad class of models, we focus on particular realizations and show numerically that they exhibit topological order, by observing topological ground-state cross-overs as well as the appearance of corresponding invariants. Apart from potentially being crucial for the interpretation of forthcoming cold-atom experiments, our results also hint at unexplored possibilities for the realization of topologically ordered matter. A further implication, relevant to fractional quantum Hall (FQH) physics, is that the correlations responsible for FQH-like states can arise from processes other than density-density interactions.

1Financial support from EPSRC (Grant No.EP/K028960/1) and ICAM Branch Contributions

Tuesday, March 3, 2015 11:15AM - 2:15PM –
Session G37 GQI: Focus Session: Semiconductor Qubits - SiGe, Isotopic Purification, and Electrical Control 212A - Andrea Morello, University of New South Wales

11:15AM G37.00001 An Exchange-Only Qubit in Isotopically Enriched $^{28}$Si. MARK GYURE, HRL Laboratories, LLC — We demonstrate coherent manipulation and universal control of a qubit composed of a triple quantum dot implemented in an isotopically enhanced Si/Ge heterostructure, which requires no local DC magnetic fields for operation. Strong control over tunnel rates is enabled by a dopantless, accumulation-only device design, and an integrated measurement dot enables single-shot measurement. Reduction of magnetic noise is achieved via isotopic purification of the silicon quantum well. We demonstrate universal control using composite pulses and employ these pulses for spin-echo-type sequences to measure both magnetic noise and charge noise. The noise measured is sufficiently low to enable the long pulse sequences required for exchange-only quantum information processing. Sponsored by United States Department of Defense. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressly or implied, of the United States Department of Defense or the U.S. Government. Approved for public release, distribution unlimited.

11:51AM G37.00002 Accumulation-Only Device Architecture for Si/Ge Single Quantum Dots. T.M. HAZARD, D. ZAJAC, X. MI, J.R. PETTA, Department of Physics, Princeton University — Accumulation mode devices with overlapping gate architectures have been successfully realized in both Si/Ge heterostructures [1] and Si MOS devices [2]. The increased control of tunneling rates, inter-dot tunnel couplings and confinement potentials over previous depletion mode designs make the overlapping gate architecture preferable. Material quality and device geometry have important implications for Si/Ge quantum dots as potential hosts for spin qubits. Here we have fabricated and characterized quantum dots made with this accumulation mode architecture. We also perform numerical simulations to optimize device geometry for tight confinement potentials and reduced cross-coupling between accumulation gates. In addition to device improvements, we have also implemented a compact filtering system on the DC gate lines to achieve sub-40 mK electron temperatures.


1Research was supported by the Sloan and Packard Foundations, Army Research Office and DARPA.

12:03PM G37.00003 A Reconfigurable Device Architecture for Si/Ge Quantum Dots. D. ZAJAC, T.M. HAZARD, X. MI, J.R. PETTA, Department of Physics, Princeton University — Depletion mode architectures for gate-defined quantum dots have been successful in the implementation of single, double and triple quantum dots. However, scaling up to more complicated devices presents serious lithographic challenges for depletion mode devices. We present a reconfigurable, accumulation-only mode lateral quantum dot device. We demonstrate full control of the device as both a single quantum dot with a single dot sensor and a double quantum dot with a single dot sensor. We reach the few electron regime in both operating modes.

1Sponsored by the Sloan and Packard Foundation, Army Research Office and DARPA.

12:15PM G37.00004 Probing the mobility-limiting mechanisms in undoped Si/Ge heterostructures. XIAO MI, THOMAS M. HAZARD, CHRISTOPHER M. PAYETTE, KE WANG, DAVID M. ZAJAC, JEFFREY V. CADY, JASON R. PETTA, Department of Physics, Princeton University — Silicon is an ideal host material for spin-based semiconductor quantum dot qubits due to weak hyperfine coupling and a route to isotopic purification. Si quantum dots formed in undoped Si/Ge quantum wells have recently allowed measurements that were previously only possible in the GaAs system [1, 2]. We report the growth of Si/Ge quantum wells with mobilities reaching 260,000 cm$^2$/Vs at a density of $7 \times 10^{11}$ cm$^{-2}$. We systematically investigate a series of 26 wafers with different growth profiles and impurity levels, and find that the mobility is limited by scattering from both oxygen impurities in the quantum wells and interface charges at the surface of the wafer.


1This work is sponsored by the United States Department of Defense with partial support from the NSF through the Princeton Center for Complex Materials (DMR-0819860) and CAREER program (DMR-0846341).

12:27PM G37.00005 Understanding the Fong-Wandzura Sequence. DANIEL ZEUCH, N.E. BONESTEEL, Department of Physics and NHMFL, Florida State University — In exchange-only spin quantum computation, qubits are encoded into the Hilbert space of three or more spin-1/2 particles (e.g. electron spins in quantum dots), and quantum gates are realized by sequences of Heisenberg exchange operations, or “exchange-pulses,” acting on pairs of spins. It is easy to obtain pulse sequences for single-qubit gates, but difficult for entangling 2-qubit gates due to the large Hilbert space of six spins. The shortest known 2-qubit gate sequence, obtained by Fong and Wandzura via a numerical search [1], consists of 12 exchange pulses. Unlike a longer 2-qubit gate sequence constructed analytically in [2], this 12-pulse sequence has, until now, escaped intuitive explanation. Here, we analyze this sequence using techniques introduced in [2]. We find the 12-pulse sequence naturally decomposes into three parts, each consisting of the same partial pulse sequence acting on four spins at a time. This reduced sequence preserves certain total spin quantum numbers in a way that naturally suggests how it can be used to construct a leakage free entangling 2-qubit gate.

12:39PM G37.00006 Entangling multi-dot spin qubits\(^1\). V. SRINIVASA, Laboratory for Physical Sciences, University of Maryland, College Park, MD. J.M. TAYLOR, Joint Center for Quantum Information and Computer Science, Joint Quantum Institute, National Institute of Standards and Technology, Gaithersburg, MD. C. TAHAN, Laboratory for Physical Sciences, College Park, MD — Single quantum bits encoded in the spins of two or three electrons confined within multiple semiconductor quantum dots provide practical advantages over individual electron spin qubits, in terms of both faster control via applied electric fields and protection from collective decoherence mechanisms. However, implementing rapid and robust entangling gates between these multi-electron, multi-dot qubits remains a current challenge. While the exchange interaction gives rise to rapid gates, it is limited in range and requires accompanying methods for suppressing leakage. Alternatively, the long-range Coulomb interaction can be used to couple both adjacent and spatially separated qubits, and rapid gates are possible through microwave manipulation of the extended charge distribution associated with a multi-dot system. We theoretically investigate different approaches for entangling qubits in double [1] and triple dots. By analyzing the coupling in the presence of charge noise and relaxation, we identify optimal regimes of operation for two-qubit gates and compare their performance for GaAs and Si quantum dots.

\(^1\)Support from DARPA MTO and the NSF-funded Physics Frontier Center at the JQI is gratefully acknowledged.

12:51PM G37.00007 Full-scope modeling of semiconductor devices for quantum information processing. JOHN KING GAMBLE, ANDREW BACZEWSKI, Sandia National Labs, ADAM FREES, University of Wisconsin-Madison, N. TOBIAS JACOBSON, INES MONTANO, RICHARD P. MULLER, ERIK NIELSEN, Sandia National Labs — Recent outstanding experimental advances in semiconductor-based quantum information processing have placed the fundamental building blocks of a quantum computer within reach. Typical computational simulation of these devices either focuses on the large-scale, semiclassical device physics or more detailed quantum mechanics within an idealized physical system. Here, we present results for full-scope simulation, where detailed multi-valley effective mass theory is coupled to large-scale device physics. This enables the simulation of the quantum properties and operation of a device directly from a physical design. This work opens the door for physics-targeted device optimization and an unprecedented level of predictive power. The authors gratefully acknowledge support from the Sandia National Laboratories Truman Fellowship Program, which is funded by the Laboratory Directed Research and Development (LDRD) Program. Sandia is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

1:03PM G37.00008 Electron Spin Resonation in Si/SiGe Quantum Dot Ensembles. RYAN M. JOCK, J.-H. HE, A.M. TYRYSKIN, S.A. LYON, Princeton University, C.-H. LEE, S.-H. HUANG, C.W. LIU, National Taiwan University — Single electron spin states in Si/SiGe quantum dots have shown promise as qubits for quantum information processing. Our previous ensemble microwave measurements of electron spins in gated Si/SiGe quantum dots have displayed relaxation (\(T_1\)) and coherence (\(T_2\)) times of 250 \(\mu\)s at 350 mK. These experiments used conventional X-band (10 GHz) pulsed Electron Spin Resonance (eESR), on a large area, double-gated, undoped Si/SiGe heterostructure, in which holes with a 300 nm diameter and 700 nm period were lithographically defined in the lower gate. Quantum dots were electrostatically induced in a natural Si quantum well, with their confinement potential controlled by the gates. Electron spin coherence in these first generation quantum dot devices was observed to be \(T_1\)-limited at stronger confining potentials. By tailoring the quantum dot size and spacing we can modify the electron confinement barrier and electron wave function size, helping us probe the mechanisms limiting coherence in silicon quantum dots. We will report results on dots with lithographic diameters of 150 to 300 nm and a 375 to 700 nm period. The device with smaller dots and larger spacing displays an extended electron relaxation times (\(T_1 = 1-2\) ms) at 350 mK. Furthermore, we observe a \(T_2\) of 310 \(\mu\)s, that is neither \(T_1\)-limited nor temperature dependent. This narrows the field of possible coherence limiting mechanisms, which will be discussed.

1:15PM G37.00009 Electrical assessments of \(^{28}\)Si enriched and deposited in situ to <1 ppm. \(^{29}\)Si, JOSHUA POMEROY, National Institute of Standards and Technology, KEVIN DWYER, HYUN-SOOG KIM, University of Maryland — We are enriching \(^{29}\)Si to better than 99.99999%, depositing epitaxial films, and measuring materials properties to improve our deposition process so that our enriched films can be used to fabricate quantum devices. Recent reports of spin-echo measurements in donor ensembles and single spins have both demonstrated spectacular coherence time and line width improvements due to enriched \(^{28}\)Si. In order to realize the benefits of our enrichment, the electrical properties of our films need to be similar quality to commercial wafers. Therefore, we are using C-V, g-V, Hall and other techniques commonly used for quantifying defect densities, mobility, carrier density, etc. to benchmark the viability of using our enriched films for quantum device fabrication.

1:27PM G37.00010 Dependence of \(^{28}\)Si concentration on deposition temperature in \(^{29}\)Si epilayers. KEVIN DWYER, JOSHUA POMEROY, HYUN SOO KIM, DAVID SIMONS, National Institute of Standards and Technology — In an effort to gain predictive power for the enrichment of \(^{29}\)Si epilayers deposited at elevated temperatures, we correlate the \(^{28}\)Si concentration due to natural abundance silane adsorption with measured IMS values. We have previously shown very high enrichments up to 99.99996 % (0.3 ppm \(^{28}\)Si) using mass filtered ion beam deposition. However, the incorporation at higher deposition temperatures of naturally abundant silane gas from our ion source has the potential to reduce the final film enrichment. Knowledge of the expected reduction in \(^{28}\)Si concentration is important because removal of the 4.7% \(^{29}\)Si nuclear spins in natural silicon allows for exceedingly long coherence (\(T_2\)) times of qubits, approaching an hour at room temperature for \(^{11}\)B nuclear spins. This makes incorporation of highly enriched \(^{28}\)Si into devices critical for solid state quantum information.

1:39PM G37.00011 Feasibility study of simultaneous capacitance detection during STM of silicon. HYUN KIM, KEVIN DWYER, Univ of Maryland-College Park, JOSHUA POMEROY, National institute of standards and technology — We are examining the feasibility of capacitance detection during STM to image buried metal nanostructures in silicon. As the hydrogen STM lithography for quantum information enables us to fabricate the atomically precise devices such as single atom qubits, the accurate alignment of metal contacts such as electrodes to the buried nanostructures on the surface becomes very challenging. Using SCM with STM gives benefits to locate the buried nanostructures and image the surface morphology simultaneously.

1:51PM G37.00012 Two-Dimensional Electron Gases in Nanomembrane-based Epitaxial Si/SiGe Heterostructures\(^1\). YIZE LI, PORNATIT SOOKCHOO, XIAORUI CUI, ROBERT MOHR, DONALD SAVAGE, RYAN FOOTE, R.B. JACOBSON, JOSE SANCHEZ-PEREZ, XIAN WU, DAN WARD, SUSAN COPPERSMITH, MARK ERIKSSON, MAX LAGALLY, University of Wisconsin-Madison — To assess possible improvements in the electronic performance of two-dimensional electron gases (2DEGs) in silicon, SiGe/Si/SiGe heterostructures are grown on fully elastically relaxed single-crystal Si nanomembranes fabricated through a strain engineering approach. This procedure eliminates the formation of dislocations in the heterostructure. Top-gated Hall bar devices are fabricated to enable magnetoresistance and Hall effect measurements. Both Shubnikov de Haas oscillations and the quantum Hall effect are observed at low temperatures, demonstrating the formation of high-quality 2DEGs. Values of charge carrier mobility as a function of carrier density extracted from these measurements are at least as high or higher than those obtained from companion measurements made on heterostructures grown on conventional strain graded substrates. In all samples impurity scattering appears to limit the mobility.

\(^1\)Supported by U.S. Dept. of Defense. The views and conclusions are those of the authors and should not be interpreted as representing the official policies, either expressly or implied, of the U.S. Government. Facilities support: DOE
The spin-2 AKLT state on the square lattice is a universal resource for quantum computation. This work was supported in part by the National Science Foundation.
12:15PM G38.00006 Quantum Circuit Complexity of Random Singlet Phases1, NOAH BRAY-ALI, Joint Quantum Institute, University of Maryland, College Park and National Institute of Standards and Technology, Gaithersburg, MD 20899 — We use quantum circuit complexity to characterize the entanglement of random singlet phases in one-dimension. Random singlet phases are infinite-randomness fixed points of the strong-disorder renormalization group. They arise in strongly-correlated, quantum many-body systems of bosons, fermions, or anyons, and have long-range entanglement. We compute the depth of the local quantum circuit required to generate the random singlet phase and find that it scales as a super-linear, universal power of the system size.

1Supported by NRC Post-doctoral Research Associateship, Visiting Research Scientist at Department of Physics and Astronomy, California Institute of Technology, Pasadena, CA

12:27PM G38.00007 An Efficient Construction of a Matrix Product State for a Free Fermion Ground State1, MATTHEW FISCHMAN, Applied Physics, California Institute of Technology, Pasadena, California 91125, USA, STEVEN WHITE, Department of Physics and Astronomy, University of California, Irvine, California 92697, USA — Here we present an efficient and numerically stable procedure for creating the Matrix Product State of a pure fermionic Gaussian state, such as the ground state of a quadratic Hamiltonian. The algorithm produces a minimal number of nearest neighbor gates that, when applied to a product state, forms the many-body ground state. We will cover the procedure for both number conserving Hamiltonians as well as more general parity conserving Hamiltonians, where we will utilize the formalism of Majorana modes. Comparisons to previous methods and applications will be discussed.

1MF is thankful for funding from the NSF Graduate Research Fellowship.

12:39PM G38.00008 What constitutes a resource state for measurement-based quantum computation?2, ELEANOR RIEFFEL, NASA Ames Research Center, HOWARD WIEMAN, Griffith University — Support for universal measurement-based quantum computation (MBQC) is a sufficient condition for states to be considered resources for MBQC, but seems too strong as a necessary condition given known classes of MBQCs that appear to give an advantage over classical computing but which are not universal. We propose some minimal criteria that states must meet in order to be considered resource states for MBQC. We introduce (PRA 89, 032323 (2014)) the notion of inherently measurement-based computations, and give a series of necessary conditions for families of MBQCs to be considered inherently measurement-based. We propose that for a state to be considered a resource for MBQC it must, at minimum, support a family of MBQCs that is inherently measurement-based. Using these criteria, we explain why discord-free states cannot be resources for MBQC, in spite of claims to the contrary. We conclude with some open questions.

2Supported by IARPA, ARO, and NSF.

12:51PM G38.00009 Shortcuts to Adiabaticity in Quantum Many-Body Systems, ADOLFO DEL CAMPO, University of Massachusetts Boston — The nonadiabatic dynamics of a many-body system driven through a quantum critical point leads unavoidably to the formation of excitations, in agreement with the Kibble-Zurek mechanism. A way out of this scenario relies on the use of shortcuts to adiabaticity, where the formation of excitations is suppressed by assisting the dynamics with auxiliary multiple-body nonlocal interactions. We propose an alternative scheme which circumvents practical challenges to realize shortcuts to adiabaticity in mesoscopic systems by tailoring the functional form of the auxiliary counterdiabatic interactions. A driving scheme resorting in few-body short-range interactions is shown to generate an effectively adiabatic dynamics.


1:27PM G38.00010 Quantum algorithms, quantum field theory, and computational complexity . KEITH LEE, CQIQC — Quantum field theory provides the framework for the Standard Model of particle physics and plays a key role in physics. However, calculations are generally computationally complex and limited to weak interaction strengths. I’ll describe an extension of our quantum algorithm for computing relativistic scattering amplitudes in scalar quantum field theories to fermionic theories. The algorithms run in polynomial time and thus achieve exponential speedup over known classical methods. One of the motivations for this work comes from computational complexity theory. Ultimately, we wish to know what is the computational power of our universe. Studying such quantum algorithms probes whether a universal quantum computer is powerful enough to represent quantum field theory; in other words, is quantum field theory in BQP? Conversely, one can ask whether a given quantum field theory can implement a universal quantum computer; is quantum field theory BQP-hard? I’ll describe our approach to addressing the question of BQP-hardness.

2:03PM G38.00011 Are Qubits Fundamentally Flawed for General-purpose Quantum Computing? , CHENG-HSIAO WU, Missouri Univ. of Science and Technology — When two qubits are employed for the addition operation of two bits, it is not the superposition of 4 states that are relevant for the quantum computing. Rather, it is the 4 symbolic substitution rules that are contained in 2 bits. Thus general-purpose quantum paralleling computing is rule-based, not logic-gate based. This is a great departure. The quantum processor (US patent 8,525,544) contains 4 instructions and stores two data. The flaws of qubit concept are explained. Internal coupling (the entanglement) and external coupling (the readouts) must be integrated as one system. The quantum computing architecture is thus in cellular automata with one such processor in each cell. When the cell-to-cell interconnections are altered, a “new kind of science” appears and explained. Reversible quantum computing is not as stringent as the unitary operation implies.


11:15AM G39.00001 Improving the dynamic range of the Josephson Bifurcation Amplifier1, LASZLO SZOCS, MICHAEL HATRIDGE, SHYAM SHANKAR, ANIRUDH NARLA, KATRINA SLIWA, MICHEL DEVORET, Yale Univ — The dynamic range of the Josephson Bifurcation Amplifier (JBA), acting as a phase-sensitive amplifier, can be improved by combination of several junctions in series and parallel in place of the single junction present in the original device. By analyzing the circuit Hamiltonian for a system with many amplifiers tiled in parallel, each containing junctions wired in series, a potential increase in the amplifier’s dynamic range can be obtained while maintaining GHz-range tunability. Theoretical results and preliminary experimental data will be presented.

1Work supported by IARPA, ARO, and NSF.
11:27AM G39.00002 Multi-mode directional parametric devices, LEONARDO RANZANI, ADAM SIROIS, NIST, Boulder - University of Colorado, Boulder, MANUEL CASTELLANOS-BELTRAN, RAYMOND SIMMONDS, JOHN TEUFEL, JOSE AUMENTADO, NIST, Boulder — Josephson parametric amplifiers (JPAs) are very common in quantum information measurement systems, because they can operate close to the standard quantum limit, but require an external circulator to achieve unidirectionality. A possible way to achieve directional amplification without a circulator is to increase the number of coupled modes. By parametrically coupling three or more modes, and selecting the right amplitude and phase for the mode coupling rates, we can realize a non-trivial interference between different internal parametric processes and obtain unidirectional frequency conversion or amplification. In this talk we are going to discuss some recent progress on the experimental implementation of directional lumped-element Josephson parametric devices based on multiple coupled modes.

11:39AM G39.00003 Directional Amplification using Josephson Ring Modulators1, M. HATRIDGE, K.M. SLIWA, A. NARLA, S. SHANKAR, M.H. DEVORET, Department of Applied Physics, Yale University — Quantum limited parametric amplifiers usually amplify in reflection, so that the input and output signals travel on the same physical port. Circulators and isolators are thus required both to separate input and output signals with minimal loss of signal-to-noise ratio and to avoid backward irradiation of the signal source. These devices are bulky, dissipative, and operate in large magnetic fields which make them incompatible with integration on chip. By interfering the non-reciprocal mixing processes present in Josephson Ring Modulators, directional amplification can be realized. The theory and performance of a novel directional amplifier will be presented.

1Work supported by: IARPA, ARO, and ONR.

11:51AM G39.00004 A new implementation of a Josephson microwave circulator1, K.M. SLIWA, M. HATRIDGE, A. NARLA, S. SHANKAR, M.H. DEVORET, Department of Applied Physics, Yale University — Circulators are essential microwave components in superconducting qubit experiments, particularly those which also use parametric amplifiers. These amplifiers typically operate in reflection, and circulators both separate input from output, and protect the qubit from dephasing due to tones reflected off the amplifier. Unfortunately, their large size and the large magnetic fields they need to operate make them impossible to integrate on chip. Here we present the theory and experimental performance of a microwave circulator based not on ferrite materials, but on the interference of non-reciprocal mixing processes present in Josephson Ring Modulators.

1Work supported by: IARPA, ARO, and ONR.

12:03PM G39.00005 Qubit readout with Josephson Photomultipliers, GUILLAUME RIBEILL, IVAN PECHENIKSKII, TED THORBECK, University of Wisconsin, Madison, CALEB HOWINGTON, MATTHEW HUTCHINGS, Syracuse University, LUKE GOVIA, FRANK WILHELM, Saarland University, B.L.T. PLOURDE, Syracuse University, ROBERT MCDERMOTT, University of Wisconsin, Madison — Continued progress in superconducting qubits will require the development of scalable quantum-limited measurement tools. We have recently introduced a scalable superconducting qubit measurement protocol involving the state-selective ringup of a readout cavity followed by photodetection with the Josephson photomultiplier (JPM), a current-biased Josephson junction. Here we describe the experimental realization of this protocol. We discuss JPM optimization for high quantum efficiency, and describe integration of the JPM with a transmon qubit for high-fidelity dispersive readout. In addition, we discuss prospects for JPM readout of larger multi-qubit circuits.

12:15PM G39.00006 Readout of superconducting qubits with a Josephson photomultiplier1, CALEB HOWINGTON, MATTHEW HUTCHINGS, Syracuse University, GUILLAUME RIBEILL, ROBERT MCDERMOTT, University of Wisconsin, Madison, B.L.T. PLOURDE, Syracuse University — A Josephson photomultiplier (JPM) formed from a current-biased Josephson junction is the centerpiece of an alternative method for measuring the state of a superconducting qubit in a microwave cavity compared to conventional linear amplification followed by heterodyne readout. This approach, which involves mapping the qubit state onto the cavity photon occupation followed by photon detection with the JPM, reduces the requirements on bulky microwave hardware and amplifiers in the cryostat. We will discuss the implementation of superconducting microwave cavities and transmon qubits tailored for this readout technique. Furthermore, we will present steps towards the readout of multiple qubits in a common cavity with the JPM-based protocol.

1We acknowledge support from ARO under contract W911NF-14-1-0080.

12:27PM G39.00007 Efficient photon detection with a Josephson Parametric Amplifier, W.F. KINDEL, JILA, University of Colorado, M.D. SCHROER, JILA, M.R. VISSERS, J. GAO, D.P. PAPPAS, NIST, K.W. LEHNERT, JILA, University of Colorado — Josephson Parametric Amplifiers (JPAs) are an important resource in quantum limited measurement, feedback and nonclassical state generation. To study the JPA transformation, we use a superconducting qubit-cavity system to launch single photons or, n=1 Fock states, into a JPA, which measures the state. From repeated measurements, we can infer the state’s loss of purity as a results of the JPA transformation. We will present our estimates of the JPA’s efficiency as a photon detector in comparison to Gaussian characterization methods.

12:39PM G39.00008 Towards a lossless and integrable circulator for quantum superconducting microwave systems: Theory of operation1, JOSEPH KERCKHOFF, BENJAMIN J. CHAPMAN, JILA, University of Colorado, KEVIN LALUMIERE, ALEXANDRE BLAIS, Université de Sherbrooke, K.W. LEHNERT, JILA, University of Colorado and NIST — Lossless and integrable microwave circulators operating in the 4-8 GHz band are a critical, missing component in superconducting microwave quantum technology. Circulators are non-reciprocal devices used to impose a unidirectional flow of microwave signals. We report on progress towards an all-superconducting microwave circuit potentially capable of integrating with other quantum technologies and replacing many instances of the lossy and non-integrable ferrite circulators used in all contemporary quantum microwave experiments. Non-reciprocity is achieved through relatively weak (sub-Gauss) and slow (∼ 100 MHz) dynamically-modulated magnetic fields that tune the linear susceptibility of SQUID arrays in a four-port, resonant circuit. Our design’s basic theory of operation will be covered in this presentation.

1This work is supported by ARO under the contract W911NF-14-1-0079.
Towards a lossless and integrable circulator for quantum superconducting microwave systems: design and initial testing\(^1\), BENJAMIN J. CHAPMAN, JOSEPH KERCKHOFF, JILA, University of Colorado Boulder, KEVIN LALUMIERE, ALEXANDRE BLAIS, Sherbrooke University, K.W. LEHNERT, JILA, National Institute of Standards, Boulder, CO, University of Colorado Boulder — Microwave circulators enforce a single propagation direction for the signals in an electrical network. Commercial circulators, however, are lossy and cannot be integrated near superconducting circuits because of the large magnetic fields they emit. We report on progress toward the development of a lossless, on-chip, active circulator for superconducting microwave circuits in the 4-8 GHz band. Non-reciprocity is achieved by the active modulation of circuit elements on a slow time scale (100 MHz). The circulator’s active components are dynamically tunable inductors constructed from series arrays of SQUIDs. SQUID inductance is tuned by varying the magnetic flux through the SQUID’s loop with fields weaker than 1 G. Device features include a tunable bandwidth between 10-100 MHz, a tunable center frequency between 4-8 GHz, a high (-93 dBm) saturation power, a factor of 50 separation between the center and reverse isolation frequencies, low loss, and 1 mm\(^2\) footprint. This presentation will cover the design and initial testing of the device.

\(^1\)This work is supported by the ARO under contract W911NF-14-1-0079.
Using photovoltage to measure device-relevant exciton diffusion in luminescent and non-luminescent organic semiconducting materials. Tyler Mullenbach, Russell Holmes, University of Minnesota — Exciton diffusion is a prominent component of many emerging organic optoelectronic devices and is commonly described by the exciton diffusion length ($L_D$). Excitons are commonly tracked by measuring their end-of-life products: photons (from radiative decay) or charge carriers (from exciton dissociation). While tracking luminescence provides an accepted means of measuring $L_D$ for many materials, non-luminescent (dark) materials and states are inaccessible via such techniques. For dark materials, the charge carriers generated from exciton dissociation are tracked to estimate $L_D$ (e.g., by fitting device external quantum efficiency), despite the fact that photogenerated carriers are often subject to recombination events prior to collection as current. Here, we present an alternate method of measuring $L_D$, equally applicable to luminescent and dark materials, that uses photovoltage instead of current to determine the number of excitons reaching the dissociating interface in an organic photovoltaic device. Use of the photovoltage sidesteps charge carrier recombination providing an unbiased measurement of $L_D$. The technique is verified against previous luminescence-based methods, and measurements of $L_D$ are presented for a variety of dark materials including fullerenes.

Using Mass Transport to Guide the Purification of Small Molecule Organic Semiconductors via Sublimation. N. T. Morgan, Y. Zhang, University of Minnesota, Minneapolis, Matthew L. Grandbois, Engineering & Process Sciences, Core R&D, The Dow Chemical Company, Bruce M. Bell, Analytical Sciences, Core R&D, The Dow Chemical Company, Russell J. Holmes, E. L. Cussler, University of Minnesota, Minneapolis — Organic electronic materials have garnered considerable commercial attention for next generation display and solid-state lighting applications. Widespread adoption of these technologies is slowed by considerable production costs, partially due to an expensive purification step. This work explores the current method of industrial purification, thermal gradient sublimation, in order to isolate the fundamental mechanisms limiting sublimation rate and controlling product deposition. For the archetypical hole transport materials, N,N'-bis(naphthalen-1-yl)-N,N'-bis(phenyl)-benzidine (NPD) and 4,4',4''-tris(carbazol-9-yl) triphenylamine (TCTA), a combination of viscous flow and physical vapor deposition are shown to be rate-limiting at constant sublimation temperature. Surprisingly, diffusion through the solid feed, reaction at the feed particle surface, and mass transfer within the bed of feed particles are not rate limiting in the case. This mechanism is different from that which is observed in many industrial sublimation systems. These results can be used to guide the design and operation of future large-scale purification systems, which are critical for the widespread adoption of organic optoelectronic devices.

Separation of Carrier-Transport and Light-Emission Functions in a Light-Emitting Organic Transistor with Bilayer Configuration. Hui Shang, Hidekazu Shimotani, Department of Physics, Tohoku University, Japan, Kanagasekaran Thangavel, Katsumi Tanigaki, WPI-AIMAR, Tohoku University, Japan, Nano Solid State Physics Team — Organic single crystal based ambipolar light-emitting field effect transistors is treated as the candidate to realize laser. However, the active layer should contain both superb luminescent property and high charge-carrier mobility, which are always competing with each other in one material. Our basic concept for solving this problem is divide these two factors into two layers, and the combination of these two layers acts as the active layer of LEFET. Bottom layer with high carrier mobility can be assigned as carrier transporter, and top layer with high PL efficiency was assigned as light emitter. After injection, the carriers will have a recombination in the bottom layer and formed exciton will transfer into the top layer with light emission. In this work, we fabricated bilayer structure device, in which tetracene was used as bottom crystal and 4-(dicyanomethylene)-2-methyl-6-(p-dimethylaminostyryl)-4H-pyran (DCM) doped tetracene was laminated on tetracene as light emitter. We have successfully observed light emission from top crystal, from which our aforementioned hypothesis was preliminary proved. Details will be reported in the presentation.

Tuning the opto-electronic properties of donor-acceptor polymers with molecular doping. Elizabeth Von Hauff, VU Amsterdam — Organic semiconductors offer vast potential for low cost, flexible energy production. The photocurrents in organic solar cells, however, are inherently limited by the poor electrical properties of the active layer. In this talk, strategies to increase the power conversion efficiency of polymer-fullerene solar cells by microscopically tuning the transport properties of the donor material are discussed. We observe that molecular doping the active layer of the device leads to increased charge separation efficiency and photocurrents. To investigate the influence of doping on the transport properties, impedance spectroscopy, a powerful, non-destructive technique, was applied. This allows us to probe carrier dynamics at different operational points in the current-voltage characteristics, and thereby correlate material properties with device performance.

12:27PM G41.00005 Polymorphism in Core-Chlorinated Naphthalene Tetracarboxylic Diamide Thin Films. Geoffrey Purdum, Dept. of Chemical and Biological Engineering, Princeton University, Princeton, NJ 08544, Falk May, BASF SE, GVM/M - B009, 67056 Ludwigshafen, Germany, Nan Yao, Princeton Institute for Science and Technology of Materials, Princeton University, Princeton, NJ 08544, Thomas Weitz, BASF SE, GVE/F - J542, 67056 Ludwigshafen, Germany, Yueh-Lin LoO, Dept. of Chemical and Biological Engineering, Princeton University, Princeton, NJ 08544 — Polymorphism within organic semiconductors can play a critical role in device performance, as some packing motifs may be more favorable to charge transport than others. As-evaporated polycrystalline thin-films of core-chlorinated naphthalene tetracarboxylic diimides (NTCDI-I) adopt a triclinic polymorph that is not different from those of single crystals grown via physical-vapor transport. Exposing these thin-films to saturated vapors of select organic solvents, such as those of acetone and chloroform, induces structural transformation; thermally evaporated films convert from the triclinic polymorph to a monoclinic polymorph that was reported for solution-grown single crystals. Isothermal transformations are well described by second-order Avrami kinetics; molecular dynamic simulations give us insight into how solvents induce different kinds of favorable molecule-molecule interactions. Interestingly, the surface energy of the underlying substrate also plays a role in determining the rate of transformation; the rate of transformation is 2× and 4× faster on hexamethyldisilazane modified-Si/SiO$_2$ compared to on Si/SiO$_2$ and octadecyltrichlorosilane modified-Si/SiO$_2$ respectively.

12:39PM G41.00006 Small Conjugated Molecules: Orbital Energy Modeling Using Tuned Range-Separated Functional. Ram Bhatta, Mesfin Tsige, Department of Polymer Science, The University of Akron — Small conjugated molecules (SCMs) have potential to be efficient electron donors for organic solar cells because of their structural simplicity, good control over synthetic reproducibility and low purification cost. Density functional theory (DFT) and time dependent DFT (TD-DFT) computations can guide for designing high-performing SCMs by modeling their orbital energies. However, the accuracy of computed orbital energies depends on the choice of the level of the theory. We present DFT and TD-DFT calculations on 12 different SCMs using range-separated functional, LC-BLYP and the popular hybrid functional, B3LYP. Systematic calculations of the highest occupied molecular orbital (HOMO) energies, the lowest unoccupied molecular orbital (LUMO) energies as well as the singlet and triplet excitation energies are performed. We found that the LC-BLYP results are strongly dependent on the range-separation parameter. The computed results are compared with experimental data.

Work supported by the National Science Foundation (Grant No. DMR0847580)
12:51PM G41.00007 Low Field Electronic Behavior and Contact Impedance of Organic Single Crystal Transistors, EMMILY BITTLE, JAMES BASHAM, National Institute of Standards and Technology, THOMAS JACKSON, Penn State University, ANNA JURCHESCU, Wake Forest University, DAVID GUNDLACH, National Institute of Standards and Technology — Organic electronic devices are attractive for a range of existing and emerging electronic applications. Most technological demonstrations of organic transistors rely on their large signal response for pixel control or logic. However, considerable application space requires analog circuits, e.g., distributed signal conditioning in sensor arrays. Charge transfer and trapping mechanisms differ significantly in organic as compared to inorganic transistors, and as a result commonly used analogies to inorganic band transport are not directly applicable. In this work, we present a detailed investigation of organic transistor behavior at small signals to understand this behavior at the device level.

1:03PM G41.00008 Site energies and charge transfer rates near pentacene grain boundaries from first-principles calculations, HAJIME KOBAYASHI, YUICHI TOKITA, Sony Co. — Charge transfer rates near pentacene grain boundaries are determined by calculating the site energies and transfer integrals of 37 pentacene molecules using first-principles calculations. The site energies decrease considerably near the grain boundaries, and electron traps of up to 300 meV and hole barriers of up to 400 meV are generated. The charge transfer rates across the grain boundaries are found to be reduced by three to five orders of magnitude with a grain boundary gap of 4 Å because of the reduction in the transfer integrals. The electron traps and hole barriers also reduce the electron and hole transfer rates by factors of up to 10 and 50, respectively. It is essential to take the site energies into consideration to determine charge transport near the grain boundaries. We show that the complex site energy distributions near the grain boundaries can be represented by an equivalent site energy difference, which is a constant for any charge transfer pass. When equivalent site energy differences are obtained for various grain boundary structures by first-principles calculations, the effects of the grain boundaries on the charge transfer rates are introduced exactly into charge transport simulations, such as the kinetic Monte Carlo method.

1:15PM G41.00009 Nanoscale domains in thin-film pentacene seen by mid-infrared near-field spectroscopy, FRITZ KEILMANN, BERT NICKEL, CHRISTIAN WESTERMEIER, CLEMENS LIEWALD, Ludwig-Maximilians-Universitaet Muenden, SERGIU AMARIE, ADRIAN CERNESCU, Neaspec GmbH Martinsried — The coexistence of structural phases in thin-film pentacene was known from X-ray diffraction, yet the scale of domain sizes remained unknown due to large-scale averaging. Infrared spectroscopy (classical FTIR) can distinguish different structural phases by slightly shifted molecular vibrational resonances but with spatial resolution not better than about 10 micrometer. When FTIR is paired with near-field microscopy performed by back-scattering infrared radiation from an AFM tip (“nano-FTIR” allowing 20 nm resolution), Bulk-Phase (BP) domains were readily observed to form <100 to 300 nm wide ellipsoids which significantly grow over months at atmospheric conditions, at the cost of the surrounding Thin-Phase (TFP) pentacene. Both the domain interfaces and their continuing dimensional evolution may point to hidden problems for solar conversion systems development, possibly also with molecular materials beyond pentacene. C. Westermeier, A. Cernescu, S. Amarie, C. Liewald, F. Keilmann, B and B. Nickel, Sub-micron phase coexistence in small-molecule organic thin films revealed by infrared nano-imaging, Nature Communications 5, 4101, DOI:10.1038/ncomms5101 (2014)

1:27PM G41.00010 Tunable Molecular Orientation and Elevated Thermal Stability of Vapor-Deposited Organic Semiconductors, DIANE WALTERS, SHAKEEL DALAL, University of Wisconsin-Madison, IVAN LYUBIMOV, JUAN DE PABLO, University of Chicago, MARK EDIGER, University of Wisconsin-Madison — Physical vapor deposition is commonly used to prepare organic glasses that serve as active layers in organic electronic devices. Orienting the molecules in such layers can significantly enhance device performance. We apply a high-throughput characterization scheme to investigate the effect of the substrate temperature (T_substrate) on glasses of three organic materials utilized as semiconductors. Using spectroscopic ellipsometry, we find that molecular orientation in these glasses is continuously tunable and controlled by T_substrate/T_g, where T_g is the glass transition temperature. All three molecules can produce highly anisotropic glasses; the dependence of molecular orientation upon substrate temperature is remarkably similar and nearly independent of molecular length. All three compounds form “stable glasses” with high density and thermal stability similar to stable glasses of model glass formers. Simulations reproduce the experimental trends and explain molecular orientation in the deposited glasses in terms of the surface properties of the equilibrium liquid. By showing that organic semiconductors form highly oriented stable glasses, these results provide an avenue for systematic performance optimization of active layers in organic electronics.

1:39PM G41.00011 GIWAXS characterization of amorphous, anisotropic, vapor-deposited organic semiconductor films, ANKIT GUJRAL, University of Wisconsin-Madison, KATHRYN O’HARA, MICHAEL CHABINYC, University of California, Santa Barbara, MARK EDIGER, University of Wisconsin-Madison — Vapor-deposited organic glasses can be produced with enhanced thermal stability and tunable molecular packing by controlling deposition conditions, such as the rate of deposition and the substrate temperature. Recent work in organic electronics has also shown improved charge carrier mobility associated with anisotropic molecular packing. In this work, grazing-incidence wide angle x-ray scattering (GIWAXS) is used to characterize the structural anisotropy in glasses of a hole transport material, TPD, prepared by physical vapor deposition. A Hermans’ order parameter is used to quantify the changes observed in the scattering patterns of glasses prepared at different substrate temperatures. The order parameter correlates closely with spectroscopic ellipsometry measurements showing different molecular orientations depending upon the substrate temperature during deposition. Additionally, the GIWAXS measurements indicate there is a change in structure at the surface of the film compared with the bulk, providing insight into the formation of stable glasses. These findings may contribute in understanding the enhanced charge carrier mobility observed for anisotropic glasses used in OLEDs.

1:51PM G41.00012 Device applications and structural and optical properties of Indigo – A biodegradable, low-cost organic semiconductor, ZHENGJUN WANG, KELLY L. PISANE, Department of Physics and Astronomy, West Virginia University, CONSTANTINOS SIERROS, Department of Mechanical and Aerospace Engineering, West Virginia University, MOHINDAR S. SHERARA, Department of Physics and Astronomy, West Virginia University, DIMITRIS KORAKAKIS, Lane Department of Computer Science and Electrical Engineering, West Virginia University — Currently, memory devices based on organic materials are attracting great attention due to their simplicity in device structure, mechanical flexibility, potential for scalability, low-cost potential, low-power operation, and large capacity for data storage [1]. In a recent paper from our group, Indigo-based nonvolatile organic write-once-read-many-times (WORM) memory device, consisting of a 100nm layer of indigo sandwiched between an indium tin oxide (ITO) cathode and an Al anode, has been reported [2]. This device is found to be at its low resistance state (ON state) and can be switched to high resistance state (OFF state) by applying a positive bias. In this work, the time constant for the current ratio of the device being up to 1.02 × e6. A summary of the results along with the structural and optical properties of indigo powder will be reported. Analysis of x-ray diffraction shows a monoclinic structure with lattice parameters a=0.924(0.577) , b=0.1222nm and β=117°. Optical absorption shows a band edge at 1.70 eV with peak of absorption occurring at 1.90 eV. These results will be interpreted in terms of the HOMO-LUMO bands of Indigo.

11:15AM G42.00001 Get in Line: Orienting Cylinders in Block Copolymer Thin Films via Shear, RALEIGH DAVIS, RICHARD REGISTER, Princeton University, PAUL CHAIKIN, New York University — Block copolymer thin films have garnered much attention for their potential as nanolithographic masks. For many patterning applications, however, the need to impart well-defined order to the microdomains is paramount. One method to achieve long-range orientational order in thin films is through the use of shear. The ease with which orientation is achieved as well as the ultimate quality of alignment is strongly influenced by the copolymer composition and molecular weight, film thickness, and shearing conditions, as revealed using a series of cylinder-forming poly(styrene)-poly(hexylmethacrylate) (PS-PHMA) copolymers. Quality of in-plane alignment is assessed via atomic force microscopy, quantified through an orientational order parameter \( \psi \). The ease with which alignment is achieved is determined by measuring \( \psi \) as a function of applied shear stress and comparing the results to a melting-recrystallization model which allows for the determination of two key alignment parameters: the critical stress needed for alignment \( \sigma_c \), and an orientation rate constant \( \Gamma \). The \( \psi \) vs. stress behavior, including the time-dependence, is well captured by the model. For monolayers, as \( \psi \) stress fraction or overall molecular weight increases, \( \sigma_c \) also increases, while \( \Gamma \) greatly decreases. As the number of cylinder layers is increased, \( \sigma_c \) decreases to a plateau. The ultimate quality of alignment is studied by comparing \( \psi \) vs. lattice defect density for well-aligned films; \( \psi \) is limited by both undulations in the cylinder trajectories as well as the present of isolated dislocations.

11:27AM G42.00002 How Mechanical Deformation of Polymers during Vitrification Alters the Subsequent Stability of the Glass, LAURA A. G. GRAY, CONNIE B. ROTH, Dept. of Physics, Emory University, Atlanta, GA — How stress and mechanical deformation impart mobility to polymer glasses have been studied primarily for materials where the glassy state was formed stress free. Here, we investigate the stability of polymer glasses where a stress condition is applied during the formation of the glassy state (thermal quench). Previously we found [Gray et al., Macromolecules 2014, 47, 6686] that poly(styrene) macromolecularly imprinted by elongational flow deforms to form a non-conducting polystyrene phase and (often unintended) stress [Macromolecules 2012, 45, 1701]. We constructed a unique jig to apply a known stress to free-standing films during the thermal quench. We used ellipsometry to measure the physical aging rate of polystyrene films by quantifying the time-dependent decrease in film thickness that results from an increase in average film density during aging. As the magnitude of stress during vitrification increases, the physical aging rate quickly transitions over a small range of stresses to a faster aging rate, indicating the resulting glass is less stable [Soft Matter 2014, 10, 1572]. To explore this unique finding, we have constructed a computer-controlled apparatus to measure and apply stress and strain to polymer films during aging in order to characterize the temperature-dependent stress build up.

11:39AM G42.00003 Lithium dendrite growth through solid polymer electrolyte membranes, KATHERINE HARRY, NICOLE SCHAUSER, NITASH BALSA, UC Berkeley — Replacing the graphite-based anode in current batteries with a lithium foil will result in a qualitative increase in the energy density of lithium batteries. The primary reason for not adopting lithium-foil anodes is the formation of dendrites during charging. In this study, stop-motion X-ray microtomography experiments were used to directly monitor the growth of lithium dendrites during electrochemical cycling of symmetric lithium-lithium cells with a block copolymer electrolyte. In an attempt to understand the relationship between viscoelastic properties of the electrolyte on dendrite formation, a series of complementary experiments including cell cycling, tomography, and rheology, were conducted above and below the glass transition temperature of the non-conducting poly(styrene) block; the conducting phase is a mixture of rubbery poly(ethylene oxide) and a lithium salt. The tomography experiments enable quantification of the evolution of strain in the block copolymer electrolyte. Our work provides fundamental insight into the dynamics of electrochemical deposition of metallic films in contact with high modulus polymer electrolytes. Rational approaches for slowing down and, perhaps, eliminating dendrite growth are proposed.

11:51AM G42.00004 DNA-programmed Nanoparticle Self-Assembly and Crystallization via Multi-Scale Modelling & Simulation, TING LI, MONICA OLVERA DE LA CRUZ, Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, USA, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, NORTHWESTERN UNIVERSITY TEAM — In the past decades, DNA hybridization has proven promising to rationally guide nanoparticles to assemble into 1D, 2D and 3D structures, lattices and recently, faceted single crystals. In this sense, a gold nanoparticle coated by a dense shell of DNA behaves as a “programmable atom equivalent.” Using a scale-accurate coarse-grained model with explicit DNA chains, we identify that the key ingredient for achieving successful 3D crystallization is in the kinetics of DNA hybridization. We predict phase diagrams and propose suitable DNA linker sequences for optimal assembly. We determine the equilibrium shape of single crystals by computing surface energies. Surface energy fluctuations are further estimated for different surface orientations, and are shown to be critical in determining the equilibrium shape of a crystal. In addition, we apply a model with implicit DNA chains to study the kinetics of crystalization into faceted single crystals.

12:03PM G42.00005 Chain exchange in triblock copolymer micelles, JIE LU, TIMOTHY LODGE, FRANK BATES, University of Minnesota — Block polymer micelles offer a host of technological applications including drug delivery, viscosity modification, toughening of plastics, and colloidal stabilization. Molecular exchange between micelles directly influences the stability, structure and access to an equilibrium state in such systems and this property recently has been shown to be extraordinarily sensitive to the core block molecular weight in diblock copolymers. The dependence of micelle chain exchange dynamics on molecular architecture has not been reported. The present work conclusively addresses this issue using time-resolved small-angle neutron scattering (TR-SANS) applied to complimentary S-EP-S and EP-S-EP triblock copolymers dissolved in squalane, a selective solvent for the EP blocks, where S and EP refer to poly(styrene) and poly(ethylene-propylene), respectively. Following the overall SANS intensity as a function of time from judiciously deuterium labelled polymer and solvent mixtures directly probes the rate of molecular exchange. Remarkably, the two triblocks display exchange rates that differ by approximately ten orders of magnitude, even though the solvophilic S blocks are of comparable size. This discovery is considered in the context of a model that successfully explains S-EP diblock exchange dynamics.

12:15PM G42.00006 Mechanics of helical mesostructures from polymer-nanoparticle hybrids, JONATHAN PHAM, JIMMY LAWRENCE, GREGORY GRASON, TODD EMRICK, ALFRED CROSBY, University of Massachusetts Amherst — We describe the fabrication and mechanics of polymer and nanoparticle (NP)-based high-aspect ratio mesostructures, which we refer to as ribbons, with nm-scale cross-sections and up to cm-scale lengths. When placed into a fluid like water, interfacial tension associated with the ribbons’ intrinsic geometric asymmetry balances the elastic cost of bending, turning ribbons into helices with tunable preferred curvature. This universal, elastocapillary-based mechanism enables the reversible formation of helices from a variety of polymer and NP compositions, as demonstrated with specific examples of poly(methyl methacrylate), CdSe quantum dots, and gold NPs with polystyrene-azide and undecene ligands. Using custom-designed characterization methods, we quantitatively show that helices are highly stretchable with force-stretch relationships described by a nonlinear spring of finite extensibility. At small strains, these helices generate nN forces, offering mesostructures with a stiffness similar to single polymer chains (ca. 10^-6 N/m), and when fully stretched, they display properties similar to synthetic polymer nanofibers. These mesostructures offer a novel platform for engineering tunable materials with a broad range of mechanical properties and organic or inorganic functionality.
12:27PM G42.00007 Simple, generalizable route to highly aligned block copolymer thin films
, ZHE QIANG, KEVIN CAVICCHI, BRYAN VOGT, Univ of Akron — Macroscopic alignment of block copolymer domains in thin films is desired for many applications, such as cell responsive surfaces or optical polarizers. Alignment generally requires specialized tools that apply external fields, shear force gradient, or produce topological patterned substrates. This requirement limits the broad academic application of aligned BCPs. Here, we describe a simple modification of commonly utilized solvent vapor annealing (SVA) process for macroscopic alignment of BCPs. Adhering a flat, crossed elastics layer to the BCP film leads to partial alignment of the ordered BCP domains. The role of elastomer properties, solvent quality, drying rate and degree of segregation of the block copolymer will be discussed to provide generalized rules for alignment with this technique. Cylindrical nanostructures formed in polystyrene-block-polydimethylsiloxane can be transformed into arrays of silica lines and increasing the thickness from a monolayer to bilayer can effectively halve the spacing of the lines. These results illustrate a generalized method for BCP alignment and a potential route for the generation of complex hierarchical assembled structures.

12:39PM G42.00008 Nanoscale physical properties of polymer glasses formed by solvent-assisted laser depo

, KIMBERLY SHEPARD, CRAIG ARNOLD, RODNEY PRIESTLEY, Princeton University — High-energy, low-density nanostructured polymer glasses are formed via the solvent-assisted laser deposition technique MAPLE (Matrix Assisted Pulsed Laser Evaporation). During film deposition, micro- to nano-size polymer/solvent clusters are ejected via laser ablation from a frozen dilute polymer solution. During flight to the substrate under vacuum, the clusters experience rapid cooling and solvent stripping, forming polymer nanoglobules. Bulk polymer films are formed via the gradual assembly of these spherical-like nanostructured building blocks (i.e. nanoglobules). The MAPLE process thus enables investigation of the exceptional properties of glasses formed under extreme processing conditions. In the bulk state, we probe the effect of process parameters and chemical identity of the thermal behavior of a series of methacrylate polymers. We also employ multiple techniques to directly measure the properties of the polymer nanoglobules and connect the results to the global film properties.

Tuesday, March 3, 2015 11:15AM - 2:03PM –
Session G43 DPOLY DBIO GSOFT: Focus Session: Fluids Under Confinement and in Biological Systems

11:15AM G43.00001 Stiff Filamentous Viruses Probe the Mobility of Counterions During Nanopore Translocations , ANGUS MCMULLEN, JAY TANG, DEREK STEIN, Brown University — We study the electrophoresis of two different filamentous viruses and double-stranded DNA through solid-state nanopores. The two viruses we examine, fd and M13, are both 880 nm in length, 6.6 nm in diameter, very stiff, and monodisperse. They only differ in their linear charge density, which is 30% lower for M13 than for fd. Filamentous viruses are therefore ideal for testing transport models and for comparisons with DNA dynamics. We find that the mean translocation speed of fd virus is related to the nanopore diameter, D, and the virus diameter, d, as ln([D/d])−1, in agreement with the conventional electrokinetic model of translocations. In order to obtain quantitative agreement between that electrokinetic model and the measured translocation dynamics, however, one must conclude that the mobility of counterions within a few Angstroms of the polymer surface is strongly reduced from the bulk value. Similar reductions in counterion mobility near fd, M13, and dsDNA explain their dynamics over a wide range of ionic strengths. This work was supported by NSF Grant CBET0846505, NSF Grant PHY1069375 and Oxford Nanopore Technologies.

11:27AM G43.00002 Salmonella detection in a microfluidic channel using orbiting magnetic beads1. MATT BALLARD, ZACHARY MILLS, DREW OWEN, SRINIVAS HANASOGO, PETER HESKETH, ALEXANDER ALEXEEV, Georgia Institute of Technology — We use three-dimensional simulations to model the detection of salmonella in a complex fluid sample in a microfluidic channel. Salmonella is captured using magnetic microbeads orbiting around soft ferromagnetic discs at the microchannel bottom subjected to a rotating external magnetic field. Numerical simulations are used to model the dynamics of salmonella and microbeads throughout the detection process. We examine the effect of the channel geometry on the salmonella capture, and the forces applied to the salmonella as it is dragged through the fluid after capture. Our findings guide the design of a lab-on-a-chip device to be used for detection of salmonella in food samples in a way that ensures that salmonella captured by orbiting microbeads are preserved until they can be extracted from the system for testing, and are not washed away by the fluid flow or damaged due to the experience of excessive stresses. Such a device is needed to detect bacteria at the food source and prevent of consumption of contaminated food, and also can be used for the detection of a variety of biomaterials of interest from complex fluid samples.

1Support from USDA and NSF is gratefully acknowledged

11:39AM G43.00003 Sequencing proteins with transverse ionic transport , PAUL BOYNTON, MASSIMILIANO DI VENTRA, University of California, San Diego — De novo protein sequencing is essential for understanding cellular processes that govern the function of living organisms. By obtaining the order of the amino acids in the protein, one can determine both its secondary and tertiary structures through protein structure prediction, which is used to create models for protein aggregation diseases such as Alzheimer’s Disease [1]. Mass spectrometry is the current technique of choice for de novo sequencing, but because some amino acids have the same mass the sequence cannot be completely determined in many cases. In this paper we propose a new technique for de novo protein sequencing that involves translocating a polypeptide through a synthetic nanochannel and measuring the ionic current of each amino acid through an intersecting perpendicular nanochannel, similar to that proposed in [2] for DNA sequencing. Indeed, we find that the distribution of ionic currents for each of the 20 proteinogenic amino acids encoded by eukaryotic genes is statistically distinct, showing this technique’s potential for de novo protein sequencing.

11:51 AM G43.00004 Nanoscale Electrospray Ion Sources and a New DNA Sequencing Technique. WILLIAM MAULBETSCHE, Brown University, JOSEPH BUSH, Bronx Community College, DEREK STEIN, Brown University, STEIN LAB TEAM — Electrospray ion sources are used to transfer biochemical samples from solution into a charged gas phase for analysis, especially by mass spectrometry. Traditional ion sources require a background gas and high voltages, and waste most of the sample passed through the source’s micrometer-scale tip. However, by scaling down the ion source to the nanoscale, we greatly reduce voltage and sample volume requirements, while eliminating the need for a background gas to desolvate droplets. We report experiments investigating the onset and characteristics of electrospray from glass capillaries whose tips were pulled down to an inner diameter on the order of 100 nanometers. Nanoscale ion sources serve as an integral part of a DNA sequencing technique we will describe, whereby DNA bases are identified by the molecular masses of the nucleotides. This work was supported by NIH grant 1R21HG005100-01 and by Oxford Nanopore Technologies, Ltd.

12:03PM G43.00005 Statics and dynamics of softly confined polymers. ANDREA SCAGLIRANI, MAURO SBRAGAGLIA, Department of Physics, University of Rome “Tor Vergata”, MARCELLO SEGA, Department of Computational Biological Chemistry, University of Vienna — A variety of biological and technological problems where long chain molecules are constrained in spaces small compared to the molecule size (like membrane nanopores or nanofluidic slits) motivated recently a growing effort to understand the dynamics and structural scaling properties of polymers confined by solid walls. Our focus is, instead, on polymers confined in different geometries by soft interfaces, mimicking, e.g., DNA packaging inside cell nuclei or, mutatis mutandis, viral capsids. Soft-confinement is achieved by a proper choice of the solvation energies such that the polymer is trapped in one of the two phases of a binary mixture of immiscible liquids. We perform Molecular Dynamics simulations of polymers coupled with a fluctuating lattice Boltzmann method for the embedding matrix. Slab and droplet configurations are considered. In the former case we address the transition among various regimes of size scaling at changing the slab width. Under shear, the droplet is distorted from its equilibrium spherical shape and we explore how the transition from an isotropic geometry to a quasi-tube-like one affects polymer size scaling and knotting degree. Finally, we show how the feedback on the solvent induces viscoelastic rheology that can be related to polymer entanglement.

12:15PM G43.00006 Threading moieties play a significant role in determining the DNA binding properties of binuclear ruthenium complexes. THAYAPARAN PARAMANATHAN, Department of Physics, Bridgewater State University, Bridgewater, MA, ANDREW CLARK, Department of Physics, Northeastern University, Boston, MA, FREDRIK WESTERLUND, PER LINCOLN, Department of Chemical and Biological Engineering, Chalmers University of Technology, Gothenburg, MICAH J. MCCAULEY, Department of Physics, Northeastern University, Boston, MA, IOULIA ROUZINA, Department of Biochemistry, Molecular Biology and Biophysics, University of Minnesota, Minneapolis, MN, MARK C. WILLIAMS, Department of Physics, Northeastern University, Boston, MA — Binuclear ruthenium complexes are of interest due to their selective DNA binding properties, which make them potential candidates for chemotherapy. These dumbbell shaped molecules have to thread through the DNA base pairs to reach their final threaded intercalation state. Here we study the binuclear ruthenium complex, \( \Delta \Lambda^\mu \text{-bidppz}(bpy)_2\text{Ru}^{4+} \), and compare it with the previously studied \( \Delta \Lambda^\mu \text{-hidppz}(phen)_2\text{Ru}^{4+} \). Both have the same intercalating bridge unit, but different threading moieties. In this study, we stretch a single DNA molecule held with optical tweezers in the presence of the ligand at various concentrations and hold the DNA at constant force until an equilibrium DNA elongation is reached. The extension of the DNA obtained as a function of time during binding yields the kinetics and equilibrium binding properties of the ligand. The preliminary data suggests that the binuclear complex with bpy in the threading moiety shows stronger affinity and an order of magnitude faster on rate, compared to its counterpart with phen in the threading moiety. This confirms the hypothesis that the extra aromatic ring of phen interferes with the threading intercalation process.

12:27PM G43.00007 Physics and (patho)physiology in confined flows: from colloidal patterns to cytoplasmic rheology and sickle cell anemia. L. MAHADEVAN, Harvard University — I will discuss a few problems that involve the interaction of fluids and solids in confined spaces. (i) Jamming in pressure-driven suspension flows that show a transition from Stokes flows to Darcy flows as the solids start to lock, as in evaporative patterning in colloids (e.g., coffee stain formation). (ii) Jamming and clogging of red blood cells, as in sickle-cell pathophysiology, with implications for other diseases that involve jamming. (iii) The mechanical response of crowded networks of filaments bathed in a fluid, as in the cytoskeleton, that can be described by poroelasticity theory. In each case, I will show how simple theories of multiphase flow and deformation can be used to explain a range of experimental observations, while failing to account for others, along with some thoughts on how to improve them.

1:03PM G43.00008 Quantifying the molecular mechanism for highly stereo-selective DNA threading intercalation. ALI ALMAQWASHI, Northeastern University, JOHANNA ANDERSSON, Uppsala University, PER LINCOLN, Chalmers University of Technology, IOULIA ROUZINA, University of Minnesota, FREDRIK WESTERLUND, Chalmers University of Technology, MARK C. WILLIAMS, Northeastern University — DNA threading intercalators, such as binuclear ruthenium complexes, are regarded as potential DNA-targeted therapeutic drugs because of slow kinetics and high affinity. Recent bulk studies reported that poly(dADT) threading intercalation by the binuclear ruthenium complex \( \mu \text{-dpzip(phen)}_2\text{Ru}^{4+} \) is highly stereo-selective. The largest fractional binding was achieved for \( \Delta \Lambda^\mu \text{-Piz} \), with the \( \Lambda \) (right handed) configuration at the distal imidazophenanthroline (ip) subunit and the \( \Lambda \) (left handed) configuration at the distal imidazophenanthroline (ip) subunit. To quantify this highly stereo-selective molecular mechanism, we used optical tweezers to probe single \( \lambda \)-DNA molecules elongation due to the threading intercalation by each of \( \Delta \Lambda^\mu \text{-Piz} \) and \( \Delta \Lambda^\mu \text{-Piz} \). While maintaining a DNA stretching force of 30 pN and a ligand concentration of 5 nM, the elongation was traced until reaching equilibrium. Then it was traced back to the free DNA extension by rinsing out the bound ligands. We found that the equilibrium elongation for \( \Delta \Lambda^\mu \text{-Piz} \) is 30% larger, and the affinity is 50% higher relative to \( \Delta \Lambda^\mu \text{-Piz} \). Further force-dependent study will quantitatively determine the differences in the zero-force binding site size, affinity and the DNA structural dynamics for association and dissociation.

1:15PM G43.00009 Improving signal-to-noise performance for DNA translocation in solid-state nanofluidic channels. THOLOMEOUS MACHIELSE, ADRIAN BALAN, University of Pennsylvania, JIANXUN LIN, PEIJIE ONG, Columbia University, REBECCA ENGELKE, Univ of Pennsylvania, KENNETH SHEPARD, Columbia University, MARIJA DRNĐIC, Univ of Pennsylvania — DNA sequencing using solid-state nanofluidic channels is impeded by the relatively high noise and low bandwidth of the current state-of-the-art translocation measurements. We measure the ion current noise through SiN nanofluidic channels at bandwidths up to 1 MHz. At these bandwidths, the input-referred current noise is dominated by the amplifier’s voltage noise acting across the total capacitance at the amplifier input. By reducing the nanopore membrane capacitance we are able to transition to a regime in which current noise is dominated by the effects of the capacitance of the amplifier itself. Advances in bandwidth and signal-to-noise ratio necessary for DNA sequencing will require lower capacitance devices as well as new amplifier designs with reduced input capacitance and noise characteristics.

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1. This work was supported by NIH Grants R21HG004767 and R01HG006879. We gratefully acknowledge use of the TEM in the NSF-MRSEC electron microscopy facility. We thank Andrew Sharo, Matthew Puster, Dr. Kimberly Venta, and Prof. Jacob Rosenstein.
2. These authors contributed equally.
3. These authors contributed equally.
1:27PM G43.00010 DNA translocation measurements through low-capacitance solid-state nanopore chips at high bandwidths, CHEN-CHI CHIEN, DAVID NIEDZWIECKI, BARTHOLOMEUS MACHIELSE, ADRIAN BALAN, University of Pennsylvania, JIANXUN LIN, PEIJIE ONG, KENNETH SHEPARD, Columbia University, MARIJA DRNDIC, University of Pennsylvania — We perform DNA translocation measurements with low-noise solid state nanopore chips. We obtain higher ion current signal-to-noise ratio and better resolution in ion current signals than previously reported in solid state nanopores at high bandwidths with chip capacitance lowering techniques of applying extra insulation on the chip surface. We show measurements of ion current during translocation of DNA molecules through thin silicon nitride (SiN) nanopores of small diameters at megahertz bandwidths with enhanced ion current signal-to-noise ratios. We further discuss how these results possibly pave the way towards identifying intramolecular DNA sequences with solid-state nanopores.

1:39PM G43.00011 Up and down events in nanoparticle translocation through solid-state nanopores, MEHDI ZANJANI, REBECCA ENGELKE, JENNIFER LUKES, MARIJA DRNDIC, University of Pennsylvania — We study translocation of nanoparticles through solid-state nanopores. Normally, nanoparticle passage is expected to decrease ion current inside the nanopores, as in the case of typical Coulter counters. However, recent experiments have reported translocation events that show an increase in the ion current. We refer to such decrease and increase in ion current as down events and up events respectively. We use theoretical methods to study such events and to determine the conditions under which they happen. A transition nanopore diameter, \( d_t \), is calculated from the theoretical model; up events are observed for nanopore diameters smaller than \( d_t \), while for nanopore diameters larger than \( d_t \), down events will occur. We also discuss how a simple mechanism can be implemented to distinguish nanoparticles of different shapes and sizes based on such up and down translocation events.

This work was supported by the NSF MRSEC grant DMR-1120901

1:51PM G43.00012 Structural Integrity of Proteins under Applied Bias during Solid-State Nanopore Translocation \( t \), MOHAMMAD R. HASAN, RAJA RAHEEL KHANZADA, MOHAMMED A. I. MAHMOOD, ADNAN ASHAFAQ, University of Texas at Arlington, SAMIR M. IQBAL, Nano-Bio Lab, Electrical Engineering, Bioengineering, University of Texas at Arlington — The translocation behavior of proteins through solid-state nanopores can be used as a new way to detect and identify proteins. The ion current through a nanopore that flows under applied bias gets perturbed when a biomolecule traverses the Nanopore. It is important for a protein detection scheme to know of any changes in the three-dimensional structure of the molecule during the process. Here we report the data on structural integrity of protein during translocation through nanopore under different applied biases. Nanoscale Molecular Dynamic was used to establish a framework to study the changes in protein structures as these travelled across the nanopore. The analysis revealed the contributions of structural changes of protein to its ion current signature. As a model, thymopin protein crystalline structure was imported and positioned inside a 6 nm diameter pore in a 6 nm thick silicon nitride membrane. The protein was solvated in 1 M KCl at 295 K and the system was equilibrated for 20 ns to attain its minimum energy state. The simulation was performed at different electric fields from 0 to 1 kCal/(mol.˚A.e). RMSD, radial distribution function, movement of the center of mass and velocity of the protein were calculated. The results showed linear increments in the velocity and perturbations in ion current profile with increasing electric potential.

Support Acknowledged from NSF through ECCS-1201878

Tuesday, March 3, 2015 11:15AM - 2:03PM –
Session G44 GSNP: Focus Session: Extreme Mechanics: Contortion of Filaments, Ribbons and Bundles

11:15AM G44.00001 Spontaneous formation of singularities in twisted ribbons, JULIEN CHOPIN, ESPCI, ARSHAD KUDROLLI, Clark University — We present experimental results on the spontaneous formation of a triangular tessellation of a thin elastic ribbon which is twisted with a prescribed longitudinal tension. We find that triangular patterns arise out of a period doubling of a primary longitudinal instability as the twist is increased in contrast with theoretical development assuming infinitely thin, inextensible sheet. Using x-ray tomography, we are able to reconstruct the 3D shape of the ribbon which can then be precisely characterized by measuring locally the mean and Gaussian curvature. We discuss quantitatively the structures of singularities (d-cones and ridges) as a function of nondimensional parameters characterizing the twist, the tension, and the geometry of the ribbon. Because the observed singularities occur away from walls and boundaries, the twisted ribbon configuration provides a unique opportunity to address the spontaneous formation of localized structures with great experimental flexibility.

11:27AM G44.00002 Perversions driven spontaneous symmetry breaking in heterogeneous elastic ribbons, SHUANGPING LIU, ZHENWEI YAO, MONICA OLVERA DE LA CRUZ, Northwestern Univ — Perversion structures in an otherwise uniform helical structure are associated with several important concepts in fundamental physics and materials science, including the spontaneous symmetry breaking and the elastic buckling. They also have strong connections with biological motifs (e.g., bacteria shapes and plant tendrils) and have potential applications in micro-muscles and soft robotics. In this work, using a three-dimensional elastomeric bi-stripe model, we investigate the properties of perversions that are independent of the specific ribbon shapes. Several intrinsic features of perversions are revealed, including the spontaneous condensation of energy as well as the distinct energy transfer modes within the perversion region. These properties of perversions associated with the storage of elastic energies can be exploited in the design of actuator devices.

We thank the financial support from the U.S. Department of Commerce, National Institute of Standards and Technology, the Office of the Director of Defense Research and Engineering (DDR&E) and the Air Force Office of Scientific Research.

11:39AM G44.00003 Deswelling and buckling of a temperature-sensitive hydrogel toroid, MICHAEL DIMITRIYEV, YA-WEN CHANG, ANTÓN SÓUSLOV, ALBERTO FERNANDEZ-NIEVES, PAUL GOLDBART, Georgia Institute of Technology — Temperature-sensitive hydrogels lose volume with increasing temperature by expelling water from their polymer matrix, which becomes effectively hydrophobic above a certain critical temperature. Whilst the temperature response of a spherically shaped sample of hydrogel has been well studied, less is known about the response of a toroidal sample. We present a model for the behavior of a hydrogel toroid for two cases of heating protocol: (i) the quasistatic limit, in which the sample loses volume but is found to maintain its toroidal shape; and (ii) the rapid quench limit, after which the sample is found to have maintained its volume but may have undergone a macroscopic, qualitative change of shape to a buckled toroid. For the quench-limit case, we develop a criterion for the stability of the rotationally symmetric state of the toroid, by utilizing an effective elastic ring model. When this criterion is no longer met, a long-wavelength deformation leads to a buckling instability of the toroid in a manner analogous to the buckling of an Euler rod.
12:27PM G44.00005 Stretchability of freestanding and polymer-supported serpentine thin films\textsuperscript{1}, NANNSHU LU, SHIXUAN YANG, University of Texas at Austin — High-performance stretchable electronics integrate high-quality inorganic electronic materials such as metal, semiconductor and oxide with deformable polymer substrates. To minimize strains in inorganic materials under large deformation, metal and ceramic thin films can both be patterned into meandering serpentine ribbons which can rotate and twist to accommodate the applied strain. We have systematically investigated the effects of geometry and substrate stiffness on the stretchability of serpentine through both theoretically and experimental means. For freestanding serpentine, closed-form analytical solutions are obtained and validated by experiments. To investigate the effect of substrates, indium tin oxide (ITO) serpentine are patterned on both polyimide and elastomeric substrates with systematically changing geometries. While stiff substrates such as polyimide almost completely prevents the rotation or twist of the serpentine, soft substrates can provide serpentine with reasonable freedom of rotation and twisting, which yields stretchability of ITO ribbons beyond 100\%. But new failure mechanisms have been found on soft substrates.

\textsuperscript{1}This work is supported by the NSF NERC - NASCENT under Grant No. 1160494.

12:39PM G44.00006 Coiling of elastic rods from a geometric perspective, MOHAMMAD JAWED, PIERRE-THOMAS BRUN, PEDRO REIS, Massachusetts Institute of Technology — We present results from a systematic numerical investigation of the pattern formation of coiled obtained when a slender elastic rod is deployed onto a moving substrate; a system known as the elastic sewing machine (ESM). The Discrete Elastic Rods method is employed to explore the parameter space, construct phase diagrams, identify their phase boundaries and characterize the morphology of the patterns. The nontrivial geometric nonlinearities are described in terms of the gravito-bending length and the deployment height. Our results are interpreted using a reduced geometric model for the evolution of the position of the contact point with the belt and the curvature of the rod in its neighborhood. This geometric model reproduces all of the coiling patterns of the ESM, which allows us to establish a universal link between our elastic problem and the analogous patterns obtained when depositing a viscous thread onto a moving surface; a well-known system referred to as the fluid mechanical sewing machine.

12:51PM G44.00007 The shape of strings to come: How topological defects twist, bend, and wrinkle filament bundles\textsuperscript{1}. ISAAC BRUSS, GREGORY GRASON, Univ of Mass - Amherst — Topological defects are crucial to the thermodynamics and structure of condensed matter systems. For instance, when incorporated into crystalline membranes like graphene, 5- and 7-fold disclinations produce conical- and saddle-like geometries respectively. A recently discovered mapping between the inter-filament spacing within a deformed bundle and the metric properties of curved surfaces, suggests previously unexplored parallels between the two, specifically in regards to how 2D patterning promotes 3D shape transitions. This discovery is poised to describe the structure of a host of filamentous materials—both biological and microfabricated—that exhibit distinctive shapes and packings. Motivated by the filamentous analogs to the conical and saddles shapes found in thin membranes, we investigate for the first time the interplay between defects in the cross section of a bundle and its global structure, using a combination of continuum elasticity theory and numerical simulation of cohesive bundles with a fixed packing topology. Focusing primarily on the instability response to disclinations, we predict a host of new equilibria structures, some of which are without direct parallel to the analogous membrane, including torsional wrinkling, radial kinking, and helical winding.

\textsuperscript{1}Center for Hierarchical Manufacturing-CMMI 10-25020, NSF CAREER Award-DMR 09-55760, & UMass MРSEC

1:03PM G44.00008 Rotation of a Thin Elastic Rod Injected into a Cylindrical Constraint\textsuperscript{1}, CONNOR MULCAHY, Massachusetts Institute of Technology, TIANXIANG SU, NATHAN WICKS, JAHIR PABON, Schlumberger-Doll Research, PEDRO REIS, Massachusetts Institute of Technology — We report the results from an experimental investigation of the buckling of a thin elastic rod injected into a horizontal cylindrical constraint, with an emphasis on comparing the two cases of rotating, or not, the rod at the injection site. We are particularly interested on the total length of rod that can be injected into the pipe prior to the onset of helical buckling. This instability arises due to the frictional rod-constraint contact that eventually leads to the buildup of axial stress on the rod, above a critical value. We explore the dependence of the buckling conditions on the physical and control parameters of the system (e.g. material and geometric parameters, injection speed and rotation frequency) and rationalize the underlying physical mechanism through a reduced model.

\textsuperscript{1}Funding and support provided by Schlumberger-Doll Research.

1:15PM G44.00009 Stress localisation in annular sheets, GERT VAN DER HEIJDEN, EUGENE STAROSTIN, University College London — For very thin sheets stretching is much more costly in terms of energy than bending. The limiting behaviour of thin sheets is therefore governed by geometry only and thus applies to a wide range of materials at vastly different scales: it is equally valid for a microscopic graphene sheet and a macroscopic sail. We derive new geometrically-exact equations for the deformation of annular strips. We use a formulation in which the inextensibility constraint is used to reduce the problem to a suitably-chosen reference curve (here the circular centreline). The equations are therefore ODEs, which allow for a detailed bifurcation analysis. Closed conical solutions are found for centreline lengths \( L < L_c = 2\pi \kappa_0 \), where \( \kappa_0 \) is the geodesic curvature of the strap. For such 'short' strips we find in addition a second branch of solutions easily reproduced in a paper strip. For 'long' strips (\( L > L_c \)) we find modes of undulating solutions. All non-conical solutions turn out to feature points of stress localisation on the edge of the annulus, the outer edge for short solutions and the inner edge for long solutions. Our theory may be used to investigate singularities of constrained or loaded sheets more general than conical ones.

1:27PM G44.00010 Large-deformation dynamics of an elastic filament at a fluid interface, SRINIVASA GOPALAKRISHNAN GANGA PRASATH, JOEL MARTELOT, RAMA GOVINDARajan, TCIS, TIIFR Hyderabad and Dept. of Physics, UMass Amherst, TCIS, TIFR Hderabad and DEPT. OF PHYSICS, UMASS AMHERST COLLABORATION — We study the dynamics of a thin elastic filament at the interface of two fluids and observe the time evolution in its shape when released from an initial configuration with a large curvature. The unfolding of the filament is driven by a competition between bending energy and viscous dissipation. We experimentally study the overdamped regime of this system by varying fluid viscosity (\( \nu \)), length (\( L_f \)) diameter (\( d \)) and elastic modulus (\( E \)) of the filament with similar initial conditions and observe the kinematics of the filament straightening. The time-dependence for this process can be collapsed by scaling time by \( \nu L_f^4 / Ed \). However, the characteristic time is a very small fraction of this time-scale. We perform numerical computations parallel to the experiments to get access to the dynamics of the filament to resolve this puzzle. An understanding of the time-dependence will enable the use of this technique to measure interfacial properties.
1:39PM G44.00011 Elasto-capillary windlass: from spider web to synthetic actuators1, HERVÉ ELETTRO, ARNAUD ANTKOWIAK, SÉBASTIEN NEUKIRCH, Institut d’Alembert, FRITZ VOLLRATH, Oxford Silk Group, INSTITUT D’ALEMBERT TEAM, OXFORD SILK GROUP TEAM — Spiders’ threads display a wide range of materials properties. The glue-covered araneid capture silk is unique among all silks because it is self tensing and remains taut even if compressed, allowing both thread and web to be in a constant state of tension. Here we demonstrate how this effect is achieved by unraveling the physics allowing the nanolitre glue droplets straddling the silk thread to induce buckling, coiling and spooling of the core filaments. Our model explains this windlass activation as a structural phase transition, which shows that fibre spooling results from the interplay between elasticity and capillarity. Fibre size is the key as such a capillary windlass requires micrometer-sized fibres in order to function. Our synthetic capillary windlasses point towards design principles for new bioinspired synthetic actuators.

1The present work was supported by ANR grant ANR-09-JCJC-0022-01, “La Ville de Paris - Programme Emergence,” Royal Society International Exchanges Scheme 2013/R1 grant EI130506, and the PEPS PTI program from CNRS.

1:51PM G44.00012 Variability of Fiber Elastic Moduli in Composite Random Fiber Networks Makes the Network Softer, EHSAN BAN, CATALIN PICIU, Rensselaer Polytech Inst — Thermal fiber networks are assemblies of beams or trusses. They have been used to model mechanics of fibrous materials such as biopolymer gels and synthetic nonwovens. Elasticity of these networks has been studied in terms of various microstructural characteristics such as the stiffness of their constituent fibers. In this work we investigate the elasticity of composite fiber networks made from fibers with moduli sampled from a distribution function. We use finite elements simulations to study networks made by 3D Voronoi and Delaunay tessellations. The resulting data collapse to power laws showing that variability in fiber stiffness makes fiber networks softer. We also support the findings by analytical arguments. Finally, we apply these results to a network with curved fibers to explain the dependence of the network’s modulus on the variation of its structural parameters.

Tuesday, March 3, 2015 11:15AM - 2:15PM — Session G45 DPOLY: Focus Session: Polymers in Batteries and Electrochemical Capacitors I

11:15AM G45.00001 Electrostatic Assembly of Nanomaterials for Hybrid Electrodes and Supercapacitors, PAULA HAMMOND, Massachusetts Institute of Technology — Electrostatic assembly methods have been used to generate a range of new materials systems of interest for electrochemical energy and storage applications. Over the past several years, it has been demonstrated that carbon nanotubes, metals, metal oxides, polymeric nanomaterials, and biotemplated materials systems can be incorporated into ultrathin films to generate supercapacitors and battery electrodes that illustrate significant energy density and power. The unique ability to control the incorporation of such a broad range of materials at the nanometer length scale allows tailoring of the final properties of these unique composite systems, as well as the capability of creating complex micron-scale to nanoporous morphologies based on the scale of the nanomaterial that is absorbed within the structure, or the conditions of self-assembly. Recently we have expanded these capabilities to achieve new electrodes that are templated atop electrospun polymer fiber scaffolds, in which the polymer can be selectively removed to achieve highly porous materials. Spray-layer-by-layer and filtration methods of functionalized multiwall carbon nanotubes and polyaniline nanofibers enable the generation of electrode systems with unusually high surface. Incorporation of pseudocapacitive nanoparticles can enhance capacitive properties, and other catalytic or metallic nanoparticles can be implemented to enhance electrochemical or catalytic function.

11:51AM G45.00002 High Energy Density and High Temperature Multilayer Capacitor Films for Electric Vehicle Applications1, IMRE TREUFELD, MICHELLE SONG, LEI ZHU, ERIC BAER, Case Western Reserve University, JOE SNYDER, Orbital Research Inc., DEEPAK LANGHE, Polymer Plus LLC. — Multilayer films (MLFs) with high energy density and high temperature capability (>120 °C) have been developed at Case Western Reserve University. Such films offer a potential solution for electric car DC-link capacitors, where high ripple currents and high temperature tolerance are required. The current state-of-the-art capacitors used in electric cars for converting DC to AC use biaxially oriented polypropylene (BOPP), which can only operate at temperatures up to 85 °C requiring an external cooling system. The polycarbonate (PC)/poly(vinylidene fluoride) (PVDF) MLFs have a higher permittivity compared to that of BOPP (2.3), leading to higher energy density. They have good mechanical stability and reasonably low dielectric losses at 120 °C. Nonetheless, our preliminary dielectric measurements show that the MLFs exhibit appreciable dielectric losses (20%) at 120 °C, which would, despite all the other advantages, make them not suitable for practical applications. Our preliminary data showed that dielectric losses of the MLFs at 120 °C up to 400 MV/m and 1000 Hz originate mostly from impurity ionic conduction.

1This work is supported by the NSF PF1/BIC program (IIP-1237708)

12:03PM G45.00003 Orientationally Ordered Lamellar Block Copolymer Films for Electrostatic Capacitor Applications, CHRISTOPHER GRABOWSKI, Air Force Research Laboratory, SAUMIL SAMANT, ALAMGIR KARIM, Univ. of Akron, MICHAEL DURSTOCK, Air Force Research Laboratory — Improving the maximum operating voltage of an electrostatic capacitor requires materials that can better suppress breakdown initiation and/or forestall breakdown propagation. Progress has been made in developing layered architectures through polymer co-extrusion and inorganic nanocomposites, which create tortuous pathways to the applied electric field, resulting in increased breakdown strength. Block copolymer films provide another route to achieve such layered structures, while allowing more control over orientation, domain size, and morphology. We report the dielectric performance of micron-thick linear diblock copolymer films consisting of polystyrene-b-poly-2-vinylpyridine and polystyrene-b-poly methyl methacrylate, focusing on molecular weight ratios that yield lamellar and spherical morphologies. Specialized techniques such as cold-zone soft shear annealing allow for the precise control of lamellae orientation (layering parallel or perpendicular to the applied electric field). Our results indicate dielectric breakdown performance for parallel ordered lamellae is greater than comparable perpendicularly lamellae and as-cast films with no induced microphase separation, which we attribute to the presence of interfacial layers that act as barriers to the applied field.

12:15PM G45.00004 Origins of enhanced capacity retention in copolymerized sulfur-based composite cathodes for Li-S batteries, CHRISTOPHER SOLES, VLADIMIR OLESHKO, JENNY KIM, STEVEN HUDSON, NIST, KOOKEON CHAR, Seoul National University, JARED GRIEBEL, ADAM SIMMONDS, RICHARD GLASS, JEFF PYUN, University of Arizona — Poly(sulfur-random-(1,3-diisopropenylbenzene) (poly(S-r-DIB)) copolymers synthesized via inverse vulcanization form high molecular mass electrochemically active polymers capable of enhanced capacity (1005 mAh/g at 100 cycles) and lifetimes over 500 cycles as cathodes for Li-S batteries. In this presentation we characterize the morphology when the poly(S-r-DIB) copolymers are mixed conductive carbon to form functional Li-S cathodes. Scanning and transmission electron microscopy are used to demonstrate that the use elemental sulfur leads to heterogeneous aggregates of carbon nanoparticles and poor mixing with the sulfur, forming a loosely percolated network of electrically conductive pathways and extended micro- and mesoscale porosity. The poly(S-r-DIB) copolymers tend to mix more intimately with the carbon nanoparticles because of a stronger cohesion between the components. This increases the compositional homogeneity, increases the contact between the electrochemically active components and improves the physico-mechanical stability of the cathode which leads to increased capacity and enhanced cycle life in a full battery. We also introduce a new Li ion microscopy technique as a tool for characterizing battery materials.
12:27PM G45.00005 Effect of Molecular Weight on Mechanical and Electrochemical Performance of All Solid-State Polymer Electrolyte Membranes1, RUIXUAN HE, University of Akron, DANIEL WARD, Miami University, MAURICIO ECHEVERRI, Kent Displays Inc., THEIR KYU, University of Akron — Guided by ternary phase diagrams of polyethylene glycol diacrylate (PEGDA), succinonitrile plasticizer, and LiTFSI salt, completely amorphous solid-state transparent polymer electrolyte membranes (ss-PEM) were fabricated by UV irradiation in the isotropic melt state. Effects of PEGDA molecular weight (700 vs 6000 g/mol) on ss-PEM performance were investigated. These amorphous PEMs have superionic room temperature ionic conductivity of $\sim 10^{-3}$ S/cm, whereby PEGDA6000-PEM outperforms its PEGDA700 counterpart, which may be ascribed to lower crosslinking density and greater segmental mobility. The longer chain between crosslinked points of PEGDA6000-PEM is responsible for greater extensibility of $\sim 80\%$ versus $\sim 7\%$ of PEGDA700-PEM. Besides, both PEMs exhibited thermal stability up to 120 °C and electrochemical stability versus Li$^+$/Li up to 4.7V. LiFePO$_4$/PEM/Li and Li$_2$Ti$_3$O$_7$ /PEM/Li half-cells exhibited stable cyclic behavior up to 50 cycles tested with a capacity of $\sim 140\text{mAh/g}$, suggesting that LiFePO$_4$/PEM/Li$_2$Ti$_3$O$_7$ may be a promising full-cell for all solid-state lithium battery.

1We thank NSF-DMR 1161070 for providing funding of this project.

12:39PM G45.00006 Stacked Polymer nanofiber array for high-performance supercapacitors1, SHIREN WANG, Texas A&M Univ, JENNY QIU, Texas Tech University — The vertically aligned polyaniline (PANI) nanowires arrays and monolayer graphene sheets were layer-by-layered deposited to specific substrate for tailored structures. Driven by external voltage, aniline molecules and graphene oxide were alternatively assembled for hierarchical porous three-dimensional nanostructures while graphene oxide was in-situ reduced to graphene during the assembly process. As-produced stacked arrays were used as the electrodes of an ultra-capacitor, and an unusual electrochemical behavior was discovered. The capacitance increases as the stack of nanowire arrays increases, resulting in high energy density and high power density at same time. Further analysis found that the distinctive electrochemical behavior originates from the electrode/electrolyte interactions and the dependence on the diffusion and charge transferring process. The specific energy density was as high as 137 Wh/Kg while power density is in excess of 2000 W/Kg. This work pointed a simple pathway to tailor polymer structure and electrochemistry for robust design of high-performance ultra-capacitor at a limited lateral size.

1National Science Foundation

12:51PM G45.00007 Sprayable, Paintable Layer-by-Layer Polyaniline Nanofiber/Graphene Electrodes for Electrowe Storage , SE RA KWON, JU-WON JEON, JODIE LUTKENHAUS, Department of Chemical Engineering, Texas A&M University — Sprayable batteries are growing in interest for applications in structural energy storage and power or flexible power. Spray-assisted layer-by-layer (LbL) assembly, in which complementary species are alternately sprayed onto a surface, is particularly amenable towards this application. Here, we report on the fabrication of composite films containing polyaniline nanofibers (PANI NF) and graphene oxide (GO) sheets fabricated via spray-assisted LbL assembly. The resulting films are electrochemical reduced to yield PANI NF/electrochemically reduced graphene (ERGO) electrodes for use as a cathode in non-aqueous energy storage systems. Through the spray-assisted LbL process, the hybrid electrodes could be fabricated 74 times faster than competing dip-assisted LbL assembly. The resulting electrodes are highly porous (0.72 void fraction), and are comprised of 67 wt% PANI NF and 33 wt% ERGO. The sprayed electrodes showed better rate capability, higher specific power, as well as more stable cycle life than dip-assisted LbL electrodes. It is shown here that the spray-assisted LbL approach is well-suited towards the fabrication of paintable electrodes containing polyaniline nanofibers and electrochemically reduced graphene oxide sheets.

1:03PM G45.00008 Superionic solid-state polymer electrolyte membrane for high temperature applications1, THEIR KYU, University of Akron, RUIXUAN HE, JINWEI CAO, University of Akron — Completely amorphous, flexible, solid-state polymer electrolyte membranes (ss-PEM) consisted of polyethylene glycol diacrylate/succinonitrile plasticizer (SCN)/lithium trifluorosulfonyl imide were fabricated via UV polymerization. The room temperature ionic conductivity of our ss-PEM is extremely high (i.e., $10^{-3}$/S/cm), which is already in the superionic conductor range of inorganic and/or liquid electrolyte counterparts. Of particular interest is that our ss-PEM is thermally stable up to 140°C, which is superior to the liquid electrolyte counterpart that degrades above 80°C. The ss-PEM exhibits cyclic stability in both LiFePO$_4$/Li and Li$_2$Ti$_3$O$_7$/Li half-cells up to 50 cycles tested. The trend of conductivity enhancement with temperature is reproducible in the repeated cycles, showing melting transitions of the SCN plastic crystals. In the compositions close to the solid (SCN plastic crystal)-liquid coexistence line, polymerization-induced crystallization occurs during photo-curing. The effect of solid-liquid segregation on ionic conductivity behavior is discussed.

1Supported by NSF-DMR 1161070

1:15PM G45.00009 Spatial position control of nanofeatures assisted by nanoporous templates fabricated by block copolymer based lithography, DONG HYUN LEE, DONG-EUN LEE, Dankook Univ — Herein, we demonstrated a unique method to control spatial arrangement of nanofeatures by using topographically patterned substrates. The thin films of block copolymers (BCPs) were firstly prepared on a thin layer of poly(vinyl alcohol) (PVA). Then to induce ordering of the BCPs, the thin films were solvent-annealed, DONG HYUN LEE, DONG-EUN LEE, Dankook Univ — Herein, we...
2:03PM G45.00013 Effect of Mobile Ions on the Electric Field Needed to Orient Charged Diblock Copolymer Thin Films, ASHKAN DEHGHAN, McMaster Univ, Michael Schick, University of Washington, An-Chang Shi, McMaster Univ, POLYMER THEORY MCMASTER UNIVERSITY TEAM, POLYMER THEORY UNIVERSITY OF WASHINGTON TEAM — We examine the behaviour of lamellar phases of charged, diblock copolymer, thin films with mobile counter-ions in the presence of an electric field. We employ self-consistent field theory, and focus on the aligning effect of the electric field on the lamellae. Of particular interest are the effects of the mobile ions on the critical field, which is the value of the field required to reorient the lamellae from the parallel configuration favoured by the surface interaction to the perpendicular orientation favoured by the electric field. We find that the critical field depends strongly on the location of the mobile ions within the system. In the case in which mobile ions are confined such that each charged lamella is electrically neutral, the presence of ions lowers the critical electric field. However, if ions are free to locate anywhere within the system, so that only the system as a whole is electrically neutral, then the presence of ions can increase the critical electric field. The presence of ions in the system introduces a new mixed phase, parallel in the bulk, parallel at the surfaces, in addition to those reported previously.

11:15AM G46.00001 Deterministic Modelling of Carbon Nanotube Near-Infrared Solar Cells, DARIN BELLISARIO, Massachusetts Institute of Technology, Dept. of Chemistry — With solution-process-ability, scale-able fabrication and purification, and cheap input materials, semiconducting single-walled carbon nanotube (SWNT) networks represent promising materials for near-IR solar cell (SC) applications. This promise has motivated a body of work not only developing solar cells but also exploring alignment/deposition methods and SWNT photovoltaic (PV) physics. Despite this interest, there is to date no quantitative model of SWNT solar cell operation analogous to bulk semiconductor p-n junction PVs, allowing a rigorous understanding of the physical tradeoffs driving experimental observations and informing what research will enable technological progress. In this work we have derived the steady state operation of planar heterojunction SWNT PVs from the fundamental light absorption, exciton transport, and free carrier transport behaviors of single nanotubes. Our method can treat arbitrary distributions of nanotube chiralities, lengths, orientations, defect types and concentration, bundle fraction and size, density, dielectric environment, electrode combinations, etc. We achieve this by treating individual SWNT properties as random variables, and describing the network by the dependent distributions of those properties, yielding coupled stochastic differential equations for light absorption, exciton transport, and free carrier transport. Applying the model to monochiral (6,5) films in aligned and isotropic configurations, we find that there is a strongly optimal film thickness less than at which photo-injecting networks transport light from the electrodes to the nanotubes and beyond the optimal thickness, the network is not efficient. The network is optimal for a SWNT exciton transport relative to exceptional intra-SWNT diffusion, vertically-aligned films are unambiguously favored at densities above 3% of close-packed; at lower densities however an optimum emerges at an intermediate angle to compensate for weaker light absorption of vertical nanotubes. Films with in-plane aligned nanotubes are unambiguously the worst design.

11:51AM G46.00002 Exotic Forms of Silicon for Energy Applications, J. P. CRAIG TAYLOR, Colorado School of Mines — Over the last few decades many exotic forms of carbon, such as carbon-60, carbon nanotubes, and graphene, have generated novel scientific discoveries and revolutionized many important applications. Similarly potential transformative breakthroughs may be expected with exotic forms of silicon. Such structures include, but are not necessarily limited to, (1) those formed under high pressure that are metastable at ambient pressure, (2) single layers of Si (silicene), (3) nanoflakes, (4) porous Si, and (5) any other structures that differ in their structural, optical or electronic properties from bulk diamond Si. Silicon is an abundant, non-toxic element around which an advanced technology exists for semiconductor devices based on diamond Si. One of these exotic forms of silicon could form the basis for the next revolution in electronics or even opto-electronics, since it comes from the exhibit direct or, nearly direct, band gaps. Recent results toward producing pure and dopable semiconductor out of Si nanodots imbedded in amorphous matrices and in clathrate Si and clathrate Si-Ge alloys will be discussed.

** footnote **

1 The author acknowledges important collaborations with R. T. Collins, C. A. Koh, L. Krishna, M. Lusk, and P. Stradins. DOE SUNSHOT program, under contract DE-EE0005326 and by the NSF MRSEC program under grant DMR-0820518.
Upon temperature changes, we observe block the binding of daidzein to nAChRs. Our FES can be a promising tool for various biomedical applications such as drug screening and therapy monitoring. Genistin or daidzein reduced Ca$^{2+}$ meaningfully measurements without errors from the device-to-device variations of the sensor characteristics. As results, that the treatment with drugs such as electrophysiological responses to nicotine compared to normal cells, which was attributed to the overexpressed nicotinic acetylcholine receptors (nAChRs) in the to measure the real-time responses of normal lung cells and small-cell lung cancer (SCLC) cells to the addition of nicotine. The SCLC cells exhibited rather large aligned single-walled carbon nanotubes, which allowed quantitatively monitoring the electrophysiological responses from nonadherent cells. The FES was used to differ between sudden temperature changes compared to slow, long-term changes implying adaptation of cytoskeletal structure. Interpreting optically induced a systematic shift of creep compliance curves J(t) for single living breast epithelial cells. We use a dual-beam laser trap (optical stretcher) to induce temperature monitoring of Nonadherent Cells.

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**Tuesday, March 3, 2015 11:15AM - 2:15PM**

**Session G47 DBIO: Focus Session: Physics of Cancer**

**217B - Rachel Lee, University of Maryland**

**11:15AM G47.00001 ABSTRACT WITHDRAWN**

**11:27AM G47.00002 Does Tensile Rupture of Tumor Basement Membrane Mark the Onset of Cancer Metastasis?**

1 SAI PRAKASH, Chemical and Biomolecular Engineering, Johns Hopkins University — Recognizing a conceptual analogy from polymer physics and reasoning via induction, we infer the plausibility that a malignant tumor (carcinoma) grows in size until a threshold determined by its mechanochemical state in relation to its microenvironment whence, peripheral cells undergo epithelial-to-mesenchymal transitions (EMT) facilitating metastasis. This state is equated to the tensile yielding/rupture of the proteolytically-weakened basement membrane (BM) that encapsulates the growing neoplasm. BMs are typically constituted of tri-continuous hydrogel networks of collagen-IV, laminin, and interstitial fluid, with connector proteins such as nidogens, and perlecans. We test this postulate by formulating a theoretical model based on continuum fluid-solid mechanics, diffusion, and biochemical kinetics of energy metabolism. Herein, a prototypical, viscous tumor spheroid grows radially, consuming metabolic nutrients while being constricted by an elastic BM ca. 0.5–2 microns-thick, and cell adhesion molecules (CAMs), chiefly cadherins and integrins. The model is computationally analyzed via Comsol[1]. Results validate the a priori conjecture, and predict subsequent crack-tip stresses shifting strains on the CAMs from compressive to tensile, that might also indicate mechanotransduced switches in their conformations, such as from non-invasive, adhesive E-cadherins to invasive, non-adhesive N-cadherin phenotypes.

**11:39AM G47.00003 Mechanical properties of growing melanocytic nevi and the progression to melanoma**

ALESSANDRO TALONI, CNR-IERI, Via R. Cozzi 53, 20125 Milano, Italy, ALEXANDER ALEMI, LASSP, Department of Physics, Clark Hall, Cornell University, EMILIO CIUSANI, Istituto Neurologico Carlo Besta, Milano, Italy, JAMES P. SETHNA, LASSP, Department of Physics, Clark Hall, Cornell University, STEFANO ZAPPETTI, CNR-IERI, Via R. Cozzi 53, 20125 Milano, Italy, CATERINA A. M. LA PORTA, Department of Biosciences, University of Milano, NATIONAL RESEARCH COUNCIL OF ITALY TEAM, LASSP, DEPARTMENT OF PHYSICS, CORNELL UNIVERSITY TEAM, ISTITUTO NEUROLOGICO CARLO BESTA COLLABORATION, DEPARTMENT OF BIOSCIENCES, UNIVERSITY OF MILANO TEAM — Melanocytic nevi are benign proliferations that sometimes turn into malignant melanoma in a way that is still unclear from the biochemical and genetic point of view. Diagnostic and prognostic tools are then mostly based on dermoscopic examination and morphological analysis of histological tissues. To investigate the role of mechanics and geometry in the morphological dynamics of melanocytic nevi, we present a computational model for cell proliferation in a layered non-linear elastic tissue. Our simulations show that the morphology of the nevus is correlated to the initial location of the proliferating cell starting the growth process and to the mechanical properties of the tissue. We also demonstrate that melanocytes are subject to compressive stresses that fluctuate widely in the nevus and depend on the growth stage. Numerical simulations of cells in the epidermis releasing matrix metalloproteinases display an accelerated invasion of the dermis by destroying the basal membrane. Moreover, we show experimentally that osmotic stress and collagen inhibit growth in primary melanoma cells while the effect is much weaker in metastatic cells.

**11:51AM G47.00004 ABSTRACT WITHDRAWN**

**12:03PM G47.00005 Reusable Floating-Electrode Sensor for Real-Time Electrophysiological Monitoring of Nonadherent Cells**

VIET ANH PHAM BA, Seoul Natl Univ, VAN-THAO TA, Hanoi Natl Univ of Education, JUHUN PARK, EUN JIN PARK, SEUNGHUN HONG, Seoul Natl Univ — We herein report the development of a reusable floating-electrode sensor (FES) based on aligned single-walled carbon nanotubes, which allowed quantitatively monitoring the electrophysiological responses to nicotine compared to normal cells, which was attributed to the overexpressed nicotinic acetylcholine receptors (nAChRs) in the SCLC cells. Importantly, using only a single device could measure repeatedly the responses of multiple individual cells to various drugs, enabling statistically meaningful measurements without errors from the device-to-device variations of the sensor characteristics. As results, that the treatment with drugs such as genistin or daidzein reduced Ca$^{2+}$ influx in SCLC cells was found. Moreover, tamoxifen, has been known as an anti-estrogen compound, was found to only partly block the binding of daidzein to nAChRs. Our FES can be a promising tool for various biomedical applications such as drug screening and therapy monitoring.

**12:15PM G47.00006 Thermorheology of living cells—impact of temperature variations on cell mechanics**

JOSEF KAS, TOBIAS KIESSLING, ANATOL FRITSCH, ROLAND STANGE, University of Leipzig — Upon temperature changes, we observe a systematic shift of creep compliance curves J(t) for single living breast epithelial cells. We use a dual-beam laser trap (optical stretcher) to induce temperature jumps within milliseconds, while simultaneously measuring the mechanical response of whole cells to optical force. The cellular mechanical response was found to differ between sudden temperature changes compared to slow, long-term changes implying adaptation of cytoskeletal structure. Interpreting optically induced cell deformation as a thermorheological experiment allows us to consistently explain data on the basis of time–temperature superposition, well known from classical polymer physics. Measured time shift factors give access to the activation energy of the viscous flow of MCF-10A breast cells, which was determined to be ~ 80 kJ/mol. The presented measurements highlight the fundamental role that temperature plays for the deformability of cellular matter. We propose thermorheology as a powerful concept to assess the inherent material properties of living cells and to investigate cell regulatory responses upon environmental changes.
generate virtual tumors and study their morphology and cell subtype populations as a function of time. Specifically, we have measured the absolute optical extinction for intra-cellular material (lysates) in aqueous suspension. Measurements were conducted over a wavelength range of 250 to 1000 nm with 1 nm resolution using Light Transmission Spectroscopy (LTS). This provides both the absolute extinction of materials under study and, with Mie inversion, the absolute number of particles of a given diameter as a function of diameter in the range of 1 to 3000 nm. Our preliminary studies show significant differences in both the extinction and particle size distributions associated with cancer versus normal cells, which appear to be correlated with differences in the particle size distribution in the range of approximately 50 to 250 nm. Especially significant is a clearly higher density of particles at about 100 nm and smaller for normal cells.

Department of Physics, Harper Cancer Research Institute, and the Office of Research at the University of Notre Dame

Role of differential physical properties in emergent behavior of 3D cell co-cultures — DAN KOLBMAN, MOUMITA DAS, Rochester Institute of Technology — The biophysics of binary cell populations is of great interest in many biological processes, whether the formation of embryos or the initiation of tumors [1]. During these processes, cells are surrounded by other cell types with different physical properties, often with important consequences. For example, recent experiments on a co-culture of breast cancer cells and healthy breast epithelial cells suggest that the mechanical mismatch between the two cell types may contribute to enhanced migration of the cancer cells [2]. Here we explore how the differential physical properties of different cell types may influence cell-cell interaction, aggregation, and migration. To this end, we study a proof of concept model—a three-dimensional binary system of interacting, active, and deformable particles with different physical properties such as elastic stiffness, contractility, and particle-particle adhesion, using Langevin Dynamics simulations. Our results may provide insights into emergent behavior such as segregation and differential migration in cell co-cultures in three dimensions.

Specifically, we explore whether leader cells are required to describe our expanding sheets of cells and whether the answer depends on individual cell activity.

Metastatic process begins when cells leave the primary tumor, either as individual cells or collectively migrating groups. Here we present data on the migration speed, but with a decrease in collective motion and increasing chaotic movement fields of groups of cells. I will describe how an underlying wave-like process of the cellular scaffolding that drives persistent migration contributes to the ability of cells to move collectively. I will further show that the same internal waves also allow cells to recognize and follow surface nanotopography on scales comparable to these internal waves. This facilitates contact guidance by the cells.

A computational model of cell-microenvironment interactions — STEPHEN BURKE, University of California, San Diego — The cell-microenvironment interaction is an important component of many biological processes, such as tissue healing, tumor invasion, and wound healing. The model is capable of representing various aspects of the interaction, including cell-cell and cell-matrix interactions, and can be used to study the effects of different microenvironments on cell behavior.

In one of the models, we consider the migration of cells through a collagen gel, which is a common extracellular matrix found in many biological environments. The model includes a three-dimensional binary system of interacting, active, and deformable particles with different physical properties such as elastic stiffness, contractility, and particle-particle adhesion, using Langevin Dynamics simulations. Our results may provide insights into emergent behavior such as segregation and differential migration in cell co-cultures in three dimensions.

12:51PM G47.00009 Modeling mechanical interactions between cancerous mammary acini — JEFFREY WANG, Harvard University, JAN LIPHARDT, Stanford University, CHRIS RYCROFT, Harvard University — The rules and mechanical forces governing cell motility and interactions with the extracellular matrix of a tissue are often critical for understanding the mechanisms by which breast cancer is able to spread through the breast tissue and eventually metastasize. Ex vivo experimentation has demonstrated the formation of long collagen fibers through collagen gels between the cancerous mammary acini responsible for milk production, providing a fiber scaffolding along which cancer cells can disorganize. We present a minimal mechanical model that serves as a potential explanation for the formation of these collagen fibers and the resultant motion. Our working hypothesis is that cancerous cells induce this fiber formation by pulling on the gel and taking advantage of the specific mechanical properties of collagen. To model this system, we employ a new Eulerian, fixed grid simulation method to model the collagen as a nonlinear viscoelastic material subject to various forces coupled with a multi-agent model to describe individual cancer cells. We find that these phenomena can be explained by two simple ideas: cells pull collagen radially inwards and move towards the tension gradient of the collagen gel, while being exposed to standard adhesive and collision forces.

12:51PM G47.00010 Wave-Based Mechanisms for Contact Guidance and Collective Cell Migration — WOLFGANG LOSERT, University of Maryland — The migration of cells in streams, and the crossover from collective behavior to individual cell migration is one of the key physical steps in cancer metastasis. This migration occurs in the context of a microenvironment with specific mechanics and texture that may guide the metastatic process. Studies on cell lines indicate that an increasing metastatic potential of cells is associated not with changes in migration speed, but with a decrease in collective motion and increasing chaotic movement fields of groups of cells. I will describe how an underlying wave-like process of the cellular scaffolding that drives persistent migration contributes to the ability of cells to move collectively. I will further show that the same internal waves also allow cells to recognize and follow surface nanotopography on scales comparable to these internal waves. This facilitates contact guidance by the cells.

12:51PM G47.00011 Computational model for chromosomal instability — STEFANO ZAPPERI, CNR-ICN, Milano, Italy, ISI Foundation, Torino, Italy. Aalto University, Finland, ZSOLT BERTALAN, ZOE BUDRIKIS, ISI Foundation, Torino, Italy., CATERINA LA PORTA, Department of Bioscience, University of Milano, Italy. — Faithful segregation of genetic material during cell division requires alignment of the chromosomes between the spindle poles and attachment of their kinetochores to each of the poles. Failure of these complex dynamical processes leads to chromosomal instability (CIN), a characteristic feature of several diseases including cancer. While a multitude of biological factors regulating chromosome congression and bi-orientation have been identified, it is still unclear how they are integrated into a coherent picture. Here we address this issue by a three dimensional computational model of motor-driven chromosome congression and bi-orientation. Our model reveals that successful cell division requires control of the total number of microtubules: if this number is too small bi-orientation fails, while if it is too large not all the chromosomes are able to congress. The optimal number of microtubules predicted by our model compares well with early observations in mammalian cell spindles. Our results shed new light on the origin of several pathological conditions related to chromosomal instability.

12:51PM G47.00012 Computational modeling of the spatiotemporal dynamics of cancer stem cells — ALEXANDRA SIGNORIELLO, MARCUS BOSENBERG, Yale University, MARK SHATTUCK, City College of New York, COREY O’HERN, Yale University — Cancer stem cells can differentiate into any cell type in a particular tumor, and thus can reform a tumor even when seeded from a single cell. Despite their importance, the identification of stem cells, their interactions, and how and why they malfunction to cause cancer and form tumors are not well understood. We have developed discrete element modeling (DEM) simulations to investigate the role of stem cells in the formation of heterogeneous cell populations in melanoma tumors. The DEM simulations include elastic, excluded volume, and signaling interactions between cells and rates for cell differentiation, apoptosis, and growth. The DEM is calibrated to results from experimental studies of melanoma tumor growth in mouse models. We use the simulations to generate virtual tumors and study their morphology and cell subtype populations as a function of time.

2:03PM G47.00013 Characterization of Collective Cell Migration Dynamics — RACHEL LEE, Univ of Maryland-College Park, HAIYCEN YUE, WOUTER-JAN RAPPEL, Univ of California-San Diego, WOLFGANG LOSERT, Univ of Maryland-College Park — During cancer progression, tumor cells invade the surrounding tissue and migrate throughout the body, forming clinically dangerous secondary tumors. This migratory process begins when cells leave the primary tumor, either as individual cells or collectively migrating groups. Here we present data on the migration dynamics of epithelial sheets composed of many cells. Using quantitative image analysis techniques, we are able to extract motion information from time-lapse images of cell lines with varying malignancy. Adapting metrics originally used to study fluid flows we are able to characterize the migration dynamics of these cell lines. By describing the migration dynamics in great detail, we are able to make a clear comparison of our results to a simulation of collective cell migration. Specifically, we explore whether leader cells are required to describe our expanding sheets of cells and whether the answer depends on individual cell activity.
Tuesday, March 3, 2015 11:15AM - 2:15PM
Session G48 DBIO: Focus Session: Physics of Proteins II
217C - Katherine Niessen, State University of New York, Buffalo

11:15AM G48.00001 Probing the conformational changes of proteins in liquid water by dielectric terahertz spectroscopy, ALI CHARKHESHT, DEEPU GEORGE, NGUYEN VINH, Virginia Tech — Proteins solvated in their biological milieu are expected to exhibit strong absorption in the terahertz range that contain information on their global and sub-global collective vibrational modes (conformational dynamics) and global dynamical correlations among solvent water molecules and proteins. Measurements in this region, however, are challenging due to the strong absorption of water and often severe interference artifacts. In response, we have developed a highly sensitive dielectric terahertz frequency-domain system and a terahertz-time domain system for probing the collective dynamics in aqueous solution. Using these techniques we explore the complex dielectric response from 5 GHz up to 3 THz that directly probes such questions as the hydration level around proteins and the large scale vibrational modes of biological polymers. We make a direct comparison to the existing molecular dynamic simulations and normal mode calculations and investigate the dependence of the terahertz frequency dynamics on protein concentration. Our measurements shed light on the macromolecular motions in a biologically relevant water environment.

11:27AM G48.00002 Nature of Light-Harvesting-System Excited States Prepared by Thermal Light, JUAN DAVID BOTERO, Univ de Antioquia, PAUL BRUMER, University of Toronto, LEONARDO PACHON, Univ de Antioquia, GRUPO DE FISICA ATOMICA Y MOLECULAR TEAM, CHEMICAL PHYSICS THEORY GROUP TEAM — The nature of excited states produced by incoherent natural thermal light is analyzed in the context of light-harvesting system. In the absence of proteomic environments or solvents, it is shown that natural thermal light generates extremely long-lasting coherent dynamics in photosynthetic light-harvesting systems provided by the super-Ohmic character of the radiation, the lack of pure dephasing dynamics and the small energy gap between donors and acceptors. Although this unexpected result has the potential of changing the entire direction of the discussion on the nature of excited states prepared by sunlight, when the environment is considered, the extremely long-lasting coherences induced by incoherent light are removed and stationary coherences are established in the photosynthetic light-harvesting system.

11:39AM G48.00003 The Hydrophobic Solvation Energies of Molecular-Scale Cavities Depend on the Detailed Structure of the Molecular Surface, ROBERT HARRIS, B. MONTGOMERY PETTITT, University of Texas Medical Branch — Both the energy \( \Delta G_{\text{vdw}} \) of inserting an uncharged molecular cavity into solution have often been assumed to increase linearly with the solvent-accessible surface area \( \mathcal{A} \), in analogy with the energy of forming macroscopic cavities in solution. Because these energies are assumed to increase with \( \mathcal{A} \), they have often been assumed to drive protein collapse during folding. However we have shown that for molecular-scale cavities neither of these energies are simple linear functions of \( \mathcal{A} \). Additionally, for both alanine and glycine peptides we have shown that \( \Delta G_{\text{vdw}} \) decreases with \( \mathcal{A} \), implying that \( \Delta G_{\text{vdw}} \) opposes folding for these systems. We also show that \( \Delta G_{\text{rep}} \) is linear in \( \mathcal{A} \) for large molecules but linear in the solvent-accessible volume \( \mathcal{V} \) for small molecules is inconsistent with our findings. Any theory that can accurately predict \( \Delta G_{\text{vdw}} \) or \( \Delta G_{\text{rep}} \) will have to consider the details of the molecular shape rather than relying on coarse measures, such as \( \mathcal{A} \) and \( \mathcal{V} \).

11:51AM G48.00004 Novel Photodynamics in Phytochrome & Cyanobacteriochrome Photosensory Proteins, DELMAR LARSEN, University of California, Davis — The photodynamics of recently characterized phytochrome and cyanobacteriochrome photoreceptors are discussed. Phytochromes are red/far-red photosensory proteins that utilize the photoisomerization of a linear tetrapyrrole (bilin) chromophore to detect the red to far-red light ratio. Cyanobacteriochromes (CBCRs) are distantly related cyanobacterial photosensors with homologous bilin-binding GAF domains, but exhibit greater spectral diversity. The excited-state mechanisms underlying the initial photoisomerization in the forward reactions of the cyanobacterial photoreceptor Cph1 from Synechocystis, the RcaE CBCR from Fremyella diplosiphon, and Npr6012g4 CBCR from Nostoc punctiforme were contrasted via multipulse pump-dump-probe transient spectroscopy. A rich excited-state dynamics are resolved involving a complex interplay of excited-state proton transfer, photoisomerization, multilayered inhomogeneity, and reactive intermediates, and Le Chatelier redistribution. NpR6012g4 exhibits a high quantum yield for its forward photoreaction (40%) that was ascribed to the activity of hidden, productive ground-state intermediates via a “second chance initiation dynamics” (SCID) mechanism.

12:27PM G48.00005 Pushing single molecule techniques to microsecond resolution proves that T4 Lysozyme is a Brownian ratchet, MAXIM V. AKHTEROV, Dept. of Physics and Astronomy, Univ of California Irvine, YONGKI CHOI, Dept. of Physics and Astronomy, Univ of California Irvine; TIVOLI J. OLSEN, Dept. of Chemistry, Univ of California Irvine, PATRICK C. SIMS, Dept. of Physics and Astronomy, Univ of California Irvine, MARIAM IFTIKHAR, Dept. of Chemistry, Univ of California Irvine, O. TOLGA GUL, BRAD L. CORSO, Dept. of Physics and Astronomy, Univ of California Irvine, GREGORY A. WEISS, Dept. of Chemistry, Univ of California Irvine, PHILIP G. COLLINS, Dept. of Physics and Astronomy, Univ of California Irvine — Single-molecule techniques can monitor conformational dynamics of proteins, but such methods usually lack the resolution to directly observe conformational pathways or intermediate conformational states. We have recently described a single-molecule electronic technique that breaks this barrier. Using a 1 MHz-bandwidth carbon nanotube transistor, the transition pathways between open and closed conformations of T4 lysozyme have been recorded with a microsecond resolution. We directly resolve a smooth, continuous transition with an average duration of 37 microseconds. Unexpectedly, the mechanical closing and re-opening of the enzyme haveidentical distributions of transition durations, and the motion is independent of the enzyme catalyzing the substrate. These results illustrate the principle of microscopic reversibility applied to a Brownian ratchet, with lysozyme tracing a single pathway for closing and the reverse pathway for enzyme opening, regardless of its instantaneous catalytic productivity.

\[ \Delta G_{\text{vdw}} = \mathcal{A} \]
12:39PM G48.00006 Detection Enhancement of Protein Structural Vibrations: Measurements and Calculations, KATHERINE NIESSEN, MENGYANG XLI, SUNY at Buffalo, Physics, EDWARD SNELL, VIVIAN CODY, JAMES PACE, Hauptman-Woodward Medical Research Institute, Buffalo, NY, MARIUS SCHMIDT, University of Wisconsin, Physics, ANDREA MARKEZL, SUNY at Buffalo, Physics. — Narrow band intramolecular protein vibrations have been successfully measured using crystal anisotropy THz microscopy (CATM), a near-field technique, on protein crystals [1]. To address the question of how these motions are related to protein function we developed a variation of this technique to rapidly measure a variety of protein crystals. The variation anisotropy measurement consists of introducing a wire-grid polarizer in the THz path and rotating the polarizer between measurements, instead of the sample. While the resulting anisotropic spectra confirm reproducibility and protein specific nature of the response the signal is not directly related to the absorption spectra and in fact shows more structure than CATM. This is due to the polarization sensitivity of the electro-optical detection crystal and the changing THz polarization direction and amplitude at the detector [2]. This combination leads to an enhancement of specific resonances and increased sensitivity to rotation of the THz polarization from the sample itself. Preliminary calculations suggest that the technique is sensitive to the birefringence associated with anisotropic absorbance. The results and significance of these measurements on protein and sucrose crystals and the calculated expected response will be discussed. 1. Acbas, G., et al. (2014). Nat Commun 5. 2. Planken, P.C.M., et al. (2001). J. Opt. Soc. Am. B. 18(3).

12:51PM G48.00007 Microtubule Severeing Stymied by Free Tubulin, JENNIFER ROSS, MEGAN BAILEY, Univ of Massachusetts - Amherst — Proper organization of the microtubule cytoskeletal network is required to perform many necessary cellular functions including mitosis, cell development, and cell motility. Network organization is achieved through filament remodeling by microtubule-associated proteins (MAPs) that control microtubule dynamics. MAPs that stabilize are relatively well understood, while less is known about destabilizing MAPs, such as severing enzymes. Katanin, the first-discovered microtubule-severing enzyme, is a AAA+ enzyme that oligomerizes into hexamers and uses ATP hydrolysis to sever microtubules. Using quantitative imaging on reconstituted microtubule severing assays in vitro we investigate how katanin can regulate microtubule dynamics. Interestingly, we find microtubule dynamics inhibits katanin severing activity; dynamic microtubules are not severed. Using systematic experiments introducing free tubulin into the assays we find that free tubulin can compete for microtubule filaments for the katanin proteins. Our work indicates that katanin could function best on stable microtubules or stable regions of microtubules in cells where free tubulin is sequesters, low, or depleted.

1:03PM G48.00008 Stereoelectronic Determinants of Color Vision: Engineering Protein Mimics of Pigmented Rhodopsins and Designing New Protein Fusion Tags, BABAK BORHAN, Michigan State University — The field of protein engineering has undergone phenomenal growth from its inception approximately 20 years ago. A wide variety of topics have been addressed, including the construction of new protein folds, the introduction of metal binding sites that are both structural and catalytic, the development of novel enzymatic activity and the creation and optimization of new ligand binding sites. However, left behind has been the issue of protein/chromophore interactions. Protein-chromophore interactions are a central component of a wide variety of critical biological processes such as color vision and photosynthesis. To understand the fundamental elements that contribute to spectral tuning of a chromophore inside the protein cavity, we redesigned small cystosolic human proteins to fully encapsulate all-trans-retinal and form a covalent bond as a protonated Schiff base. These systems, using rational mutagenesis, have led to restructurizing the electrostatic environment within the binding pocket of the host protein, enabling the regulation of the absorption maximum of the pigment over 200 nm. So far our work has shown that the manipulation of the electrostatic potential projected by the protein onto the chromophore has a powerful effect on the absorption properties of the ligand. We have parlayed these results towards developing new protein fusion tags and pH responsive protein dyes.

1:39PM G48.00009 Obtaining structural information of small proteins using solid-state nanopores and high-bandwidth measurements, DAVID NIEDZWIECI, CHRISTOPHER LANCI, JEFFERY SAVEN, MARLIA DRNDIC, University of Pennsylvania — The use of biological nanopores sensors to characterize proteins has proved a fruitful field of study. Solid-state nanopores hold several advantages over their biological counterparts, including the ability to tune pore diameter and their robustness to external conditions. Despite these advantages, the use of solid-state nanopores for protein analysis has proved difficult due to rapid translocation times of proteins and poor signal-to-noise of small peptides. Recently, improvements in high-bandwidth acquisition and in signal-to-noise have made the study of small peptides using solid-state nanopores feasible. Here we report on the detection and characterization of peptides as small as 33 amino-acids in length using sub-10 nm thin silicon nitride nanopores, giving high signal levels, combined with high-bandwidth electronics. In addition we show differentiation between monomers and dimer forms of the GCN-4 p1 leucine zipper, a coil-coil structure, and compare this with the unstructured 33-mer. The differentiation between these two forms demonstrates the possibility of extracting useful structural information from short peptide sequences using modern solid-state nanopore systems.

1:51PM G48.00010 Determination of Kinetic Isotope Effects in Yeast Alcohol Dehydrogenase Using Transition Path Sampling, MATTHEW VARGA, STEVEN SCHWARTZ, Univ of Arizona — The experimental determination of kinetic isotope effects in enzymatic systems can be a difficult, time-consuming, and expensive process. In this study, normal mode centroid molecular dynamics (CMD) was applied to the transferring hydride/deuteride in order to correctly incorporate quantum effects into the molecular simulations. Though previous studies have used rTPS to calculate reaction rate constants in various model and real systems, it has not been applied to a system as large as YADH. Due to the fact that particle transfer is not wholly indicative of the chemical step, this method cannot be used to determine reaction rate constants in YADH. However, it is possible to determine the transition rate constant of the particle transfer, and the kinetic isotope effect of that step. This method provides a set of tools to determine kinetic isotope effects with the atomistic detail of molecular simulations.

2:03PM G48.00011 ABSTRACT WITHDRAWN —

Tuesday, March 3, 2015 11:15AM - 2:15PM — Session G49 GSOFT: Fracture, Friction, and Deformation 217D - Mike Salerno, Sandia National Laboratories

11:15AM G49.00001 Popping balloons: formation of a crack network in rubber membranes, SEBASTIEN MOULINET, MOKHTAR ADDA-BEDIA, Lab. de Physique Statistique, EQUIPE MORPHOGENESE ET PHENOMENES MULTI-ECHELLE TEAM — Everyone can make the observation: a rubber balloon inflated until it spontaneously pop breaks into a large number of shreds. In contrast, a balloon pierced with a needle at an early stage of its inflation breaks into two large pieces. Using model latex balloons, we have experimentally investigated the transition between these two breaking regimes. We have showed that, above a threshold stress in the latex membrane, a single crack become unstable and separates into two new cracks. Then, a cascade of tip-splitting generates a network of cracks that eventually form a large number of fragments. We have observed that the instability of the crack occurs when it reaches a limit velocity that could the speed of sound. By studying the energy balance during the explosion, we can determine the intrinsic fracture energy of rubber, a measurement difficult to achieve with usual tensile testing.
11:27AM G49.00002 Do thermal fluctuations stabilize an extensible buckling rod? , DESHPREET BEDI, XIAOMING MAO, Univ of Michigan - Ann Arbor — The classical problem of a rod buckling under a compressive force, "Euler buckling," has long been studied and solved in physics; however, the classical theory of Euler buckling does not take into account thermal fluctuations. At small enough scales, entropic effects become significant, and a more intricate analysis incorporating thermal fluctuations is needed, for instance, in the study of biopolymers and nanotubes. In this talk, we discuss buckling of an extensible, semi-flexible rod embedded in two and three dimensions. We systematically examine the problem both analytically, using a momentum-space renormalization group procedure, and numerically, using Monte Carlo simulations, to determine the topology of the phase diagram containing the unbuckled and buckled states. In two dimensions, for instance, we determine that thermal fluctuations tend to stabilize the straight-rod state over the buckled state and that this stabilization increases with temperature. We also analyze the mechanical response of the rod in order to study the differing scaling regimes of the system.

11:39AM G49.00003 Localized Disturbance in a 2D Cohesive Granular Packing, JENNIFER RIESER, University of Pennsylvania, MATHILDE LAPLAGNE, University of Pennsylvania and Ecole Polytechnique, DOUGLAS DURIAN, University of Pennsylvania — How the local structural configuration influences large-scale deformation in disordered materials is not known. Inspired by nano-indentation experiments, we characterize the response of disordered granular packing to a localized disturbance by driving a triangular wedge into the packing. The extent of the disturbance is explored by performing experiments with several wedge angles. The two-dimensionality of the system allows for direct observation of all particle dynamics during the indentation. The grains can be cohesive, with an attraction governed by tunable capillary forces that are induced through an interstitial fluid. Topological quantities derived from a radical Voronoi diagram as well as the resulting triangulation are used to characterize local structure within the packing. Dynamics are characterized by local deformations to the triangulation as well as the local non-affine motion. For all wedge angles, a boundary develops between moving and static grains. This size and shape of this boundary depend on the indenter angle, and in all cases, the size of the boundary increases with time. During the deformation, non-affine grain motion occurs both throughout the moving region as well as along the boundary, while holes tend to develop primarily along this boundary.

11:51AM G49.00004 Shells on lattice-mismatched colloidal spheres, cubes, and peanuts, MELINDA SINDORO, STEVE GRANICK, Univ of Illinois - Urbana — Cavities form spontaneously due to geometrical frustration when crystalline shells is gradually grown on non-linear surfaces. This we conclude experimentally from growing lattice mismatched shells on colloidal spheres, cubes, and peanuts, all of them providing different local curvature. According to the core shape, the underlying interfacial curvature promotes different cavity formation which we can follow over time. During the deformation, non-affine grain motion occurs both throughout the moving region as well as along the boundary, while holes tend to develop primarily along this boundary.

12:03PM G49.00005 Adhesion and Wetting of Soft Nanoparticles on Textured Surfaces: Transition between Wenzel and Cassie-Baxter States, ZHEN CAO, University of Connecticut, MARK STEVENS, Sandia National Laboratories, JAN-MICHAEL CARRILLO, Oak Ridge National Laboratory, ANDREY DOBRYNNIN, University of Connecticut — We use a combination of the molecular dynamics simulations and scaling analysis to study interactions between gel-like nanoparticles and substrates covered with rectangular shape posts. Nanoparticle in contact with a substrate undergo a first order transition between Wenzel and Cassie-Baxter states depending on nanoparticle shear modulus. The strength of nanoparticle-substrate interactions, height of the substrate posts and nanoparticle size, $R_p$. There is a range of system parameters where these two states coexist such that the average indentation $\delta$ produced by substrate posts changes monotonically with nanoparticle shear modulus. We have developed a model that describes deformation of nanoparticle in contact with patterned substrate. The effect of the patterned substrate can be taken into account by introducing an effective work of adhesion, $W_{eff}$, which describes the first order transition between Wenzel and Cassie-Baxter states. There are two different shape deformation regimes for nanoparticles with shear modulus $G_p$ and surface tension $\gamma_p$. Shape of small nanoparticles with size $R_p < \sqrt{3} G_p / \gamma_p W_{eff}^{-1/2}$ is controlled by capillary forces while deformation of large nanoparticles, $R_p > \sqrt{3} G_p / \gamma_p W_{eff}^{-1/2}$, is determined by nanoparticle elastic and contact free energies.

12:15PM G49.00006 Self-affine parameters of fracture surfaces of high strength steels, MOISES HINOJOSA, ELISA SCHAEFFER, YOSHUA GUZMAN, JORGE ALDACO, Universidad Autónoma de Nuevo León — We report the experimental study of crack nucleation and propagation on AISI 4340 and Premoment steels, submitted to different thermal treatments that resulted in different properties and microstructures. Crack initiation and propagation under fatigue, tension and impact conditions were analyzed at different lengthscales. The SEM fractographic study allowed the correlation of the observed mechanisms with the patterns observed on the fracture surfaces. The scaling properties were explored and correlated to the observed mechanisms. Using the topographic data of 3D reconstructed surfaces obtained by laser scanning, we calculated both global and local roughness exponents using different variable-bandwidth methods, obtaining the statistical distributions as a function of the orientation. Although the results tend to the same average global value (close to 0.8) for both steels regardless of the heat-treating condition, their statistical distributions are sensitive to the anisotropy of the microstructure, we also found a correlation of the local roughness exponents with the local orientation of the microstructure and the dimples observed on the fracture surfaces.

12:27PM G49.00007 Probing Interfacial Friction and Dissipation in Granular Gold Nickel Alloys with a Quartz Crystal Oscillator in an External Magnetic Field, K.M. STEVENS, J. KRM, North Carolina State University — We present here a quartz crystal microbalance study of two-phase gold nickel alloys whose internal granular properties are probed by exposure to a fluctuating external magnetic field. The work is motivated by prior studies demonstrating that granular two-phase materials exhibited lower friction and wear than solid solution alloys with identical compositions [1]. In particular, we report a “flexing” effect which appears when an external magnetic field is applied, and is manifested as a decrease in the magnitude of oscillation amplitude that is synchronized with the applied field; the effect is not seen on the complimentary solid solution samples. The effect is consistent with internal interfacial friction between nickel and gold grains, indicating a degree of freedom which may decrease friction even in the absence of an external magnetic field. This is supported through analysis of energy dissipation in the system, using the Butterworth-Van Dyke equivalent circuit model [2]. Data and interpretation are also presented that rule out alternate explanations such as giant magnetoresistance [3] and/or other resistive phenomenon within the film.


1 NSF # DMR-1004576 DMR-1409710

Funding provided by NSF DMR0805204. Thanks to L. Pan for sample preparation.
12:39PM G49.00008 Stick-slip patterns in a model frictional interface, GEORGIOS TSEKENIS, DEMET TATAR, SHMUEL RUBINSTEIN, DAVID WEITZ, MICHAEL AZIZ, FRANS SPAEPEN, Harvard University — We present measurements of the local displacements during slip-stick motion of two rough surfaces sliding over one another. The surfaces are cast in polymer and have roughness on the order of 30 \( \mu \text{m} \). The displacements are observed by confocal microscopy of embedded fluorescent particles, and measured by PIV. The displacement patterns during large and small slip events are directly observed and analyzed by statistical methods.

12:51PM G49.00009 Stiff particles on highly compliant solid substrates: adhesion or wetting?, KATHARINE JENSEN, ERIC DUFRESNE, Yale University — The classic theories of contact mechanics with deformable materials account only for the competition between adhesion energy and elasticity. However, for compliant materials, solid surface tension also plays an important role in resisting shape change, and may significantly modify the physics of contact with soft matter. We report experiments bringing small, stiff spheres into adhesive contact with compliant silicone substrates. We observe the quasi-static deformation of the substrate in two sticky situations: with zero applied force, where the spheres are allowed to settle to an equilibrium position, and during forced withdrawal from contact starting from an initial condition of zero displacement. In both cases, we map the profiles of the deformed silicone surface, and compare to capillary and elastic theories. The similarities – and differences – between our experimental measurements and the classic theories point to a crossover form a capillary-dominated near field response close to the contact line to an elastic-dominated response in the far field.

1:03PM G49.00010 Single-asperity friction during quasi-static sliding, TRISTAN SHARP, Johns Hopkins University, LARS PASTEWKA, Karlsruhe Institute of Technology, MARK ROBBINS, Johns Hopkins University — The static friction of an asperity is investigated using atomic-scale simulations. We explore scale effects by varying the sphere radius \( R \) and the contact radius \( a \) from nanometers to micrometers. We first consider commensurate contact between bare lattices with repulsive interactions across the interface. In small contacts, all contacting atoms move coherently and the friction coefficient \( \mu \) is independent of contact radius and load. In larger contacts, interfacial slip is mediated by localized dislocations, and the static friction coefficient \( \mu \sim \left( \frac{a_0}{a} \right)^{1.2} \), where \( a_0 \) is the nearest-neighbor spacing. In very large contacts \( \mu \) stops decreasing and begins to increase with \( a \), at fixed \( R \). The results are in sharp contrast to Cattaneo-Mindlin continuum theory where \( \mu \) is independent of contact size. Separate simulations are performed to connect the results to the dislocation-based models of contact-size effects due to Hurtado and Kim, and Gao, which assume adhesion interactions between surfaces and find \( \mu \sim \left( \frac{a_0}{a} \right)^{1.5} \). Simulations for incommensurate contacts show a transition from superlubricity for rigid contacts to a finite friction associated with the Peierls stress in very large contacts. Support from: DMR-1006805; NSF IGERT-0801471; OCI-0963185; CMMI-0923018

1:15PM G49.00011 Penetration drag in loosely packed granular materials, STEPHAN BLESS, MEHDI OMIDVAR, MAGUED ISKANDER, New York University, Dept Civil & Urban Eng'ng, NEW YORK UNIVERSITY COLLABORATION — The drag coefficient for penetration of granular materials by conical-nosed penetrators was computed by assuming the particles are non-interacting and rebound elastically off of the advancing penetrator. The solution was \( C = 4 \sin(\theta) \) where \( \theta \) is the half angle of the cone. Experiments were conducted in which the drag coefficient was measured over the range 30 to 80 m/s for four types of sand: Ottawa silica sand, crushed quartz glass, coral sand, and aragonite sand. The sands were tested at relative densities of 40 and 80%. The drag coefficients for the low density materials were in excellent agreement with this simple model. The high density material had a drag considerably larger than predicted, presumably because of particle-to-particle interactions.

1:27PM G49.00012 Geometrically Frustrated Fracture Mechanics, NOAH MITCHELL, James Franck Institute, University of Chicago, VINZENZ KONING, VINCENZO VITTELI, Instituut-Lorentz, Universiteit Leiden, WILLIAM T. M. IRVINE, James Franck Institute, University of Chicago — When a flat elastic sheet is forced to conform to a surface with Gaussian curvature, stresses arise in the sheet. The mismatch between initial and final metrics gives rise to new fracture behavior which cannot be achieved by boundary loading alone. Using experiments of PDMS sheets frustrated on 3D-printed surfaces and a linearized analytical model, we demonstrate the ability of curvature to govern the sheets’ fracture phenomenology. In this talk, we first show that curvature can both stimulate and suppress fracture initiation, depending on the position and orientation of the initial slit. Secondly, we show that curvature can steer the path of a crack as it propagates through the material. Lastly, the curvature can arrest cracks which would otherwise continue to propagate.

1:39PM G49.00013 Kibble-Zurek Mechanism in Microscopic Acoustic Cracking Noises, HAMED O. GHAFFARI, University of Toronto, PHILIP BENSON, University of Portsmouth, K. XIA, R. PAUL YOUNG, University of Toronto — The fast evolution of microstructure is key to understanding “cracking” phenomena. It has been proposed that formation of a nonlinear zone around a moving crack tip controls the crack tip velocity. Progress in understanding the physics of this critical region has been limited by our lack of hard data describing the detailed physical processes that occur within. For the first time, we show that the signature of the non-linear elastic zone around a microscopic dynamic crack maps directly to generic phases of acoustic noises, supporting the formation of a strongly weak zone near the moving crack tips. We additionally show that the rate of traversing to non-linear zone controls the rate of weakening, i.e. speed of global rupture propagation. We measure the power-law dependence of nonlinear zone size on the traversing rate, and show that our observations are in agreement with the Kibble-Zurek mechanism (KZM). In addition, we illustrate that cracks exhibiting global rupture fronts with velocity faster than Rayleigh waves (i.e., super-shear rupture fronts) display a complex configuration of non-linear zone prior to the fast weakening phase.

1:51PM G49.00014 Optical Characterization of Temperature-Dependent Microstructure of Polymeric Asphalt Binders, ADAM RAMM, FARBOD SHAFIEI, Physics Dept., Univ of Texas, Austin, MARYAM ZAMANI, Physics Dept., Shahid Beheshti University, Iran, SHARMIN SULTANA, AMIT BHASIN, Civil Eng. Dept, Univ of Texas, Austin, M. C. DOWNER, Physics Dept., Univ of Texas, Austin — Asphalt binders used in construction of pavements must be chemically engineered to withstand wide climatic variations. Ideal binders possess high stiffness at high temperatures, low stiffness with high relaxation rates at low temperatures, and high resistance to fatigue cracking at intermediate temperatures. Such bulk properties are conventionally measured with rheometers, but appear to be closely connected with temperature-dependent microstructural changes. AFM has been used to observe such microstructures, but is only possible near room temperature [1]. Here we characterize asphalt binder microstructure over a wide range of temperatures and chemical compositions using noninvasive optical microscopy correlated with linear and second-harmonic optical scatter to measure statistical fluctuations. For example, micron-size “bee”-structures previously observed by AFM [1] are resolved optically, and are observed to vary as temperature and composition change, while inducing corresponding changes in optical scatter. We will present these and other optical measurements, and discuss their connection to bulk material properties. [1] Pauli et al., Internat. J. Pavement Engin. 12, 291 (2011).
2:03PM G49.00015 Rings and rackets from single-wall carbon nanotubes: manifestations of mesoscopic mechanics, YUEZOU WANG, University of Minnesota, Twin Cities, MATTHEW SEMLER, North Dakota State University, Fargo, IGOR OSTANIN, University of Minnesota, Twin Cities, ERIK HOBBIE, North Dakota State University, Fargo, TRAIAN DUMITRICĂ, University of Minnesota, Twin Cities — We combine distinct element method simulations and experiments to understand the stability of rings and rackets formed by single-wall carbon nanotubes assembled into ropes. Bending remains a soft deformation mode in ropes because intra-rope sliding of the constituent nanotubes occurs with ease. Our simulations indicate that the formation of these aggregates can be attributed to the mesoscopic mechanics of entangled nanotubes and to the sliding at the rope contacts. Statistical analysis of fluctuations in ROI indicates that the stability of the experimental aggregates can be largely explained by the competition between bending and van der Waals adhesion energies. Our results and simulation method should be useful for understanding nanoscale fibers and self-assembling process in general.

References:

Tuesday, March 3, 2015 11:15AM - 2:15PM — Session G50 DBIO: Focus Session: Physics of Neural Systems

11:15AM G50.00001 Human movement stochastic variability leads to diagnostic biomarkers In Autism Spectrum Disorders (ASD), DI WU, Physics, Indiana Univ - Bloomington, Bloomington, IN; ELIZABETH B. TORRES, Dept. of Psychology, Rutgers Univ, New Brunswick, NJ; JORGE V. JOSE, Physics, Indiana Univ - Bloomington, Bloomington, IN; cell and Integrative Physiology, Indiana Univ. School of Medicine, Indianapolis, IN — ASD is a spectrum of neurodevelopmental disorders. The high heterogeneity of the symptoms associated with the disorder impedes efficient diagnoses based on human observations. Recent advances with high-resolution MEM wearable sensors enable accurate movement measurements that may escape the naked eye. It calls for objective metrics to extract physiological relevant information from the rapidly accumulating data. In this talk we’ll discuss the statistical analysis of movement data continuously collected with high-resolution sensors at 240Hz. We calculated statistical properties of speed fluctuations within the millisecond time range that closely correlate with the subjects’ cognitive abilities. We computed the periodicity and synchronicity of the speed fluctuations from their power spectrum and ensemble averaged two-point cross-correlation function. We built a two-parameter phase space from the temporal statistical analyses of the nearest neighbor fluctuations that provided a quantitative biomarker for ASD and the periodicity and synchronicity of the speed fluctuations from their power spectrum and ensemble averaged two-point cross-correlation function. We built a two-parameter phase space from the temporal statistical analyses of the nearest neighbor fluctuations that provided a quantitative biomarker for ASD and adult normal subjects and further classified ASD severity. We also found age related developmental statistical signatures and potential ASD parental links in our movement dynamical studies. Our results may have direct clinical applications.

11:27AM G50.00002 Adaptation tunes cortical dynamics to a critical regime during vision, WOODROW SHEW, WESLEY CLAWSON, University of Arkansas, JEFF POBST, YAHYA KARIMIPANAH, NATHANIEL WRIGHT, RALF WESSEL, Washington University, St. Louis, SHEW LAB TEAM, WESSEL LAB TEAM — A long-standing hypothesis at the interface of physics and neuroscience is that neural networks self-organize to the critical point of a phase transition, thereby optimizing aspects of sensory information processing. This idea is partially supported by strong evidence for critical dynamics observed in the cerebral cortex, but has not been tested in systems with significant sensory input. Thus, the foundations of this hypothesis — the self-organization process and how it manifests during strong sensory input — remain unstudied experimentally. Here we report microelectrode array measurements from visual cortex of turtles during visual stimulation of the retina. We show experimentally and in a computational model that strong sensory input initially elicits cortical network dynamics that are not critical, but adaptive changes in the network rapidly tune the system to criticality. This conclusion is based on observations of multifaceted scaling laws predicted to occur at criticality. Our findings establish sensory adaptation as a self-organizing mechanism which maintains criticality in visual cortex during sensory information processing.

1Supported by NSF CRCNS grant 1308174.

11:39AM G50.00003 Rich club neurons dominate Information Transfer in local cortical networks, SUNNY NIGAM, MASANORI SHIMONO, OLAF SPORNS, JOHN BEGGs, Indiana Univ - Bloomington — The performance of complex networks depends on how they route their traffic. It is unknown how information is transferred in local cortical networks of hundreds of closely-spaced neurons. To address this, it is necessary to record simultaneously from hundreds of neurons at a spacing that matches typical axonal connection distances, and at a temporal resolution that matches synaptic delays. We used a 512 electrode array (60 μm spacing) to record spontaneous activity at 20 kHz, simultaneously from up to 700 neurons in slice cultures of mouse somatosensory cortex for 1 hr at a time. We used transfer entropy to quantify directed information transfer (IT) between pairs of neurons. We found an approximately lognormal distribution of firing rates as reported in in-vivo. Pairwise information transfer strengths also were nearly lognormally distributed, similar to synaptic strengths. 20% of the neurons accounted for 70% of the total IT coming into, and going out of the network and were defined as rich nodes. These rich nodes were more densely and strongly connected to each other expected by chance, forming a rich club. This highly uneven distribution of IT has implications for the efficiency and robustness of local cortical networks, and gives clues to the plastic processes that shape them.

1JSPS

11:51AM G50.00004 Clique of functional hubs orchestrates population bursts in developmentally regulated neural networks, ALESSANDRO TORCINI, STEFANO LUCCIOlI, Istituto dei Sistemi Complessi - CNR, Sesto Fiorentino (Italy), PAOLO BONIFAZI, ESHEL BEN-JACOB, Beverly and Sakler Faculty of Exact Sciences School of Physics and Astronomy, Tel Aviv University, 69978 Ramat Aviv, Israel, ARI BARZILAI, Department of Neurobiology, George S. Wise Faculty of Life Sciences and Sagol School of Neuroscience, Tel Aviv University, Israel — It has recently been discovered that single neuron stimulation can impact network dynamics in immature and adult neuronal circuits. Here we report a novel mechanism which can explain in developing neuronal circuits, typically composed of only excitatory cells, the peculiar role played by a few specific neurons in promoting/arresting the population activity. For this purpose, we consider a standard neuronal network model, with short-term synaptic plasticity whose population activity is characterized by bursting behavior. The addition of developmentally regulated constraints on single neuron excitability and connectivity leads to the emergence of functional hub neurons, whose stimulation/deletion is critical for the network activity. Functional hubs form a clique, where a precise sequential activation of the neurons is essential to ignite collective events without any need for a specific topological architecture. Unsupervised time-lagged firings of supra-threshold cells, in connection with coordinated entrainments of near-threshold neurons, are the key ingredients to orchestrate population activity.

1This work is part of the activity of the Joint Italian-Israeli Laboratory on Integrative Network Neuroscience supported by the Italian Ministry of Foreign Affairs.
12:03PM G50.00005 Neural mechanism to construct a future timeline. KARTHIK SHANKAR, Boston University — Computing the set of possible future states is an important cognitive feature that aids in planning toward a goal. The brain must perform this computation swiftly, and more importantly without destroying the current state of memory. Here we propose a neural mechanism that periodically modifies the synaptic weights in a mathematically principled way to achieve the construction of the future timeline. Preliminary evidence of synaptic modifications in synchrony with the theta rhythm suggests that this mechanism could take place in the Hippocampus. The hypothesis also predicts that the time cells observed in the Hippocampus should exhibit phase precession with respect to the theta rhythm as the future timeline is cognitively constructed.

12:15PM G50.00006 Local structure of subcellular input retinotopy in an identified visual interneuron1. YING ZHU, Structural and Computational Biology & Molecular Biophysics program, Baylor College of Medicine, Houston, TX, 77030, FABRIZIO GABBIANI, Department of Neuroscience, Baylor College of Medicine, Houston, TX, 77030, FABRIZIO GABBIANI’S LAB TEAM — How does the spatial layout of the projections that a neuron receives impact its synaptic integration and computation? What is the mapping topography of subcellular wiring at the single neuron level? The LGMD (lobula giant movement detector) neuron in the locust is an identified neuron that responds preferentially to objects approaching on a collision course. It receives excitatory inputs from the entire visual hemifield through calcium-permeable nicotinic acetylcholine receptors. Previous work showed that the projection from the locust compound eye to the LGMD preserved retinotopy down to the level of a single ommatidium (facet) by employing in vivo widefield calcium imaging. Because widefield imaging relies on global excitation of the preparation and has a relatively low resolution, previous work could not investigate this retinotopic mapping at the level of individual thin dendritic branches. Our current work employs a custom-built two-photon microscope with sub-micron resolution in conjunction with a single-facet stimulation setup that provides visual stimuli to the single ommatidium of locust adequate to explore the local structure of this retinotopy at a finer level.

1We would thank NIMH for funding this research.

12:27PM G50.00007 Nonlinear Dynamic Theory of Acute Cell Injuries and Brain Ischemia1. DOAA TAH, Department of Physics and Astronomy, Wayne State University, FIKRA ANGGRAINI, DONALD DEGRACIA, Department of Physiology, School of Medicine, Wayne State University, ZHI-FENG HUANG, Department of Physics and Astronomy, Wayne State University — Cerebral ischemia in the form of stroke and cardiac arrest brain damage affect over 1 million people per year in the USA alone. In spite of close to 200 clinical trials and decades of research, there are no treatments to stop post-ischemic neuron death. We have argued that a major weakness of current brain ischemia research is lack of a deductive theoretical framework of acute cell injury to guide empirical studies. A previously published autonomous model based on the concept of nonlinear dynamic network was shown to capture important facets of cell injury, linking the concept of therapeutic to bistable dynamics. Here we present an improved, non-autonomous formulation of the nonlinear dynamic model of cell injury that allows multiple acute injuries over time, thereby allowing simulations of both therapeutic treatment and preconditioning. Our results are connected to the experimental data of gene expression and proteomics of neuron cells. Importantly, this new model may be constructed as a novel approach to pharmacodynamics of acute cell injury. The model makes explicit that any pro-survival therapy is always a form of sub-lethal injury. This insight is expected to widely influence treatment of acute injury conditions that have defied successful treatment to date.

1This work is supported by NIH NINDS (NS081347) and Wayne State University President’s Research Enhancement Award.

12:39PM G50.00008 ABSTRACT WITHDRAWN —

12:51PM G50.00009 Interpreting collective neural activity underlying spatial navigation in virtual reality. LEENOY MESHULAM, JEFF GAUTHIER, DAVID TANK, WILLIAM BIALEK, Princeton University — Traditionally, cognitive-demanding processes like spatial navigation were studied by recording the activity of single neurons. However, recent technological progress allows imaging the simultaneous activity of large neuronal populations in awake behaving animals. This progress in experimental work calls for a similar adjustments of the modeling frameworks. To achieve a description of the “real thermodynamics” of the neural system, we construct maximum entropy models for optical imaging data spanned by the network states. The model proposes that the information that comes to be recorded in the brain is first orthogonalized (as in Gram-Schmidt orthogonalization) and then inscribed in synaptic weights. While the orthogonalized versions of input vectors with ±1 components are stored in the model brain, the original vectors/patterns are retrieved exactly when checked for retrieval. Simulations are presented that give insight into the energy landscape in the space of stored patterns ($\frac{p}{N}$). The model predicts the number of components stored in the model brain is $N$ by $p$ and become zero around $\frac{p}{N}$. The model also predicts the information that comes to be recorded in the brain is first orthogonalized and then inscribed in synaptic weights. While the orthogonalized versions of input vectors with ±1 components are stored in the model brain, the original vectors/patterns are retrieved exactly when checked for retrieval. Simulations are presented that give insight into the energy landscape in the space spanned by the network states.


1Vipin Srivastava is also at School of Physics, University of Hyderabad and a life member of Indian Physics Association.
How to generate a sound-localization map in fish

J. Leo Van Hémmen, Physik Department, TU Munich — How sound localization is represented in the fish brain is a research field largely unbiased by theoretical analysis and computational modeling. Yet, there is experimental evidence that the axes of particle acceleration due to underwater sound are represented through a map in the midbrain of fish, e.g., in the *torus semicircularis* of the rainbow trout (Wubbels et al. 1997). How does such a map arise? Fish perceive pressure gradients by their three otolithic organs, each of which comprises a dense, calcareous, stone that is bathed in endolymph and attached to a sensory epithelium. In rainbow trout, the sensory epithelia of left and right utricle lie in the horizontal plane and consist of hair cells with equally distributed preferred orientations. We model the neuronal response of this system on the basis of Schüff’s vector detection hypothesis (Schüff et al. 1975) and introduce a temporal spike code of sound direction, where optimality of hair cell orientation θj with respect to the acceleration direction θa is mapped onto spike phases via a von-Mises distribution. By learning to tune in to the earliest synchronized activity, nerve cells in the midbrain generate a map under the supervision of a locally excitatory, yet globally inhibitory visual teacher.

1Work done in collaboration with Daniel Begovic. Partially supported by BCCN – Munich.

The neural circuit and synaptic dynamics underlying perceptual decision-making

Feng Liu, School of Physics, Nanjing University — Decision-making with several choice options is central to cognition. To elucidate the neural mechanisms of multiple-choice motion discrimination, we built a continuous recurrent network model to represent a local circuit in the lateral intraparietal area (LIP). The network is composed of pyramidal cells and interneurons, which are directionally tuned. All neurons are reciprocally connected, and the synaptic connectivity strength is heterogeneous. Specifically, we assume two types of inhibitory connectivity to pyramidal cells: opposite-feature and similar-feature inhibition. The model accounted for both physiological and behavioral data from monkey experiments. The network is endowed with slow excitatory reverberation, which subserves the buildup and maintenance of persistent neural activity, and predominant feedback inhibition, which underlies the winner-take-all competition and attractor dynamics. The opposite-feature and opposite-feature inhibition have different effects on decision-making, and only their combination allows for a categorical choice among 12 alternatives. Together, our work highlights the importance of structured synaptic inhibition in multiple-choice decision-making processes. Reference: Cheng Xue and Feng Liu. J. Neurosci. 34, 13444-13457 (2014).

Tuesday, March 3, 2015 11:15AM - 2:15PM –

Session G51 GSOFT GSNP: Invited Session: Frontiers of Soft Matter II

Grand Ballroom C1 - M.

11:15AM G51.00001 Entangled active matter: from ants to living cells1, Franoise Brochard-Wyart, Institut Curie — We introduce the field of “Entangled Active Matter” where the building blocks are transiently bound. We will point out strong similarities between aggregates of ants and cells! We will use multicellular aggregates, a model system for tissues. We characterize the tissue mechanical properties using pipette aspiration technique. The aggregate exhibits a viscoelastic response. We observe aggregate reinforcement with pressure, which may results in pulsed contractions or “shivering.” We interpret this reinforcement as a mecha-sensitive active response of the acto-myosin cortex. We describe the spreading of aggregates on rigid and soft substrates, varying both intercellular and substrate adhesion. We find both partial and complete wetting, with a precursor film forming a cellular monolayer in a liquid or gas phase. We model the dynamics of spreading from a balance between active cellular driving forces and permeation of cells to enter into the film. Finally we study the motility of aggregates induced by chemical or rigidity gradients, or spontaneous: on soft substrate, the precursor film is unstable, leading to a symmetry breaking and a global motion of the aggregate. We describe the shapes of migrating aggregates, the flow and the force field responsible of the motion. We monitored the center of mass motion and we characterize the stick-slip motions.

1Work done in collaboration with Andrej Kosmrlj.

11:51AM G51.00002 Free-standing thermalized graphene: a hard/soft hybrid1, David Nelson, Department of Physics, Harvard University — Understanding deformations of macroscopic thin sheets and plates has a long and rich history, culminating with the Föppl-von Karman equations in 1904. These highly non-linear equations are characterized by a dimensionless coupling constant (the “Föppl-von Karman number”) that can easily reach $k = 10^{7}$ in an ordinary sheet of writing paper. Since the late 1980’s, it has been clear that thermal fluctuations in microscopically thin elastic membranes fundamentally alter the long wavelength physics, leading to a negative thermal expansion coefficient, and a strongly scale-dependent bending energy and Young’s modulus. Recent experiments from the McEuen group at Cornell that twist and bend individual atomically-thin free-standing graphene sheets (with $k = 10^{13}$) call for a theory of the mechanical deformation of thermally excited membranes with large Föppl-von Karman number. We present here results for the bending and pulling of thermalized graphene ribbons and tabs in the cantilever mode.

1Work done in collaboration with Andrej Kosmrlj.

12:27PM G51.00003 Liquids Gone With the Wind, David Quéré, ESPCI, Paris — Self-propelling fluidic devices naturally result from some asymmetry of wettability, geometry or temperature. Here we consider the case of motions arising from the air around, forced by some trick to flow in an asymmetric way. We first consider vapor flows generated in a Leidenfrost situation, and made anisotropic by textures decorating the hot substrate. We discuss how the force and speed arising from these rectified vapor flows can be optimized. Then, we observe drops on a fiber placed in a symmetric wind. In a well-defined window of wind speed, the drop is found to self-propel along the fiber, which is analyzed. We also show that this effect makes drops moving in opposite direction bounce on each other, which generates fascinating 1-D dynamics.

In collaboration with Guillaume Dupeux, Philippe Bourrinane, Dan Soto, Hélène de Maleprade, Pierre-Brice Bintein, Hadrien Bense and Christophe Clanet.

1:03PM G51.00004 Directed assembly in soft matter by energy stored in inclusions, Kathleen Stebe, University of Pennsylvania — We have been exploiting fields that arise spontaneously when microparticles are placed in contact with deforming matter to direct assembly. In one context, we use capillary interactions that occur between anisotropic microparticles at fluid interfaces. The fluid interface deforms owing to the particle presence, creating an area field that bears the signature of the particle shape and wetting. We use curvature fields to direct particles to migrate, orient and assemble. In another context, we exploit elastic energies and defect fields that arise in liquid crystals. When a nematic liquid crystal is confined using surfaces with complex topographies and well-defined anchoring energies, the director field and associated defect fields can be molded to store elastic energy which can be used to steer particles into rich assemblies. In a final context, we study the interaction of colloidal particles on giant vesicles under tension, in which particles interact via bending energies to interact with each other.
1:39PM G51.00005 The Extreme Mechanics of Soft Structures¹. PEDRO REIS, Massachusetts Institute of Technology — I will present a series of experimental investigations on the rich behavior of soft mechanical structures, which, similarly to soft materials, can undergo large deformations under a variety of loading conditions. Soft structures typically comprise slender elements that can readily undergo mechanical instabilities to achieve extreme flexibility and reversible reconfigurations. This field has come to be warmly known as Extreme Mechanics, where one of the fundamental challenges lies in rationalizing the geometric nonlinearities that arise in the post-buckling regime. I shall focus on problems involving thin elastic rods and shells, through examples ranging from the deployment of submarine cables onto the seabed, locomotion of unflagellated bacteria, crystallography of curved wrinkling and its usage for active aerodynamic drag reduction. The main common feature underlying this series of studies is the prominence of geometry, and its interplay with mechanics, in dictating complex mechanical behavior that is relevant and applicable over a wide range of length scales. Moreover, our findings suggest that we rethink our relationship with mechanical instabilities which, rather than modes of failure, can be embraced as opportunities for functionality that are scalable, reversible, and robust.

¹The author acknowledges financial support from the National Science Foundation, CMMI-1351449 (CAREER).

Tuesday, March 3, 2015 11:15AM - 2:15PM –

Session G52 DCMP: Invited Session: Spin-Momentum Coupling in Topological Insulator Surfaces and Semiconductors Grand Ballroom C2 - Daniel Ralph, Cornell University

11:15AM G52.00001 Spin Circuit Model for Spin Orbit Torques in 2D Channels¹. SEOKMIN HONG, School of Electrical and Computer Engineering, Purdue University — Recently, the unique coupling between charge and spin in topological insulators has been explored through various types of electrical measurements, which could have interesting applications. In this talk, we present a spin circuit model [1] for spin orbit torques in topological insulator surface states and other 2D channels. We show with a simple example that results from the circuit model agree well with those obtained from nonequilibrium Green’s function (NEGF) based quantum transport simulation. Some predictions [2] of our model have already received experimental support and we hope this model can provide a unifying framework that can be used to critically evaluate experimental results, to explore new types of devices as well as to answer fundamental questions regarding these materials. The model for spin-orbit torques described here can be incorporated into a broader spin-circuit approach [3] which, we believe, provides a natural platform for multi-physics, multi-component spintronic devices.

¹This work was supported by FAME, a Semiconductor Research Corporation program sponsored by MARCO and DARPA.

11:51AM G52.00002 Magnetization switching through giant spin-orbit torque in the magnetically doped topological insulators¹. YABIN FAN, University of California, Los Angeles — Recent demonstrations of magnetization switching induced by in-plane current in heavy metal/ferromagnetic heterostructures (HMFHs) have drawn great interest to spin torques arising from the large spin-orbit coupling (SOC)...[1-3] in heavy metals. Considering the intrinsic strong SOC, topological insulators (TIs) are expected to be promising candidates for exploring spin-orbit torque (SOT)-related physics. In this talk, we report the magnetization switching through giant SOT in the magnetically doped TI structures. In particular, we demonstrate the magnetization switching in a chromium-doped TI bilayer heterostructure, and the current induced SOT possibly has contribution from the spin-momentum locked surface states of TI. The critical current density for switching is below 8.9 × 10⁴ A/cm² at 1.9 K. Moreover, we use second-harmonic methods to measure the spin torque efficiencies which are more than three orders of magnitude larger than those reported in heavy metals. The giant SOT and efficient current-induced magnetization switching exhibited by the bilayer heterostructure may lead to innovative spintronics applications such as ultralow power dissipation memory and logic devices.

¹We are grateful to the support from the DARPA Mesos program under contract No.N66001-12-1-4034 and N66001-11-1-4105. We also acknowledge the support from the Western Institute of Nanoelectronics (WIN) and the support from the FAME center.

12:27PM G52.00003 Spin-transfer torque generated by a topological insulator. ALEX MELNNIK, Cornell Univ — Magnetic devices are a leading contender for the implementation of memory and logic technologies that are non-volatile, that can scale to high density and high speed, and that do not wear out. However, widespread application of magnetic memory and logic devices will require the development of efficient mechanisms for reorienting their magnetization using the least possible current and power. We report experiments showing that charge current flowing in-plane in a thin film of the topological insulator Bi₂Se₃ at room temperature can exert a strong spin-transfer torque on an adjacent metallic ferromagnetic layer, with a direction consistent with that expected from a topological surface state. The spin torque efficiency per unit charge current density in the Bi₂Se₃ is larger than any previously measured at room temperature. Our data suggest that topological insulators could enable very efficient electrical manipulation of magnetic materials at room temperature, for memory and logic applications. Related publications: A. R. Melnnik, J. S. Lee, A. Richar'della, J. L. Grab, P. J. Mintun, M. H. Fischer, A. Vaezi, A. Manchon, E.-A. Kim, N. Samarth, D. C. Ralph, Nature 511, 449-451 (2014).
spin-mixing conductance of \(3\) from the confined mode to the spin sink of ferromagnetic material in the surrounding film. Though unexpected for insulating systems, the measured intralayer scales like the surface-to-volume ratio of the mode, indicating an interfacial damping effect (similar to spin pumping) due to the transfer of angular momentum is created within an extended, unpatterned YIG film by means of the intense local dipolar field of a micromagnetic tip. The damping of the confined mode spin ensembles. Electron spin resonance spectroscopy corroborates spin transport in strong field gradients. These experiments, supported by microscopic Monte Carlo modeling, provide a unique insight into the intrinsic dynamics of pure spin currents needed for nanoscale devices that seek to control spins. In addition, we observe a dependence of the damping of a confined mode of precessing ferromagnetic magnetization on the size of the mode. The micron-scale mode is created within an extended, unpatterned YIG film by means of the intense local dipolar field of a micromagnetic tip. The damping of the confined mode scales like the surface-to-volume ratio of the mode, indicating an interfacial damping effect (similar to spin pumping) due to the transfer of angular momentum from the confined mode to the spin sink of ferromagnetic material in the surrounding film. Though unexpected for insulating systems, the measured intralayer spin-mixing conductance of \(3 \times 10^{11}\) m\(^{-2}\) demonstrates efficient intralayer angular momentum transfer.

1:03PM G52.00004 Observation of chiral currents at the magnetic domain boundary of a topological insulator. YIHUA WANG, Stanford University — The broken time-reversal symmetry (TRS) states on the surface of a three-dimensional topological insulator (3D-TI) promise many exotic quantum phenomena. Breaking TRS opens a band gap on the surface Dirac cone and transforms the metallic surface into a Chern insulator. The TRS-broken surface states coupled to a superconductor are predicted to lead to Majorana fermions, which are the fundamental ingredients of topological quantum computation. Just as the surface Dirac cone is a signature of the non-trivial topological bulk band structure of a time-reversal invariant 3D-TI, bulk-boundary correspondence dictates that the TRS-broken surface states with a nonzero Chern number is manifested by a gapless chiral edge state (CES) at the domain boundary. In the special case where the domain boundary is the edge of the sample surface, CES along the edge leads to a quantized anomalous Hall conductance, which was recently measured in a magnetically doped 3D-TI. More generally, a magnetic domain boundary on the surface of TI hosts a CES, which is yet to be directly demonstrated because any local change of conductivity due to the CES does not affect conductance globally. Here we use a scanning superconducting quantum interference device (SQUID) to show that in a uniformly magnetized topological insulator - ferromagnetic insulator (TI-FMI) heterostructure current flows at the edge of the surface of the topological insulator when the Fermi level is gate-tuned to the surface band gap. We further induce micron-scale magnetic structures using the field coil of the SQUID and show that there emerges a chiral edge current at the magnetic domain boundary. In both cases the magnitude of the chiral edge current depends on the chemical potential rather than the applied current. Such magnetic nano-structures, which can be readily created on a TI in an arbitrary geometry, provide a versatile platform for detecting topological magneto-electric effects and may allow the engineering of magnetically defined quantum bits and spin-based electronics. Hybridization with conventional superconductors may open the door to topological quantum computation.

1:39PM G52.00005 Current-induced spin polarization in anisotropic spin-orbit fields. VANESSA SIH, University of Michigan — Current-induced spin polarization is a phenomenon in which carrier spins are oriented when subjected to current flow. However, the mechanism that produces this spin polarization remains an open question. Existing theory predicts that the spin polarization should be proportional to the spin-orbit splitting yet no clear trend has been observed experimentally. We perform experiments on semiconductor samples designed so that the magnitude and direction of the in-plane current and applied magnetic field can be varied and measure the electrical spin generation efficiency and spin-orbit splitting using optical techniques. Contrary to expectation, the magnitude of the current-induced spin polarization is shown to be larger for momentum directions corresponding to smaller spin-orbit splitting. In addition, angle-dependent measurements demonstrate that the steady-state in-plane spin polarization is not along the direction of the spin-orbit field, which we attribute to anisotropic spin relaxation. Furthermore, we show that this electrically-generated electron spin polarization can produce a nuclear spin hyperpolarization through dynamic nuclear polarization.


11:15AM G53.00001 Atomic spin chains as testing ground for quantum magnetism, SANDER OTTE, Kavli Institute of Nanoscience, Delft University of Technology — The field of quantum magnetism aims to capture the rich emergent physics that arises when multiple spins interact, in terms of elementary models such as the spin \(\frac{1}{2}\) Heisenberg chain. Experimental platforms to verify these models are rare and generally do not provide the possibility to detect spin correlations locally. In my lab we use low-temperature scanning tunneling microscopy to design and build artificial spin lattices with atomic precision. Inelastic electron tunneling spectroscopy enables us to identify the ground state and probe spin excitations as a function of system size, location inside the lattice and coupling parameter values. Two types of collective excitations that play a role in many dynamic magnetic processes are spin waves (magnons) and spinons. Our experiments enable us to study both types of excitations. First, we have been able to map the standing spin wave modes of a ferromagnetic bit of six atoms, and to determine their role in the collective reversal process of the bit (Spinelli et al., Nature Materials 2014). More recently, we have crafted antiferromagnetic spin \(\frac{1}{2}\) XXZ chains, which allow us to observe spinon excitations, as well as the stepwise transition to a fully aligned phase beyond the critical magnetic field (Toskovic et al., in preparation). These findings create a promising experimental environment for putting quantum magnetic models to the test.

11:51AM G53.00002 Spatially-resolved measurement of spin transport across nanoscale interfaces. ROHAN ADUR, The Ohio State University — Spintronics uses spin for information processing and storage. Mechanisms for spin relaxation in bulk systems have been extensively studied. However, a clear understanding of few-spin systems remains challenging. We report spatially-resolved magnetic resonance studies of a “spin nanowire” formed by nitrogen vacancies in diamond. The result reveals that the lifetime of the spin ensemble is dominated by spin transport from the ensemble into the adjacent spin reservoir, which is in striking contrast to conventional spin-lattice relaxation measurements of isolated spin ensembles. Electron spin resonance spectroscopy corroborates spin transport in strong field gradients. These experiments, supported by microscopic Monte Carlo modeling, provide a unique insight into the intrinsic dynamics of pure spin currents needed for nanoscale devices that seek to control spins. In addition, we observe a dependence of the damping of a confined mode of precessing ferromagnetic magnetization on the size of the mode. The micron-scale mode is created within an extended, unpatterned YIG film by means of the intense local dipolar field of a micromagnetic tip. The damping of the confined mode scales like the surface-volume ratio of the mode, indicating an interfacial damping effect (similar to spin pumping) due to the transfer of angular momentum from the confined mode to the spin sink of ferromagnetic material in the surrounding film. Though unexpected for insulating systems, the measured intralayer spin-mixing conductance of \(3 \times 10^{11}\) m\(^{-2}\) demonstrates efficient intralayer angular momentum transfer.
In collaboration with Stefano Bonetti, Roopali Kukreja, Zhao Chen, Stanford University and SLAC National Accelerator Laboratory; Sergei Urazhdin, Emory University; Josef Frisch, SLAC National Accelerator Laboratory; Ferran Macià, Dirk Backes, New York University; Anders Eklund, Gunnar Malm, The Royal Institute of Technology (KTH); Fred Mancoff, Everspin Technologies Inc.; Jordan Katine, HGST; Vasyl Tyberkevich, Andrei Slavin, Oakland University; Andrew In collaboration with Stefano Bonetti, Roopali Kukreja, Zhao Chen, Stanford University and SLAC National Accelerator Laboratory; Sergei Urazhdin, Emory University; Josef Frisch, SLAC National Accelerator Laboratory; Ferran Macià, Dirk Backes, New York University; Anders Eklund, Gunnar Malm, The Royal Institute of Technology (KTH); Fred Mancoff, Everspin Technologies Inc.; Jordan Katine, HGST; Vasyl Tyberkevich, Andrei Slavin, Oakland University; Andrew

1:03PM G53.00004 Full control of the spin-wave damping in a magnetic insulator using spin orbit torque. OLIVIER KLEIN, SPINTEC, UMR CEA/CNRS/UFJ-Grenoble 1/Grenoble-INP, INAC, 38054 Grenoble, France — The spin-orbit interaction (SOI) has been an interesting and useful addition in the field of spintronics by opening it to non-metallic magnet. It capitalizes on adjoining a strong SOI normal metal next to a thin magnetic layer. The SOI introduces a charge current, $J_c$, into a spin current, $J_s$, with an efficiency parametrized by $\gamma_{SO}$. The spin Hall angle. An important benefit of the SOI is that $J_c$ and $J_s$ are linked through a cross-product, allowing a charge current flowing in-plane to produce a spin current flowing out-of-plane. Hence it enables the transfer of spin angular momentum to non-metallic materials and in particular to insulating oxides, which offer improved performance compared to their metallic counterparts. Among all oxides, Yttrium Iron Garnet (YIG) holds a special place for having the lowest known spin-wave (SW) damping factor. Recently we have observed that spin current through the YIG-Pt interface has been subject to debate. While numerous experiments have reported that $J_s$ produced by the excitation of ferromagnetic resonance (FMR) in YIG can cross efficiently the YIG-Pt interface and be converted into $J_c$ in Pt through the inverse spin Hall effect (ISHE), most attempts to observe the reciprocal effect, where $J_c$ produced in Pt by the direct spin Hall effect (SHE) is transferred to YIG, resulting in damping compensation, have failed. This has been raising fundamental questions about the reciprocity of the spin transparency of the interface between a metal and a magnetic insulator. In this talk it will be demonstrated that the threshold current for damping compensation can be reached in a 5 $\mu$m diameter YIG(20nm)—Pt(7nm) disk. Reduction of both the thickness and lateral size of a YIG-structure were key to reach the microwave generation threshold current, $J_t$. The experimental evidence rests upon the measurement of the ferromagnetic resonance linewidth as a function of $J_c$, using a magnetic resonance force microscope (MRFM). It is shown that the magnetic losses of spin-wave modes existing in the magnetic insulator can be reduced or enhanced by at least a factor of five depending on the polarity and intensity of the in-plane dc current, $J_{dc}$. Complete compensation of the damping of the fundamental mode by spin-orbit torque is reached for a current density of $J_{dc} \sim 3 \times 10^{11}$A.m$^{-2}$, in agreement with theoretical predictions. At this critical threshold the MRFM detects a small change of static magnetization, a behavior consistent with the onset of an auto-oscillation regime. This result opens up a new area of research on the electronic control of the damping of YIG-nanostructures.

1:39PM G53.00005 X-ray Imaging of Spin Wave Dynamics at the Nanoscale. HENDRIK OHLDAG, SLAC, Stanford University — Imaging current induced magnetization dynamics has so far remained an elusive task, due to the lack of microscopy techniques with combined high spatial and temporal resolution, and elemental magnetic sensitivity. Using synchrotron radiation, we have been able to create the first x-ray images of spin waves generated in nano-contact spin torque oscillators realized on different ferromagnetic thin films, using the x-ray magnetic circular dichroism (XMCD) effect as a probe. In nanocontacts with perpendicular magnetic anisotropy, we directly observed the appearance of a highly localized mode beneath the nanocontact with large precession angle. In samples with an easy-plane magnetic anisotropy, we have been able to implement time-resolution in the measured process and to create a movie of the spin waves. We observed that the spin wave dynamics is excited on the side of the nanocontact where the internal field in the thin film is at a minimum. Around this field minimum, the spin wave extends with a radius of approximately 250 nm, demonstrating the localized nature of the mode. Finally, our measurements show that the spin wave has a node in amplitude, around which the magnetic field points in two opposite out-of-plane directions.

In collaboration with Stefano Bonetti, Roopali Kukreja, Zhao Chen, Stanford University and SLAC National Accelerator Laboratory; Sergei Urazhdin, Emory University; Josef Frisch, SLAC National Accelerator Laboratory; Ferran Macià, Dirk Backes, New York University; Anders Eklund, Gunnar Malm, The Royal Institute of Technology (KTH); Fred Mancoff, Everspin Technologies Inc.; Jordan Katine, HGST; Vasyl Tyberkevich, Andrei Slavin, Oakland University; Andrew Kent, New York University; and Joachim Stöhr, Hermann Dürrr, Hendrik Ohldag, SLAC National Accelerator Laboratory.

2:00PM - 2:00PM Session H1 APS: Poster Session I (2:00 pm - 5:00 pm) Exhibit Hall C

H1.00001 UNDERGRADUATE RESEARCH

H1.00002 Electromagnetic cavities as an analog to chaos regularization of quantum tunneling rates. RACHEL O'WEN, Western Washington University, JOHN RODGERS, University of Maryland — For double-well potentials separated by a tunneling barrier, it has been shown theoretically that quantum mechanical tunneling rates vary greatly with well geometry. Chaotic wells exhibit statistically smaller fluctuations in energy level splitting than those characterized by nonchaotic dynamics. This phenomenon (chaos regularization) can be analyzed by examining the statistical spacing in symmetric and anti-symmetric wave states produced by tunneling. Exploiting the similarity of transverse electromagnetic waves in large cavities and quantum mechanical wave functions in symmetric double-wells, chaos regularization in electromagnetic structures was studied experimentally and numerically. The resonant frequencies in rectangular (integrable) and bowtie (chaotic) cavities coupled via short sections of cutoff waveguides were simulated using finite element code and measured using a vector network analyzer. The ensemble difference in the measured anti-symmetric and symmetric resonant frequencies squared (analogous to splitting in energy levels) showed remarkably good agreement with theory. In the rectangular cavity we observed quantized resonances spaced across a wide range of frequencies whereas in the bowtie cavity the resonances were grouped randomly close to the theoretical curve.
H1.00003 Quantifying the Relationship between Surface Hydrophobicity and Depletion Layer Thickness

JARED NUTTER, SHANNON PETERSEN, RYAN SAYKO, ADELE POYNOR, Allegheny College — When water comes into contact with an extended hydrophobic surface, a uniform region of low density forms, called the depletion layer. This phenomenon has only been experimentally verified on surfaces with contact angles $>100^\circ$, but understanding how the thickness of the depletion layer changes with the hydrophobicity at intermediate contact angles is one of the underlying mechanisms behind several biological systems including colloidal self-assembly, protein folding, and fluid flow across membranes. We aim to quantify this relationship by using self-assembled monolayers of 1-octadecanethiol and 1-mercaptoheptadecanoic acid on gold to produce surfaces with contact angles between $55^\circ$ and $107^\circ$. We then use surface plasmon resonance spectroscopy to determine the thickness of the depletion layer formed for each surface.

H1.00004 Dependence of the Contact Angle on Self-Assembled Monolayer Production Method

BROOKE OLLANDER, SHANNON PETERSEN, RYAN SAYKO, ADELE POYNOR, Allegheny College — When water is forced in contact with a hydrophobic surface, it attempts to reduce its contact by forming a depletion layer. A depletion layer is defined as a nanometer scale low density region of water molecules at the surface. To alter the hydrophobicity of the slide, self-assembled monolayers (SAMs) are formed by utilizing the following organothiol solutions: 11-mercaptoundecanoic acid (hydrophilic) and 1-octadecanethiol (hydrophobic). The contact angle of slides with different organothiol solution exposure times is measured using a homemade goniometer and ImageJ software.

H1.00005 Flow Rate In Microfluidic Pumps As A Function Of Tension and Pump Motor Head Speed

ANTHONY IRWIN, KRISTA MCBRIDE, Belmont University — As the use of microfluidic devices has become more common in recent years the need for standardization within the pump systems has grown. The pumps are ball bearing rotor microfluidic pumps and work off the idea of peristalsis. The rapid contraction and relaxation propagating down a tube or a microfluidic channel. The ball bearings compress the tube (occlusion) and move along part of the tube length forcing fluid to move inside of the tube in the same direction of the ball bearings. When the ball bearing rolls off the area occupied by the microfluidic channel, its walls and ceiling undergo restitution and a pocket of low pressure is briefly formed pulling more of the liquid into the pump system. Before looking to standardize the pump systems it must be known how the tension placed by the pumps bearing heads onto the PDMS inserts channels affect the pumps performance (mainly the flow rate produced). The relationship of the speed at which the bearings on the motor head spin and the flow rate must also be established. This research produced calibration curves for flow rate vs. tension and rpm. These calibration curves allow the devices to be set to optimal user settings by simply varying either the motor head tension or the motor head speed.

1 I would like to acknowledge the help and support of Vanderbilt University SyBURE program, Christina Marasco, Stacy Sherod, Franck Block and Krista McBride.

H1.00006 Photoemission spectroscopy and X-ray diffraction analysis of 3D topological and Kondo insulators

PAVEL SHIBAYEV, Princeton University, HASAN GROUP TEAM — The advantage of studying 3D topological insulators (TIs), compounds that have attracted the attention of many in the condensed matter field, is the ability for their existence at room temperature and no magnetic fields, allowing both for resolving their band structure via angle-resolved photoemission spectroscopy (ARPES) and understanding electrical transport and other properties via X-ray diffraction (XRD) and point-contact spectroscopy (PCS). A comprehensive quantitative analysis of Bi$_2$Se$_3$, a 3D TI, was carried out using these methods. The Bi$_2$Se$_3$ crystals were synthesized in-house at Princeton University. A first-principles calculation based on density functional theory, DFT, was performed using the Abinit software. The band structure of the crystal was then resolved via ARPES at the Advanced Light Source in LBNL, resulting in a surprisingly stark and clear single Dirac cone. A large band gap was confirmed, suggesting an increased potential for applications. In contrast, Kondo insulators are found in rare-earth based materials with f-electron degrees of freedom. Photon energy dependent dispersion relationships and temperature dependence studies were performed on a Kondo candidate CeB$_6$ via ARPES, showing an even number of Dirac cones and a non-TI behavior. Analysis of I-V characteristics through PCS will follow, in addition to characterization via Bruker XRD for both compounds.

2 Research group led by Professor M. Zahid Hasan (Princeton University)

H1.00007 Structure Property Relationships in Imidazole-based Deep Eutectic Mixtures

LOGAN TERHEGGEN, TYLER COSBY, JOSHUA SANGORO, Univ of Tennesse, Knoxville — Deep eutectic mixtures of levulinic acid with a systematic series of imidazoles are measured by broadband dielectric spectroscopy, differential scanning calorimetry, and Fourier transform infrared spectroscopy to investigate the impact of steric interactions on charge transport and structural dynamics. An enhancement of dc conductivity is found in each of the imidazoles upon the addition of levulinic acid. However, the extent of increase is dependent upon the alkyl substitution on the imidazole ring. These results highlight the importance of molecular structure on hydrogen bonding and charge transport in deep eutectic mixtures.

H1.00008 Laser Induced Breakdown Spectroscopy of Metals

ANDRIA PALMER, CARLOS LAWHEAD, LASZLO UJJ, University of West Florida — Laser Induced Breakdown Spectroscopy (LIBS) is a very practical spectroscopy to determine the chemical composition of materials. Recent technical developments resulted in equipment used on the MARS Rover by NASA. It is capable of measuring the emission spectra of laser induced plasma created by energetic laser pulses focused on the sample (rocks, metals, etc.). We have develop a Laser Induced Breakdown Spectroscopy setup and investigated the necessary experimental and methodological challenges needed to make such material identification measurements. 355 and 532 nm laser pulses with 5 ns temporal duration was used to generate micro-plasma from which compositions can be determined based on known elemental and molecular emission intensities and wavelengths. The performance of LIBS depends on several parameters including laser wavelength, pulse energy, pulse duration, time interval of observation, geometrical configuration of collecting optics, and the properties of ambient medium. Spectra recorded from alloys (e.g. US penny coin) and pure metals will be presented.

1 Special thanks for the financial support of the Office of Undergraduate Research of UWF

H1.00009 Differential Conductance Measurements of MgB$_2$/I/Pb Heterojunctions and all-MgB$_2$ Junctions

DAVID CUSICK, Taylor University, MATTHEW ECKHARDT, Indiana Wesleyan University, WENQING DAI, QI LI, Pennsylvania State University, KE CHEN, DANIEL CUNNANE, Temple University, C.G. ZHUANG, None, X.X. XI, Temple University, MICHIO NAITO, Tokyo University of Agriculture and Technology, ROBERTO RAMOS, Indiana Wesleyan University — We present our work characterizing several types of Magnesium Diboride Josephson junctions, including MgB$_2$/I/Pb heterojunctions and all-MgB$_2$ junctions. We report on the I-V and dI/dV-V data collected at various temperatures using both a cryocooler-based experimental platform between 2 and 20 Kelvin and using a $^3$He probe platform between 0.3 and 1.0 Kelvin. These were both developed by undergraduates in a liberal arts university. Using high-sampling rates with a 24-bit data acquisition card and access to a broad range of temperatures, we track and report energy gap distributions and temperature-dependent features of dI/dV peaks of MgB$_2$, comparing these with theoretical predictions.

1 R.C.R. acknowledges support from National Science Foundation Grant # DMR-1206561.

2 David Cusick is a Taylor University student interning at Indiana Wesleyan University.
Volume phase transition and corresponding change in composition of polymeric microgels. Janna Mino, Christian Gunder, Kiril Streletzky, Cleveland State University — Temperature sensitive polysaccharide microgels and parent amphiphilic polymer solution were studied in parallel with Dynamic (DLS) and Static Light Scattering (SLS) spectroscopies. The microgels showed a reversible volume phase transition which was accompanied by a significant change in microgel volume and composition. Coupling DLS and SLS techniques on microgels and polymer solutions allowed to deduce microgel size, structure, molecular weight and a relative change in microgel water content during the volume phase transition. It also allowed comparing controlled dewetting transition in microgels with corresponding phase transition in parent polymer solution. Light scattering findings were tested with SEM imaging.

Synthesis and Characterization of Tetraphiafulvalene Derivatives, Mark Bartolo, Stephen Tsui, Cal State Univ - San Marcos, Eric Reinheimer, Rigaku — We synthesize tetraphiafulvalene (TTF) derivative materials in an effort to identify conducting and magnetic properties. The doping of these TTF derivatives include tetracyanoethylene (TCN), 7,7,8,8-tetracyanoquinodimethane (TCNQ), and para-dinitrobenzene (pDNB). We examine these TTF containing donor-acceptor complexes through their structural and electronic transport characteristics.

Determination of stimulation focality in heterogeneous head models during transcranial magnetic stimulation (TMS), Erikl Lee, Ravi Hadimani, David Jiles, Department of Electrical and Computer Engineering, Iowa State University — Transcranial Magnetic Stimulation (TMS) is an increasingly popular tool used by both the scientific and medical community to understand and treat the brain. TMS has the potential to help people with a wide range of diseases such as Parkinson's, Alzheimer's, and PTSD, while currently being used to treat people with chronic, drug-resistant depression. Through computer simulations, we are able to see the electric field that TMS induces in anatomical human models, but there is no measure to quantify this electric field in a way that relates to a specific patient undergoing TMS therapy. We propose a way to quantify the focality of the induced electric field in a heterogeneous head model during TMS by relating the surface area of the brain being stimulated to the total volume of the brain being stimulated. This figure would be obtained by conducting finite element analysis (FEA) simulations of TMS therapy on a patient specific head model. Using this figure to assist in TMS therapy will allow clinicians and researchers to more accurately stimulate the desired region of a patient's brain and be more equipped to do comparative studies on the effects of TMS across different patients.

Electronic Resonance Enhancement in Raman and CARS Spectroscopy: Surface Enhanced Scattering of Highly Fluorescent Molecules, Carlos Lawhead, Laszlo Ujj, University of West Florida — Surface enhanced Raman spectroscopy (SERS) is an extremely useful tool in increasing sensitivity of Raman spectroscopy; this technique significantly increases the signal from vibrational resonances which can overcome background fluororesces. Silver nanoparticles coated substrates and the silver nanoparticles in solution were used on a variety of fluorescent molecules in order to overcome sample complexities and measure the vibrational spectra. The possible enhancement of SERS using a coherent Raman (CARS) method was investigated, but enhancement factors due to Surface Enhanced CARS have yet to be verified. The instrument used was developed in the University of West Florida Physics Department utilized the second harmonic of a Nd:YAG laser to provide the excitation wavelength at 532 nm and is capable of both transmission and reflection Raman measurements.

Fluorescence and Bonding of Quantum Dots on DNA Origami Constructs, Matthew Kessinger, Timothy Corigan, Concord, David Neff, Michael Norton, Marshall University, CONCORD UNIVERSITY COLLABORATION — Semiconductor quantum dots (QDots) have historically been of interest to the scientific community since their creation for various applications ranging from solar energy to optical labeling. In this study, bioconjugated CdSe/ZnS core/shell QDots were synthesized and functionalized with 3-mercappropionic acid using both traditional ligand exchange as well as newly developed in situ functionalization techniques used to increase the quantum yield of the QDots. Their fluorescence and bonding to both gold as well as DNA origami were investigated for use in self assembled DNA constructs. It is believed that controlling the attachment and spacing of these nanoparticles on DNA origami could be used in a variety of optical labeling and sensing applications. Commercially available biotin and streptavidin functionalized quantum dots were also examined, and subject to the same experiments with gold nanoparticles as the MPA functionalized QDots.

Analysis of layer-by-layer thin-film oxide growth using RHEED and Atomic Force Microscopy, Eli Adler, M.C. Sullivan, Ithaca College, Department of Physics and Astronomy, Araceli Gutierrez-Llorente, H. Jiores, A. Woll, J.D. Brock, Cornell High Energy Synchrotron Source, Cornell University — Reflection high energy electron diffraction (RHEED) is commonly used as an in situ analysis tool for layer-by-layer thin-film growth. Atomic force microscopy is an equally common ex situ tool for analysis of the film surface, providing visual evidence of the surface morphology. During growth, the RHEED intensity oscillates as the film surface changes in roughness. It is often assumed that the maxima of the RHEED oscillations signify a complete layer, however, the oscillations in oxide systems can be misleading. Thus, using only the RHEED maxima is insufficient. X-ray reflectivity can also be used to analyze growth, as the intensity oscillates in phase with the smoothness of the surface. Using x-ray reflectivity to determine the thin film layer deposition, we grew three films where the x-ray and RHEED oscillations were nearly exactly out of phase and halted deposition at different points in the growth. Pre-growth and post-growth AFM images emphasize the fact that the maxima in RHEED are not a justification for determining layer completion.

Enhanced Scattering of Highly Fluorescent Molecules, Stephen Tsui, Cal State Univ - San Marcos, Eric Reinheimer, Rigaku — We synthesize tetraphiafulvalene (TTF) derivative materials in an effort to identify conducting and magnetic properties. The doping of these TTF derivatives include tetracyanoethylene (TCN), 7,7,8,8-tetracyanoquinodimethane (TCNQ), and para-dinitrobenzene (pDNB). We examine these TTF containing donor-acceptor complexes through their structural and electronic transport characteristics.

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Electronic Resonance Enhancement in Raman and CARS Spectroscopy: Surface Enhanced Scattering of Highly Fluorescent Molecules, Carlos Lawhead, Laszlo Ujj, University of West Florida — Surface enhanced Raman spectroscopy (SERS) is an extremely useful tool in increasing sensitivity of Raman spectroscopy; this technique significantly increases the signal from vibrational resonances which can overcome background fluororesces. Silver nanoparticles coated substrates and the silver nanoparticles in solution were used on a variety of fluorescent molecules in order to overcome sample complexities and measure the vibrational spectra. The possible enhancement of SERS using a coherent Raman (CARS) method was investigated, but enhancement factors due to Surface Enhanced CARS have yet to be verified. The instrument used was developed in the University of West Florida Physics Department utilized the second harmonic of a Nd:YAG laser to provide the excitation wavelength at 532 nm and is capable of both transmission and reflection Raman measurements.

Fluorescence and Bonding of Quantum Dots on DNA Origami Constructs, Matthew Kessinger, Timothy Corigan, Concord, David Neff, Michael Norton, Marshall University, CONCORD UNIVERSITY COLLABORATION — Semiconductor quantum dots (QDots) have historically been of interest to the scientific community since their creation for various applications ranging from solar energy to optical labeling. In this study, bioconjugated CdSe/ZnS core/shell QDots were synthesized and functionalized with 3-mercappropionic acid using both traditional ligand exchange as well as newly developed in situ functionalization techniques used to increase the quantum yield of the QDots. Their fluorescence and bonding to both gold as well as DNA origami were investigated for use in self assembled DNA constructs. It is believed that controlling the attachment and spacing of these nanoparticles on DNA origami could be used in a variety of optical labeling and sensing applications. Commercially available biotin and streptavidin functionalized quantum dots were also examined, and subject to the same experiments with gold nanoparticles as the MPA functionalized QDots.

Analysis of layer-by-layer thin-film oxide growth using RHEED and Atomic Force Microscopy, Eli Adler, M.C. Sullivan, Ithaca College, Department of Physics and Astronomy, Araceli Gutierrez-Llorente, H. Jiores, A. Woll, J.D. Brock, Cornell High Energy Synchrotron Source, Cornell University — Reflection high energy electron diffraction (RHEED) is commonly used as an in situ analysis tool for layer-by-layer thin-film growth. Atomic force microscopy is an equally common ex situ tool for analysis of the film surface, providing visual evidence of the surface morphology. During growth, the RHEED intensity oscillates as the film surface changes in roughness. It is often assumed that the maxima of the RHEED oscillations signify a complete layer, however, the oscillations in oxide systems can be misleading. Thus, using only the RHEED maxima is insufficient. X-ray reflectivity can also be used to analyze growth, as the intensity oscillates in phase with the smoothness of the surface. Using x-ray reflectivity to determine the thin film layer deposition, we grew three films where the x-ray and RHEED oscillations were nearly exactly out of phase and halted deposition at different points in the growth. Pre-growth and post-growth AFM images emphasize the fact that the maxima in RHEED are not a justification for determining layer completion.

Enhanced Scattering of Highly Fluorescent Molecules, Stephen Tsui, Cal State Univ - San Marcos, Eric Reinheimer, Rigaku — We synthesize tetraphiafulvalene (TTF) derivative materials in an effort to identify conducting and magnetic properties. The doping of these TTF derivatives include tetracyanoethylene (TCN), 7,7,8,8-tetracyanoquinodimethane (TCNQ), and para-dinitrobenzene (pDNB). We examine these TTF containing donor-acceptor complexes through their structural and electronic transport characteristics.
H1.00016 Developing a protocol for creating microfluidic devices with a 3D printer, PDMS, and glass

H1.00017 Highly Porous Regenerated Cellulose Fiber Mats via the Co-Forcespinning of Cellulose Acetate for Separator Applications. ALEJANDRO CASTILLO, YUANBING MAO, University of Texas Pan-American Chemistry — Improvements in battery technology are necessary for the transition away from a fossil fuel based economy. An important bottle-neck in battery efficiency is the quality of the separator, which separates the cathode and anode to prevent a short-circuit while still allowing the ions in solution to flow as close to unobstructed as possible. In this work solutions of cellulose acetate, polyvinylidifluorine (pvdf), and polyvinylpyrrolidone (ppv) dissolved in a 2:1 v/v acetone/dimethylacetamide solvent mixture were Forcespun to create nonwoven fiber mats of nanoscale diameter. These mats were then soaked in a NaOH solution so as to both strip the ppv from the fiber as well as regenerate cellulose from its acetate derivative for the purpose of creating high surface area, nanoporoporous, hydrophilic, and ionically conductive cellulose/pvdf nonwoven mats for the purposes of testing their suitability as battery separators.

H1.00018 IR spectroscopy of an OH hindered rotor in ZnO

H1.00019 Temperature dependence measurements for Cadmium Telluride (CdTe) solar cells. FERNANDA DUARTE, WEINING WANG, Department of Physics, Seton Hall University — Traditional silicon (Si)-based solar cells have been studied broadly and have already reached their maximum efficiency. However, their cost is relatively high, preventing them from being widely used. Unlike Si-based solar cells, Cadmium Telluride (CdTe) solar cells are considerably cheap, yet the record efficiency is still lower than that of traditional silicon-based solar cells. More studies are needed to understand and improve the efficiency of CdTe solar cells. In this work, we report our studies of the temperature dependence of CdTe solar cell parameters using the temperature-varying apparatus designed and built by us in-house. This temperature-varying apparatus will be incorporated with a solar cell testing station in order to measure the solar cell parameters while varying the temperature. The solar cell parameters will be measured at different temperatures (within a 100 K temperature range), and the effects of temperature on the open-circuit voltage, short-circuit current and efficiency of the solar cells will be reported. These results allow us to further understand the physics of CdTe solar cells and shine light on how to improve the efficiency of CdTe solar cells.

H1.00020 Systematic Studies of Phase Transitions in Thermos-Responsive Polymers Used in Targeted Drug Delivery. JANAE BRADLEY, Univ of Missouri - Columbia, DANIEL DENMARK, SARATH WITANACHCHI, University of South Florida — Thermoresponsive polymers such as poly-N-isopropylacrylamide (PNIPAM) can undergo reversible phase transitions in aqueous solutions under varying temperature. They are ideal candidates for the polymer shell of a targeted drug delivery capsule. Concentration and pH can affect the lower critical solution temperature (LCST) of the PNIPAM polymer and its physical properties. In this work, a systematic study of the factors that influence the LCST of the PNIPAM polymer mixed with Fe304 nanoparticles (MNPs) during thermal bath heating is presented. A series of PNIPAM solutions with varying concentrations of PNIPAM with MNPs were prepared and characterized using scanning electron microscopy. In-situ transmission measurements were used to determine the LCST of PNIPAM concentrations. A systematic decrease in the LCST was observed as the concentration of PNIPAM was increased. In addition, the impact of pH on the LCST of PNIPAM was examined by increasing the basicity of the PNIPAM solutions by adding adjusted KOH pellets. An increase in the thermal stability of the LCST was observed when the basicity of the PNIPAM solution was increased. The results from this study provide valuable information towards using these thermo-responsive polymers in targeted drug delivery.

H1.00021 Superconducting Resonators: Protecting Schrodinger’s Cat

H1.00022 Capacitance measurements of defects in solar cells: checking the model assumptions
H1.00023 Does a simple lattice protein exhibit self-organized criticality? , DANA GIBBON, ALISSA RUNYON, ARUN BAJRACHARYA, JOËLLE MURRAY, Linfield College — There are many unanswered questions when it comes to protein folding. These questions are interesting because the tertiary structure of proteins determines its functionality in living organisms. How do proteins consistently reach their final tertiary structure from the primary sequence of amino acids? What explains the complexity of tertiary structures? Our research uses a simple hydrophobic-polar lattice-bound computational model to investigate self-organized criticality as a possible mechanism for generating complexity in protein folding and protein tertiary structures.

H1.00024 Development of TiO$_2$-Xwt\%InVO$_4$ Photocatalytic Nano-composites for Ambient Light Assisted Water Detoxification , SESHA SRINIVASAN, Florida Polytechnic University, College of Innovation and Technology, JEREMIAH WILSON, Tuskegee University, Department of Physics, ERIC VICKERS, RYAN INTELLIGA, Florida Polytechnic University, College of Engineering — We have developed nano-composites of TiO$_2$-Xwt\%InVO$_4$ for environmental and biomedical research applications. TiO$_2$ is commonly used as catalyst that utilizes the UV portion of the sun light spectrum to induce photo-oxidation and photo-reduction processes. We hypothesized that the combination of InVO$_4$ and TiO$_2$ will result in a material that will catalyze organic contaminants through photo-oxidation under visible light. We combined TiO$_2$ with 2,4,6,8,10wt\% of InVO$_4$ via wet ball milling process. We have compared the various concentrations of InVO$_4$ on TiO$_2$ matrix by SEM, BET surface area analyzer, FTIR, XRD, and photodegradation of the organic contaminant Methyl Orange. After characterization we found that 4wt\% InVO$_4$-TiO$_2$ mixture displayed the most promising characteristics for photo-oxidation under visible light. From the BET surface area analysis it showed the largest surface area out of the prior mentioned TiO$_2$ = Xwt\%InVO$_4$ mixtures and a degradation amount equivalent to 50\% of Methyl Orange contaminant over 7 hours under visible light. In conclusion, TiO$_2$-Xwt\%InVO$_4$ displayed evidence of photo-oxidation under visible light conditions.

1 Authors would like to acknowledge the support from Sigma Pi Sigma and Society of Physics Students. National Science Foundation and Florida Energy Systems Consortium are gratefully acknowledged for the research and education grants.

H1.00025 Toward a Rb MOT for Undergrad Research and Advanced labs at Bridgewater State University , EDWARD DEVENEY, Bridgewater State University — The seminal paper for the undergraduate MOT appeared in AJP (63 (4), 1995) by C. Wieman, G. Flowers and S. Gilbert; ‘Inexpensive laser cooling and trapping experiment for undergraduate laboratories’. They wrote: “Because of this visual appeal and the current research excitement in this area, we felt that it was highly desirable to develop an atom trapping apparatus that could be incorporated into the undergraduate laboratory classes.” From our observations, it seems that while there are extraordinary examples of MOTs thriving in a few undergraduate labs, MOT experiments have yet to be widely incorporated into the undergraduate curriculum – likely because they are, in fact, not trivial to make. With the benefit of 20 years evolution since this 1st undergraduate MOT paper, we report the progress at BSU of constructing a 85Rb MOT that incorporates significant simplifications and straightforward techniques that include: using a single ECDL laser for both trapping and re-pumping (using an EOM to add FM sidebands) and combining a purchased stabilized HeNe with the ECDL in a Fabry-Perot Interferometer to correct and sufficiently stabilize the ECDL for trapping. When completed we will revisit the question of do-ability for the undergraduate research/advanced lab. The BSU MOT was planned with and is currently being built with the help and guidance of David DeMille and his research group at Yale University [including J. Barry Thesis, Yale].

H1.00026 Optical V-Band Observations of Active Galactic Nuclei , TAYLOR HUTCHISON, RAINA MUSSO, FRANCIS MACINNIS, MARK BOTTORFF, Southwestern University — Students at Southwestern University participated in an international observing campaign to study twelve active galactic nuclei (AGN). As part of this project, the students measured optical V-band light variations of four targets within the range of 4.5° to 8° from the Galactic Center. The students used the 18.2-meter studentscope at the Tenerife Astronomical Observatory and the Cerro Tololo Inter-American Observatory. The students analyzed the data using statistical methods and compared their results with previous studies. The students’ observations provided new insights into the optical variations of AGN and contributed to our understanding of the dynamics of active galactic nuclei.

H1.00027 ABSTRACT WITHDRAWN –

H1.00028 ABSTRACT WITHDRAWN –

H1.00029 ABSTRACT WITHDRAWN –

H1.00030 Origins of Nonlinearity in Superconductive Passive Circuits , SEAN HAMILTON, Grand Valley State University, STEPHEN REMILLARD, Hope College — The distinct origins of even and odd order nonlinear behavior in type II cuprate superconductors have yet to be fully elucidated. Microwave intermodulation distortion (IMD) was examined in a YBCO superconducting thin-film hairpin resonator at 840 MHz. Measurements of the temperature dependence of IMD near Tc support the view that the nonlinear Meissner effect is responsible for the occurrence of both 2\textsuperscript{nd} and 3\textsuperscript{rd} order IMD tones near Tc as well as their suppression in an applied magnetic field. However, at lower reduced temperatures (T/Tc less than 0.95), where the influence of the nonlinear Meissner effect is less pronounced, 3\textsuperscript{rd} order IMD is unaffected by a static magnetic field, while 2\textsuperscript{nd} order IMD decays exponentially after a static magnetic field is removed with a temperature dependent time constant. It is apparent that the magnetically induced remnant vortex state contributes to the 2\textsuperscript{nd} order nonlinearity, but not to the 3\textsuperscript{rd} order nonlinearity, and that this effect is diminished close to Tc due to degradation of the remnant vortex state.

1 This research was funded by the National Science Foundation under grant number DMR-1206149.

H1.00031 Measuring and Modeling the Plasma Temperature and Density in WIRX , MICHAEL MORKEN, DARREN CRAIG, Wheaton College (IL) — We develop a theoretical model and experimental techniques to provide a better picture of how the adjustable parameters such as the current, and electrode geometry affect the temperature and density of WIRX plasmas. Our model predicts the plasma temperature and density by balancing the Ohmic heating with convective losses. The Ohmic heating is measured directly as the product of the voltage drop between the electrodes and the plasma current. Temperature and density are measured independently using spectroscopic methods. Stark broadening of the H-\beta line is used to measure density. To measure the electron temperature of the plasma the line ratios of various hydrogen transitions were compared with the predictions of the Boltzmann thermal equilibrium model and the coronal equilibrium model. Preliminary experimental results are consistent with the plasma parameters predicted by our model. This work will be used to inform future modifications to the experiment with the intent of producing higher temperatures in WIRX plasma, making magnetic reconnection more probable. Work supported by US DOE.
H1.00032 Two Dimensional Intermodulation Distortion Scanning of Superconducting Filter Resonators, MICHAEL BISCHAK, STEPHEN REMILLARD, Hope College — Nonlinear superconducting conductivity produces distortion that has usually been measured globally across the entire sample. In order to fully understand the origin of non-linearity, local methods must be used to examine specific points in the sample. The nonlinear Ohm’s law, \( V = IZ(I) \) includes the current dependence in the impedance. The method in this work raster scans a magnetic loop probe across a sample. In order to address limited resolution, we reduced the size of the magnetic loop probe. Using the electromagnetic field solver, sonnet, two dimensional current simulations of superconducting microwave filters composed of Ti2Ba2CaCu2O8 or of YBa2Cu3O7 reveal microwave current which is bunched up at the corners and sides of the sample. Two dimensional images of third order intermodulation distortion made with the magnetic probe at the same corners and edges reveal elevated distortion in the same places. Using the magnetic probe, third order intermodulation was seen to come from the same corners and edges where the current is bunched. This research was funded by the National Science Foundation under grant number DMR-1260149.

H1.00033 Raman spectroscopy of single-walled carbon nanotubes of different lengths exposed to microwave radiation, P. BHATNAGAR, Angelo State Univ, S. FERGUSON, University of Texas - Dallas, G. SESTRIC, I. WRIGHT, S. WILLIAMS, Angelo State Univ — Carbon nanotubes have been observed to emit ultraviolet, visible, and infrared radiation when exposed to microwave fields. Although there is considerable controversy concerning the mechanism responsible for the emissions, the results of recently-performed experiments suggest that the emissions may be the result of field emission-induced luminescence. We have performed experiments in which both short (0.5 \( \mu \)m - 2 \( \mu \)m) and long (5 \( \mu \)m - 30 \( \mu \)m) single and double-walled carbon nanotubes were exposed to 2.46 GHz microwaves at a pressure of approximately \( 10^{-6} \) torr. A comparison of the spectra of the radiation emitted from the nanotubes suggests that the longer nanotubes emitted radiation of greater intensity than the shorter nanotubes, which is consistent with field emission-induced luminescence. Moreover, structural modification of the carbon nanotubes due to microwave irradiation has been studied using the Raman spectroscopy G-band and D-band intensities, which suggests that microwave radiation at relatively low powers can lead to new nanotube defects, especially in the case of the long nanotube samples.

H1.00034 Study of the angular distributions of X-rays emitted following L3 ionization of gold atoms by electron impact, I. WRIGHT, G. SESTRIC, S. FERGUSON, S. WILLIAMS, Angelo State University — Theoretical work suggests that when an atomic inner-shell vacancy with total angular momentum \( j \) greater than 1/2 is created by interaction with a photon or charged particle the vacancy will be aligned due to the magnetic sublevels of the ion having nonstatistical populations. The experiments we performed, testing this theory, involved measurements of the angular distributions of gold L\( \alpha \), L\( \beta \), and L\( \gamma \) X-rays at forward angles in the range 0 degrees to 25 degrees emitted after being bombarded with 15-keV electrons. After corrections for absorption of the characteristic X-rays within the gold target, our results suggest that the angular distributions of the L\( \alpha \), L\( \beta \), and L\( \gamma \) X-rays are essentially isotropic, as no angular dependence was observed in our data outside of experimental uncertainties. However, the results of our experiments suggest that the angular distribution of the gold L\( \beta \) X-rays may be weakly anisotropic.

H1.00035 A Study of Two Dimensional Electron Gas Using 2D Fourier Transform Spectroscopy, CARL MCINTYRE, Colorado Mesa University, JAGANNATH PAUL, DENIS KARAISKAJ. University of South Florida — The dephasing of FES was measured in a symmetrically modulated doped 12 nm single quantum well GaAs/AlGaAs two dimensional electron gas system using time integrated four wave mixing (TIFWM) and a two dimensional Fourier transform spectroscopy (2DFTS). At high in-well carrier densities of \( \sim 4 \times 10^{11} \) cm\(^{-2}\), many body effects that are prevalent and measurable with non-linear optical spectroscopy. Effects of exciton-exciton and exciton-phonon scattering events, exciton populations, and biexciton formation are detectable at these carrier concentrations. Homogeneous linewidths obtained from 2DFT and TIFWM yield a zero Kelvin linewidth of 1.42 meV and an acoustic phonon scattering coefficient of 158 \( \mu \) eV/K. These observations indicate a rapid increase in homogeneous linewidth with increased temperature.

H1.00036 Analytically Evaluating Sums in Quantum and Statistical Physics Using Integral Transforms, JOHN VASTOLA, University of Central Florida — Evaluating sums analytically is a problem that is easy to pose and to give approximate solutions to, but that is difficult to exactly solve in general. Many results that are known are byproducts of Fourier analysis, which requires guessing that a series corresponds to a function. A more systematic method of evaluating sums using integral transforms is proposed which can reproduce many results obtained using other techniques. In particular, representing polynomials as Laplace transforms gives some nontrivial exact results. Some applications of the method are demonstrated, and extensions of the method using integral representations of frequently appearing functions are suggested. One useful representation of the gamma function is supplied, and used to provide both well-known and more obscure results. Interestingly, the application of this integral representation to evaluating sums suggests the introduction of a novel integral transform, which itself can be used to evaluate sums. Some of the transform’s properties are given, and its usefulness in other areas (like solving differential equations) is touched upon. Some physical problems involving the partition functions of statistical mechanics, and some infinite sums appearing in quantum mechanics, are considered.

H1.00037 In-air Rutherford Backscattering and Particle Induced X-ray Emission for Biophysics and Material Science Research, JAMES BECKER, None — Rutherford Backscattering (RBS) and Particle Induced X-ray Emission (PIXE) are methods of nondestructive analysis of elemental composition. Rebounding particles or emitted x-rays can be “collected” and then analyzed to reveal the number ratio of the elements in a sample. Due to the nondestructive feature of these processes, RBS and PIXE are useful in many diverse fields of study such as archaeology, art, and biology; however, these experiments usually require large, expensive particle accelerators and detectors. Instead, I am attempting to use a radioactive source, photodiodes, and computer software to perform the same methods at a fraction of the cost. I am exploring cost, time, and resolution benefits and losses of my approach versus the traditional accelerator-based approach.

H1.00038 Relativistic Quantum Mechanical Calculations on Alkali Atoms and Dimers from Cesium to Ununennium, CHUKVUNOSO ARINZE, WALTER ERLMLER, University of Texas at San Antonio — Ab initio calculations using relativistic effective core potentials, and intermediate angular momentum coupling of electrons are carried out on the alkali metal atoms, and dimers from cesium through ununennium. A spin-orbit configuration interaction (SOCl) method is employed that includes a spin-orbit coupling operator and a relativistic effective core potential in the Schrodinger Hamiltonian operator. The energy levels from these calculation are found to reproduce the positions of the experimental spectral lines and predict lines not heretofore observed for both of these atoms.
H1.00039 Re-Examining Gravitational Tunneling Radiation when taking into account Quantum Gravity Effects\footnote{H1.00039 Re-Examining Gravitational Tunneling Radiation when taking into account Quantum Gravity Effects}, JOHN VALENTINE, TREVOR PRESCOTT, GARDO BLADO, Houston Baptist Univ — Although shown to theoretically exist, Hawking Radiation has yet to be detected. The paper entitled “Gravitational Tunneling Radiation”\cite{rabinowitz1999} by Mario Rabinowitz proposed a possible explanation by considering the gravitational tunneling effects in the presence of other bodies in the vicinity of the black hole. Rabinowitz showed that the power radiated (through gravitational radiation) by a black hole, $P_{\text{H}}$, is related to the power generated by Hawking Radiation, $P_{\text{SH}}$ by $P_{\text{H}} \approx \frac{T^3}{16\pi} \sim P_{\text{SH}}$ where $T$ is the gravitational tunneling probability. The presence of other bodies lowers the gravitational barrier which in turn increases the gravitational tunneling probability thereby decreasing the Hawking radiation, $P_{\text{H}}$. In this paper, we examine the modification of $T$ in the presence of quantum gravity effects by incorporating the Generalized Uncertainty Principle.

\begin{equation}
\text{H1.00040 A Novel Method of Line Detection using Image Integration Method},
\end{equation}

DAVISON LIN, BO SUN, Oregon State University — We developed a novel line detection algorithm based on image integration method. Hough Transformation uses spatial image gradient method to detect lines on an image. This is problematic because if the image has a region of high noise intensity, the gradient would point towards the noisy region. Denoising the noisy image requires an application of sophisticated noise reduction algorithm which increases computation complexity. Our algorithm can remedy this problem by averaging the pixels around the image region of interest. We were able to detect collagen fiber lines on an image produced by confocal microscope.

\begin{equation}
\text{H1.00041 Exploring the Power Output of Small Wind Turbines in Urban San Antonio, Texas},
\end{equation}

JOSE CASILLAS, STEPHANIE SPERDUTI, ROSA CARDENAS, The University of the Incarnate Word — The means of transporting power from a centralized power plant by transmission lines has several disadvantages. Electricity transmission and distribution networks are costly, require long planning processes and are unsightly to residents. These networks are also susceptible to natural disasters creating massive disruptions to consumers. For these reasons distributed power sources such as solar panels and small wind turbines are becoming a more desirable and viable means of energy production. We report on the status of a study to determine the maximum output power of small wind turbines in urban San Antonio, Texas. Wind speed data along with power measurements from small wind turbines in urban San Antonio will be reported.

\begin{equation}
\text{H1.00042 Analyzing Hurricane Sandy},
\end{equation}

ANGELYN CONVERTINO, STEPHAN MEYER, BECCA EDWARDS, Southwestern University — Post-tropical Storm Sandy underwent extratropical transition shortly before making landfall in southern New Jersey October 29 2012. Data from this system was compared with data from Hurricane Ike (2008) which represents a classic hurricane with a clear eye wall and symmetry after landfall. Storm Sandy collided with a low pressure system coming in from the north as the hurricane made landfall on the US East coast. This contributed to Storm Sandy acting as a non-typical hurricane when it made landfall. Time histories of wind speed and wind direction were generated from data provided by Texas Tech’s StickNet probes for both storms. The NOAA Weather and Climate program were used to generate radar loops of reflectivity during the landfall for both storms; these loops were compared with time histories for both Ike and Sandy to identify a relationship between time series data and storm-scale features identified on radar.

\begin{equation}
\text{H1.00043 Using budget-friendly methods to analyze sport specific movements},
\end{equation}

LINDSAY JACKSON, SARAH WILLIAMS, DAVON FERRARA, Belmont University — When breaking down the physics behind sport specific movements, athletes, usually professional, are often assessed in multimillion-dollar laboratories and facilities. Budget-friendly methods, such as video analysis using low-cost cameras, iPhone sensors, or inexpensive force sensors can make this process more accessible to amateur athletes, which in-turn can give insight into injury mechanisms. Here we present a comparison of two methods of determining the forces experienced by a cheerleader during co-education stuntng and soccer goailes while side-diving. For the cheerleader, accelerometer measurements were taken by an iPhone 5 and compared to video analysis. The measurements done on the soccer players were taken using FlexiForce force sensors and again compared to video analysis. While these budget-friendly methods could use some refining, they show promise for producing usable measurements for possibly increasing our understanding of injury in amateur players. Furthermore, low-cost physics experiments with sports can foster an active learning environment for students with minimum physics and mathematical background.

\begin{equation}
\text{H1.00044 Porphyrin Induced Laser Deactivation of Trypsinogen-Trypsin Conversion},
\end{equation}

JOANNA PERIDO, Undergraduate Researcher, LORENZO BRANCALEON, Professor, PI — Pancreatitis is caused by the inflammation of the pancreas, where the digestive enzyme trypsin is activated from the precursor enzyme trypsinogen while still in the pancreas. The presence of trypsin in the pancreas causes auto-activation of trypsinogen, resulting in greater inflammation and auto-digestion of the pancreas. In severe cases, this cascade effect can lead to organ failure, diabetes, and pancreatic cancer. Our hypothesis is that if trypsinogen is prevented from auto-activating into trypsin, then this cascade can be stopped. We propose to do this by inducing conformational changes in trypsinogen when bound to a photoactive porphyrin dye. Porphyrins are comprised of four linked heterocyclic groups forming a flat ring, and bind well with proteins such as trypsinogen. In this study we used spectroscopic techniques to probe the binding of meso-tetrakis (4-sulfonatophenyl) porphyrin (TSP) to trypsinogen in vitro, as a preliminary step to then prompt and characterize conformational changes of trypsinogen through irradiation. If conformational changes are detected the trypsinogen will be tested for trypsin inactivation. This investigation may provide promising initial results to the possible use of porphyrins as an inhibitor of the self-activation of trypsinogen into trypsin, and a potential inhibitor of pancreatitis.

\begin{equation}
\text{H1.00045 Synthesizing new, high-temperature superconductors},
\end{equation}

CLAIRE WEAVER, Hofstra University, MEIGAN ARONSON, Brookhaven National Laboratory and Stony Brook University — Currently, there is no accepted theory behind type-II, high-temperature superconductors, but there is a distinct relationship between anti-ferromagnetism and superconductivity. Our research focuses on synthesizing new superconducting materials by observing the link between atomic structure and magnetic moments of anti-ferromagnetic compounds and attempting to reproduce the molecular physics of these known materials in new compounds. Consider the square-planar arrangement of the transition metal Fe in the Fe-pnictide superconductors of the ZrCuSiAs “11 11” and the ThCrSi “122” structure types. We believe that the physics behind this superconductor, where Fe has d$^6$ valence electrons, contributes to the superconducting state, not the presence of Fe itself. For this reason, we are synthesizing materials containing neighboring transition metals, like Mn and Co, combined with other elements in similar crystal lattice arrangements, having ionization properties that hopefully impose d$^6$ valence electrons on the transition metals.

\begin{equation}
\text{1 This project was supported in part by the U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists (WDTS) under the Science Undergraduate Laboratory Internships Program (SULI)}
\end{equation}

\begin{equation}
\text{H1.00046 Re-Examining Gravitational Tunneling Radiation when taking into account Quantum Gravity Effects},
\end{equation}


\begin{equation}
\end{equation}
Our newly developed mathematical methods of extracting vector correlation information from sliced imaging anisotropy will permit detailed study of a variety of photodissociation systems. Comparisons between these simulations and our experimental images will be presented. We are optimistic that induced chemical reactions require detailed experimental results which measure vector properties. Sliced velocity mapped ion imaging is a powerful method to about excited states symmetry, non-adiabatic dynamics and the forces and torques operating during fragmentation. Accurate molecular descriptions of photo- - Vector correlations between parent molecule transition dipole moments, photofragment velocity angular momentum vectors, can provide valuable information about excited states symmetry, non-adiabatic dynamics and the forces and torques operating during fragmentation. Accurate molecular descriptions of photo-induced chemical reactions require detailed and experimentally investigated as a function of a sharp spectral phase-step. The phase-step introduces asymmetric diagonal and off-diagonal features into the stimulated emission spectra that are sensitive to the single-photon transitions of IR-125. The sharp phase-step causes enhanced absorption of the high frequency components and a sharp narrow-band emission of low frequency. We calculate the frequency-dispersed nonlinear spectrum versus the phase step to fourth-order in the field. We show that the third-order polarization of the sample is sensitive to phase changes in the excitation spectrum and it is responsible for the observed narrowband feature in the experiments.

H1.00048 Adsorption of CO Molecules on Si(001) at Room Temperature

EONMI SEO, Korea University of Science & Technology, Korea Research Institute of Standards and Science, DAEJEON EOM, Korea Research Institute of Standards and Science, HANCHUL KIM, Department of Physics, SooMyung Women's University, Korea. JA-YONG KOO, Korea University of Science & Technology, Korea Research Institute of Standards and Science — Initial adsorption of CO molecules on Si(001) is investigated by using room-temperature (RT) scanning tunneling microscopy (STM) and density functional theory calculations. Theoretical calculations show that only one adsorption configuration of terminal-bond CO (T-CO) is stable and that the bridge-bond CO is unstable. All the abundantly observed STM features due to CO adsorption can be identified as differentially configured T-CO. The initial sticking probability of CO molecules on Si(001) at RT is estimated to be as small as ~ 1 x 10^-4 monolayer/Langmuir, which is significantly increased at high-temperature adsorption experiments implying a finite activation barrier for adsorption. Thermal annealing at 900 K for 5 min results in the dissociation of the adsorbed CO molecules with the probability of 60-70% instead of desorption, indicating both a strong chemisorption state and an activated dissociation process. The unique adsorption state with a large binding energy, a tiny sticking probability, and a finite adsorption barrier is in stark contrast with the previous low-temperature (below 100 K) observations of a weak binding, a high sticking probability, and a barrierless adsorption. We speculate that the low-temperature results might be a signature of a physisorption state in the condensed phase.

H1.00049 Multidimensional stimulated emission with a single phase-shaped pulse

ARKAPRABHA KONAR, RACHEL GLENN, VADIM. V. LOZOVOY, MARCOS DANTUS, Michigan State University — Two-dimensional optical signals from a single-pulse excitation are experimentally and theoretically investigated as a function of a sharp spectral phase-step. The phase-step introduces asymmetric diagonal and off-diagonal features into the stimulated emission spectra that are sensitive to the single-photon transitions of IR-125. The sharp phase-step causes enhanced absorption of the high frequency components and a sharp narrow-band emission of low frequency. We calculate the frequency-dispersed nonlinear spectrum versus the phase step to fourth-order in the field. We show that the third-order polarization of the sample is sensitive to phase changes in the excitation spectrum and it is responsible for the observed narrowband feature in the experiments.

H1.00050 Spectroscopic Studies of Imidizolium and Pyridinium Based Ionic Liquids

RYAN BOOTH, JAIME STEARNS, Air Force Research Laboratory — Ionic liquids (ILs) have been shown to be extremely useful in areas ranging from chemical synthesis to energetic materials. Furthermore, ILs are thought to be a potential replacement for hydrazine as satellite propellants because a subset are hypergolic with nitric acid. While ILs are useful, however, there is a lack of understanding of the microscopic origins for their macroscopic properties (e.g. viscosity). An example of this is that [emim]⁺[tf2N⁻] is three times less viscous than its methylated counterpart [emim]⁺[tf2N⁻] and there is some discord regarding the reason. We have investigated the molecular properties of such IL pairs using UV and IR spectroscopy in the gas phase on both imidazolium and pyridinium-based (pyr) ILs. UV data show that the photophysics of [emim]⁺[tf2N⁻] is different than [emim]⁺[tf2N⁻] in that there is a lack of evidence for the existence of a charge transfer (CT) state (as was seen in [emim]⁺[tf2N⁻]). Preliminary UV spectra for the [pyr]⁺ILs show at least two distinct peaks in the region from 208-270 nm, which are tentatively established as CT states between the anion and cation. IR spectra deliver structural information for both sets of ILs and should provide insight into the correlation between microscopic and macroscopic properties.

H1.00051 Strong field ionization tomography with two-color circularly polarized femtosecond laser fields

MAITHREYI GOPALAKRISHNAN, CHRIS MANCUSO, DANIEL HICKSTEIN, PATRIK GRYCHTOL, RONNY KNUT, FRANKLIN DOLLAR, DMITRIY ZUSIN, CHRISTIAN GENTRY, EMRAH TURGUT, JENNIFER ELLIS, HENRY KAPTEYN, MARGARET MURNANE, JILA and Department of Physics, University of Colorado Boulder and NIST, OFFER KFIR, OREN COHEN, Solid State Institute and Physics Department, Technion and Department of Physics and Optical Engineering, Ort Braude College, XIAO-MIN TONG, Division of Material Science, Faculty of Pure and Applied Science, Institute of Tsukuba, MING-CHANG CHEN, Institute of Photonics Technologies, National Tsing Hua University — Recent experiments using two-color circularly polarized laser fields have demonstrated that high-harmonic generation (HHG), a versatile spectroscopy and tomographic reconstruction techniques, we identify low-energy structures in the 3D photoelectron angular distributions that correspond to the rescattering of electrons with the ion. The observation of rescattering structures confirms the proposed explanation for HHG under two-color fields and paves the way for next-generation spectroscopies to investigate molecular structure.

H1.00052 DC Sliced Ion Imaging Study of Photodissociation Dynamics: Comparison between Conditions of Simulations and Experiments

COLIN J. WALLACE, WEI WEL, SIMON W. NORTH, Texas A&M — College Station — Vector correlations between parent molecule transition dipole moments, photofragment velocity angular momentum vectors, can provide valuable information about excited states symmetry, non-adiabatic dynamics and the forces and torques operating during fragmentation. Accurate molecular descriptions of photo-induced chemical reactions require detailed and experimentally investigated as a function of a sharp spectral phase-step. The phase-step introduces asymmetric diagonal and off-diagonal features into the stimulated emission spectra that are sensitive to the single-photon transitions of IR-125. The sharp phase-step causes enhanced absorption of the high frequency components and a sharp narrow-band emission of low frequency. We calculate the frequency-dispersed nonlinear spectrum versus the phase step to fourth-order in the field. We show that the third-order polarization of the sample is sensitive to phase changes in the excitation spectrum and it is responsible for the observed narrowband feature in the experiments.

H1.00053 ABSTRACT WITHDRAWN —
1. Measure support a model of core-hole decay in which charge is redistributed from Xe to the F ligands and energetic F ions are produced by Coulombic

2. Rostock, Germany, CHRISTOPH SCHICK, Institute of Physics, University of Rostock, Germany — We present a new method for the determination of the vapour

3. Rostock, Germany, OLAF KESSLER, Faculty of Mechanical Engineering, University of Rostock, Germany, UDO KRAGL, Institute of Chemistry, University of

4. MATHIAS AHRENBERG, Institute of Physics, University of Rostock, Germany, MARTIN BECK, Ludwig Maximilian University, ZOU FINFROCK, Argonne National Laboratory, ANTHONY DIAZ, Central Washington University, GERALD SEIDLER, University of Washington, JOSEPH PACOLD, Lawrence Berkeley National Laboratory, DEVON MORTENSEN, University of Washington, WILLIAM REICHLIN, Central Washington University, ZOU FINFROCK, Argonne National Laboratory, ANTHONY DIAZ, Central Washington University, GERALD SEIDLER, University of Washington — Compounds, molecules, and nanoparticles containing lanthanides as primary constituents or as dopants are widely used in applications including luminescent
dyes and lighting phosphors. Recent work has shown that x-ray spectroscopy methods can be used to monitor the sequence of excited states that leads to luminescence in lanthanide materials. Here, we use x-ray spectroscopy methods to monitor the sequence of excited states that leads to luminescence in lanthanide materials. Here, we use x-ray spectroscopy methods to monitor the sequence of excited states that leads to luminescence in lanthanide materials.
Intermolecular coupling and dynamics through infrared nano-spectroscopic imaging

Benjamin Pollard, Eric A. Muller, Omar Khatib, Markus B. Raschke, Univ. of Colorado - Boulder — Intermolecular interactions and coupling on the nanoscale lead to a variety of structural phases and degrees of crystallinity in soft-matter and biological systems, producing unique functional properties. We combine multi-spectral vibrational scattering-scanning near-field optical microscopy (s-SNOM) with multimodal scanning probe imaging to investigate structure-function relationships in soft matter. Using vibrational resonances as sensitive reporters of local structure, coupling, and dynamics, we resolve spectral shifts and line broadening on the nanoscale. These spectral shifts allow us to map intermolecular electric fields across nanoscale domains through solvatochromism or transition dipole coupling. Similarly, linewidths relate directly to the spatially-varying coupling dynamics of vibrational oscillators. Comparing spectral maps of peak position and linewidth to maps of adhesion and Young's modulus, for example, provides insight into the structure-function relationship dictating nanoscale self assembly in, e.g., block copolymer thin films.

Sucralose Destabilization of Protein Structure

Inha Cho, Lee Chen, Nimesh Shukla, Christina Othon, Wesleyan Univ — Sucralose is a commonly employed artificial sweetener. Sucralose behaves very differently than its natural disaccharide counterpart, sucrose, in terms of its interaction with biomolecules. The presence of sucralose in solution is found to destabilize the native structure of the globular protein Bovine Serum Albumin (BSA). The melting temperature decreases as a linear function of sucralose concentration. We correlate this destabilization with the increased polarity of the sucralose molecule as compared to sucrose. The strongly polar nature is observed as a large dielectric friction exerted on the excited state rotational diffusion of tryptophan using time-resolved fluorescence anisotropy. Tryptophan exhibits rotational diffusion proportional to the measured bulk viscosity for sucrose solutions over a wide range of concentrations, consistent with a Stokes-Einstein diffusional model. For sucralose solutions however, the diffusion is linearly dependent with the concentration, strongly diverging from the viscosity predictions. The polar nature of sucralose causes a dramatically different interaction with biomolecules than natural disaccharide molecules.

Time-resolved phase-sensitive second harmonic generation spectroscopy of electron injection at the water/air interface

Jan Verlet, Durham University — A new methodology is developed to probe the real-time dynamics of species at interfaces based on phase-sensitive second harmonic generation. The key attributes of the method are that the measured signal is linear with concentration and can independently measure the real and imaginary part of the second-order non-linear susceptibility. We apply this methodology to probing the dynamics of the hydrated electron at the water/air interface, produced by charge-transfer-to-solvent from a precursor ion (iodide in this case). Preliminary results indicate a fast decay on a sub-picosecond timescale of the real (non-resonant) part of the second-order non-linear susceptibility, which we associate with the charge-transfer dynamics at the water/air interface.

Electric Field: Maker and Breaker of Molecular co-operativity: the paradigm of (CH\(_3\)OH)\(_n\)−(H\(_2\)O)\(_n\) \(n = 1-4\) hetero-clusters

Rajeev Pathak, Dept of Physics, University of Pune — Hydrogen-bonded hetero-clusters of methanol and water: (CH\(_3\)OH)\(_n\)−(H\(_2\)O)\(_n\) \(n = 1-4\), when subjected to an externally applied dipolar electrostatic field, exhibit remarkable stability up to their characteristic maximal field threshold strengths. Moderate fields below the threshold endow a given cluster with enhanced stability against dissociation, whereas beyond the threshold its HOMO-LUMO gap abruptly closes down, resulting into structural breakdown. The electric field thus plays a dual role of a maker and breaker of molecular co-operativity in a hydrogen-bonding scenario. Ab initio investigations on these clusters employing M06-2X hybrid functional with a 6-311++G(2d, 2p) basis set reveal the structural evolution of the conformers with increasing electric field strengths: structural deformations, enhancement in their dipole moments with concomitant decrease in their HOMO-LUMO gaps interspersed with abrupt changes in these attributes when the clusters “open out.” Energetics quantify the stability of the clusters in field, while the IR vibrational spectra bring out shifts in the normal modes with marked emergence of exotic low-frequency O-H stretches as precursors of breakdown at the threshold field strengths.

Hose sucralose destabilizes the native structure of the globular protein Bovine Serum Albumin (BSA), the melting temperature decreases as a linear function of sucralose concentration. We correlate this destabilization with the increased polarity of the sucralose molecule as compared to sucrose. The strongly polar nature is observed as a large dielectric friction exerted on the excited state rotational diffusion of tryptophan using time-resolved fluorescence anisotropy. Tryptophan exhibits rotational diffusion proportional to the measured bulk viscosity for sucrose solutions over a wide range of concentrations, consistent with a Stokes-Einstein diffusional model. For sucralose solutions however, the diffusion is linearly dependent with the concentration, strongly diverging from the viscosity predictions. The polar nature of sucralose causes a dramatically different interaction with biomolecules than natural disaccharide molecules.

We use a 2D Ising lattice gas model to conduct Monte Carlo simulations of the heterogeneous nucleation of a liquid droplet from the supersaturated vapor phase, as triggered by a soluble nanoscopic aerosol particle. The liquid droplet that forms is a cluster of both solvent and solute particles. As a function of the size n of the droplet, we observe a solubility transition: At smaller n, the droplet consists of a compact solute cluster wetted by solvent, while at larger n the solute dissolves and is more uniformly distributed within the droplet. We evaluate the free energy of formation of a droplet as a function of n, and identify conditions at which nucleation is a two-step process. That is, two free energy barriers are encountered as the droplet grows, one associated with the solubility transition, and the other with the nucleation of the bulk solvent phase. We also evaluate the nucleation rate from the mean first passage time for the droplet to reach the critical size for the formation of the bulk phase, and quantify the influence on the rate due to solute solubility, and due to the relative heights of the barriers for the solubility and bulk transitions.

Two-step nucleation: Monte Carlo simulation of heterogeneous nucleation of liquid droplets on soluble nanoscopic aerosols

Oleksandr Zavalov, Sophie McGibbon-Gardner, Peter Poole, Dept of Physics, St. Francis Xavier University, Antigonish, Nova Scotia, Canada, Richard Bowles, Dept of Chemistry, University of Saskatchewan, Saskatoon, Saskatchewan, Canada, Ivan Saka-Voivod, Dept of Physics and Physical Oceanography, Memorial University of Newfoundland, St. John's, Newfoundland, Canada — We use a 2D Ising lattice gas model to conduct Monte Carlo simulations of the heterogeneous nucleation of a liquid droplet from the supersaturated vapor phase, as triggered by a soluble nanoscopic aerosol particle. The liquid droplet that forms is a cluster of both solvent and solute particles. As a function of the size n of the droplet, we observe a solubility transition: At smaller n, the droplet consists of a compact solute cluster wetted by solvent, while at larger n the solute dissolves and is more uniformly distributed within the droplet. We evaluate the free energy of formation of a droplet as a function of n, and identify conditions at which nucleation is a two-step process. That is, two free energy barriers are encountered as the droplet grows, one associated with the solubility transition, and the other with the nucleation of the bulk solvent phase. We also evaluate the nucleation rate from the mean first passage time for the droplet to reach the critical size for the formation of the bulk phase, and quantify the influence on the rate due to solute solubility, and due to the relative heights of the barriers for the solubility and bulk transitions.

Landscapes, kinetics, paths and statistics of curl flux, coherence, entanglement and energy transfer in non-equilibrium quantum systems

Zhedong Zhang, Jinhui Wang, Suny Stony Brook — We developed a population and flux landscape theory for general non-equilibrium quantum systems. We illustrated our theory by modelling the quantum transport of donor-acceptor energy transfer. We found two driving forces for the non-equilibrium quantum dynamics. The symmetric part of the driving force corresponds to the population landscape contribution which mainly governs the equilibrium part of dynamics while the anti-symmetric part of the driving force generates the non-equilibrium curl quantum flux which leads to the detailed-balance-breaking and time-irreversibility. The multi-loop structure of the flux emerges which forms the flux-landscape. Improving the voltage and electronic coupling in general facilitates the quantum transport by reducing the population landscape barriers.
H1.00067 Sensitivity of chiral 3-methylcyclopentanone structure, electric moment and thermodynamic parameters to medium polarity. WATHEQ AL-BASHEER, Department of Physics, King Fahd University of Petroleum & Minerals, SAID AL AZAR, Basic Sciences Department, Dar Al Uloom University. The location of Ni is one of the tasks of this kind of catalyst. R(+)-3-methylcyclopentanone (R3MCP) is a chiral ketone which can exist in as many as five conformers with two dominant conformers at room temperature: equatorial-methyl and axial-methyl. Density Functional Theory (DFT) calculations of the optimized geometries of R(+)-3-methylcyclopentanone (R3MCP) individual dominant conformers were performed in 10 common solvents of wide polarity range, under the framework of polarizable continuum model (PCM). DFT correlation function type B3LYP using a powerful basis set (aug-cc-pVDZ) yielded different linear correlation between solvent polarity and R3MCP equatorial and axial conformers Gibbs free and zero-point energies, entropies, vibrational modes frequencies, in addition to heat capacity resulting from translational, electronic, rotational and vibrational motion. Furthermore, DFT calculations of the R3MCP equator and axial conformers electric dipole and quadrupole moments components in 3D were also carried out and found to have a linear correlation with solvent polarity and cavitation energy. An observed trend for the standard Gibbs energies for the rotational equilibrium of R3MCP to be strongly-solvent dependent will be presented.

H1.00068 1 D Simulation of Capacitively Coupled Water Vapor Plasma. ZIANE KECHIDI1, None, A.H. BELBACHI TEAM, M. ANNOUN COLLABORATION, W.W. GRAHAM COLLABORATION. The results of a 1D simulation of a capacitively coupled water vapor discharge is reported. The simulated plasma consists of two electrodes separated by gap distance of 1 mm operating at 13.56 MHz with 26 species and 62 dominant reaction channels. The input parameters under which the plasma can be created is explored and space and time profiles of the electron densities are presented. The model finds that plasma ignition cannot be obtained in the present configuration and at pressures of greater than 0.1 atmosphere. The model has also be used to demonstrate the impact of rotational and vibrational excitation of water molecules in suppressing electrical breakdown.

H1.00069 Charge Conservation in BDG Formalism and its Effect in Calculating Berry Phase of Transporting a Localized BDG Quasiparticle around a Vortex in Superfluids/Superconductors. YIRUO LIN, TONY LEGGETT, University of Illinois at Urbana-Champaign. We examine charge conservation in BDG formalism and discuss the consequence of violating the charge conservation in Berry phase calculation of transporting a localized BdG quasiparticle around a vortex in superfluids/superconductors. We calculate explicitly the Berry phase in a model system in which the vortex is replaced by a 1D annulus ring geometry with quantized superfluid center-of-mass winding number and a localized Zeeman field is imposed to trap a quasiparticle with definite spin orientation.

H1.00070 Parahydrogen Induced Polarization by Pairwise Replacement on Pt and Ir Nanoparticles. CLIFFORD BOWERS, RONGHUI ZHOU, EVAN ZHAO, WEI CHENG, LUKE NEAL, HELENA WEAVER, Univ of Florida - Gainesville. Parahydrogen Induced Polarization (PHIP) is a robust and scalable method for production of bulk quantities of hyperpolarized fluids. The symmetrization order inherent in parahydrogen is transformed via symmetry breaking hydrogenation reaction into NMR-observable hyperpolarization. Spin polarization of order unity can be obtained. A key requirement of PHIP is pairwise hydrogenation by addition of H atoms originating from the same H2 molecule. PHIP using supported metal catalysts is a promising recent development because it exploits the advantages over homogeneous and supported metal complexes. The present work demonstrates a new PHIP mechanism involving the pairwise replacement of parahydrogen into propane (the substrate) over TiO2 supported Ir and Pt nanoparticle catalysts. Analysis of the stereoselectivity of the pairwise replacement process is facilitated by density matrix spectral simulations. The cis and trans dispositions of the symmetrization order give strikingly different PHIP spectra. The observed stereoselectivity of the pairwise replacement step, together with control experiments, rule out an alternative mechanism involving dehydrogenation of free propane over the catalyst.

H1.00071 Promoting alkali and alkaline-earth metals on MgO for enhancing CO2 capture by first-principles calculations. HYOSEOK KIM, WON BO LEE, KIWOONG KIM, Sogang Univ. The CO2 capture properties of Alkali(Li, Na, K, Rb, and Cs-) and Alkaline-Earth metal(Ba, Ca, Sr, and Ba-) promoted MgO sorbents are investigated by first principles density functional theory on the basis of PW91/GGA augmented with DFT+D2. Calculated Adsorption energy on the metal-promoted MgO sorbents is higher than Pure MgO sorbents, except for the Na-promoter. These results indicate that the CO2 capture capacity is improved by metal promotion. Li, Ca, and Sr were identified as adequate promoters among 9 metals, considering bind stability and regenerability.

H1.00072 Diffusion of a particle on a static rugged energy landscape with spatial correlations. BIMAN BAGCHI, SAIKAT BANERJEE, Indian Institute of Science. Despite the broad applicability of the problem, we have limited knowledge about the effect of ruggedness on diffusion at a quantitative level. Every study seems to use the expression of Zwanzig [Proc. Natl. Acad. U.S.A. 85, 2029 (1988)] who derived the effective diffusion coefficient, \[ D_{eff} = D_0 \exp(-3\beta \epsilon^2) \] We introduce and study two models of Gaussian random energy surface; a discrete lattice and a continuous field. Our simulations show that Zwanzig's expression overestimates diffusion in the uncorrelated Gaussian random lattice. The disparity originates from the presence of "three-site traps" (TST) on the energy landscape – which are formed by the presence of deep minima flanked by high barriers on either side. Using mean first passage time (MFPT) formalism, we derive a general expression for the effective diffusion coefficient, \[ D_{eff} = D_0 \exp(-3\beta \epsilon^2) \{ 1 + \text{erf}(\beta \epsilon / 2)^2 \}^{-1} \] in the presence of TST. In presence of spatial correlation we derive a more general form of the expression, which reduces to Zwanzig's form in certain limit. We characterize the same using non-Gaussian order parameter, and show that this "breakdown" scales with ruggedness following an asymptotic power law. The breakdown of Zwanzig's elegant expression was perhaps anticipated but was not clearly demonstrated earlier.

H1.00073 New insides in the characterization of HDS industrial catalysts by HAADF-STEM. PAZ DEL ANGEL, ARTURO PONCE, JOSEFINA ARELLANO, MIGUEL J. YACAMAN, Universidad de Texas, San Antonio. MARTHA HERNANDEZ-PICHARDO, Instituto Politecnico Nacional. The role of Ni is one of the tasks of this kind of catalyst. The used catalysts was a state-of- the-art commercial nickel-molybdenum alumina-supported formulation, including organic agent modifier. This type of material belongs to a novel family of catalysts specially designed for ultra-low sulfur production from straight-run gas oil (SRGO), cycle oil, coker gas oil, or their combinations at operating conditions of commercial interest in hydrotreating units at industrial scale. Aberration corrected HAADF-STEM allowed to observe the nanostructure and location of MoS2 and its interaction with the alumina. The results indicate that the MoS2 is highly dispersed on the alumina, however the location of Ni is one of the task of this kind of catalyst.
AuCl

We conclude that the origin of the p-type doping in as well as the effect of the adsorbate concentration. As a result, we find that especially AuCl mechanisms while considering all possible configurations and concentrations. In particular, we show that the formation of the tetrahedral subunits are important

We thank NSERC for financial support and Compute Canada for computational resources.

AuCl

We investigate the rectification behavior of the diblock dipyrimidinyldiphenyl molecule and its derivates with computing free energies of both face-centered cubic (FCC) and hexagonal close-packed (HCP) hard sphere crystals with a precision of 10^{-6} hartree. The finite models prefer a rippled/twisted structure morphology over the planar or helical ones. The rippled/twisted models appear to be structurally more stable. We simulated STEM images of the theoretical models to compare it with the experimental ones. In contrast with infinite models, the finite models predict a rippled/twisted structure morphology over the planar or helical ones. The rippled/twisted models appear to be structurally more stable.

We thank NSERC for financial support and Compute Canada for computational resources.

1. We thank NSERC for financial support and Compute Canada for computational resources.

2. This research is supported by the National Science Foundation (USA) under grants CHE-0841557 and DMR-1206971.

3. This work is supported by National Science Foundation of China and "973" project.
H.1.00081 First-Principles Investigations of Lead-Free Formamidinium Based Hybrid Perovskites, ALTYNBEK MURAT, UDO SCHWINGENSCHLOGL, PSE Division, KAUST, Saudi Arabia — Hybrid organic-inorganic perovskite solar cells have recently emerged as the next-generation photovoltaic technology. Most of the research work has been focused on the prototype MAPbI$_3$ perovskite (MA = Methylammonium = CH$_3$NH$_3$) and its analogues that have lead to power conversion efficiencies in excess of 15%. Despite the huge success, these materials are still non-optimal in terms of optical absorption where the bandgaps are greater than 1.6 eV as well as the toxicology issue of lead. Thus, investigation and development of lead-free perovskites with bandgaps closer to optimal, allowing greater spectral absorption, is of great interest. In this work, we perform first principles calculations to study the structural, optical, and electronic properties of new derivatives of MAPbI$_3$ in which the organic MA cation is replaced by other organic amines of similar size such as Formamidinium (FA) and/or the Pb cation replaced by similar elements such as Sn. In particular, we investigate the role and effect of FA and Pb cations on the electronic and optical properties and analyze to which extend the bandgaps can be tuned.

H.1.00082 Dye attached fullerene and P3HT complexes, AMANDA GARNICA, LUIS BASURTO, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — We study the electronic structure of C60 fullerenes functionalized with thiophene-diketo-pyrrolopypyropheophorbide based chromophores using density functional theory combined with large polarized basis sets. These chromophores have electron donor character and thus the functionalization of the fullerene produces donor-acceptor (DA) systems. We examine in detail the effect of the linker and the addition site on the electronic structure of the fullerenes. We further study how the charge transfer excited states of these DA complexes and also that of the complexes of these functionalized fullerenes with the poly(-3-ethylthiophene-2,5-diyl) (P3HT) are studied using the perturbative A-$\Delta$-SCF method. The exciton binding energies in the functionalized fullerene-P3HT complexes are found to be smaller compared to similarly prepared phenyl-C61-butyric acid methyl ester (PCBM)-P3HT complex.

H1.00083 Electronic structure and charge transfer excitation energies of three endohedral fullerene- ZnTPP/ZnPc dyads, FATEMEH AMERIKHEIRABADI, LUIS BASURTO, RAJENDRA ZOPE, TUNNA BARUAH, The University of Texas at El Paso — Organic donor-acceptor (D-A) moieties make up the main component of organic photovoltaics (OPVs). It has been proved that the open circuit voltage of these devices which is a parameter in efficiency determination, is directly related to the charge transfer excited states of the D-A pairs. Fullerenes having lots of interesting acceptor properties and porphyrins as well as phthalocyanines possessing intriguing donor characteristics, are shown to be promising nominees. In this work, we computationally analyze three donor-acceptor dyads of Zn-tetraphenyl porphyrin and Zn-phthalocyanine with novel endohedral fullerenes: Sc$_2$NOC$_8$H$_{38}$ZnP, Y$_3$NOC$_8$H$_{38}$ZnP and Sc$_2$NOC$_8$H$_{38}$ZnP. The Sc$_2$NOC$_8$H$_{38}$ and Y$_3$NOC$_8$H$_{38}$ belong to a particular class of fullerenes called trimaltic nitride endohedral fullerenes where the trimalletic nitrides form the endohedral units. Density functional theory, as implemented in NRLMOL code, is used to study the electronic structure and the related properties of these DA complexes. The charge transfer excitation energies are calculated using the perturbative delta self-consistent method recently developed in our group. We find that the CT excitation energies are larger for endohedral fullerene based dyads compared to similar C$_60$ based dyads.

H.1.00084 Current flow in biased bilayer graphene: the role of sublattices, CARLOS PAEZ, Universidad Estadual de Campinas-FCA, DARIO BAHAMON, MacGrafe -Graphene and Nano-Materials Research Center, Mackenzie Presbyterian University, ANA PEREIRA, Universidade Estadual de Campinas-FCA — We investigate here how the current flows over a bilayer graphene in the presence of an external electric field perpendicularly applied (biased bilayer). Charge density polarization between layers in these systems is known to create a layer pseudospin, which can be manipulated by the electric field. Our results show that current does not necessarily flow over regions of the system with higher charge density. Charge can be predominantly concentrated over one layer, while current flows over the other layer. We find that this phenomenon occurs when the charge density becomes highly concentrated over only one of the sublattices, as the electric field breaks layer and sublattice symmetries for a Bernal-stacked bilayer. For bilayer nanoribbons, the situation is even more complex, with a competition between edge and bulk effects for the definition of the current flow. We show that, in spite of not flowing trough the layer where charge is polarized to, the current in these systems also defines a controllable layer pseudospin.

H.1.00085 PHYSICS EDUCATION

H.1.00086 Visualizations of Illinois Educational Data, CACEY STEVENS, The James Franck Institute and Department of Physics, University of Chicago, MICHAEL MARDER, Department of Physics, The University of Texas at Austin, SIDNEY NAGEL, The James Franck Institute and Department of Physics, University of Chicago — We examine data from scores on standardized exams taken by students in the state of Illinois. In order to analyze the factors affecting school performance in mathematics, we represent the data through visualizations, an approach commonly used to identify patterns in studies of physical systems. Exam scores for different schools are shown to depend on program type, location, and poverty concentration. For most schools in Illinois, test scores decline linearly with increased poverty concentration. However schools in Chicago show deviations from the linear trend. For any given poverty level, schools in Chicago perform better than those in other communities of Illinois. We also compare different school types, such as neighborhood, magnet, and charter programs, at each grade level. The city’s selective enrollment programs show notably superior achievement at the high school level. This is less pronounced at earlier grades.

H.1.00087 Lab-in-a-box @ school: Exiting hands-on experiments in soft matter physics1, KARIN JACOBS, MARTIN BRINKMANN, FRANK MULLER, Experimental Physics, Saarland University, Saarbruecken, Germany — Soft materials like liquids and polymers are part of everyday life, yet at school, this topic is rarely touched. Within the priority program SPP 1064 ‘Nanos- and Microfluidics’ of the German Science Foundation, we designed an outreach project that allows pupils (age 14 to 18) to perform hands-on experiments (www.labinabox.de). The experiments allow them e.g. to feel viscosity and viscoelasticity, experience surface tension or see structure formation. We call the modulus operandi ‘subjective experiments’ especially catch the attention of girls without disadvantaging boys. Both are fascinated by the hands-on experiments. We further study the charge transfer excited states of these DA complexes and also that of the complexes of these functionalized fullerenes with the poly(-3-ethylthiophene-2,5-diyl) (P3HT) are studied using the perturbative A-$\Delta$-SCF method. The exciton binding energies in the functionalized fullerene-P3HT complexes are found to be smaller compared to similarly prepared phenyl-C61-butyric acid methyl ester (PCBM)-P3HT complex.

1Financial support of the German Science Foundation DFG is acknowledged.

H.1.00088 QUANTUM INFORMATION, CONCEPTS AND COMPUTATION
H1.00089 Approach to solving spin-boson dynamics via non-Markovian quantum trajectories
- ZENG-ZHAO LI, Beijing Computational Science Research Center, CHO-TUNG YIP, Hong Kong Polytechnic University, HAI-YAO DENG, Hong Kong Polytechnic University and National Institute for Materials Science, MI CHEN, Fudan University, TING YU, Stevens Institute of Technology, J. Q.’ YOU, Beijing Computational Science Research Center, CHI-HANG LAM, Hong Kong Polytechnic University — We develop a systematic and efficient approach for numerically solving the non-Markovian quantum state diffusion equation for an open quantum system that can be strongly coupled to an environment. As an important application, we consider a real-time simulation of a spin-boson model in a strong coupling regime that is difficult to deal with using conventional methods. We show that the non-Markovian stochastic Schrödinger equation can be efficiently implemented as a real-time simulation for this model, so as to give an accurate description of spin-boson dynamics beyond the rotating-wave approximation.

H1.00090 Relation between Full Counting Statistics and the flow of Shannon entropy
- MOHAMMAD ANSARI, YULI NAZAROV, Kavli Institute for nanoscience, Delft University of Technology — We show that microscopic theory of counting statistics that is applicable for many quantum noise analysis, has an internal and fundamental correspondence to the Renyi entropy flow in the quantum system. This analogy reveals an interesting step towards understanding quantum thermodynamics. We also further extend the formulation for the flows of entropy using full counting statistics and determine novel quantum terms in the statistical moment measurements.

H1.00091 Coherent control of multipartite excitonic entanglement in quantum dot arrays
- JUAN E. ROLON, JOAQUIN E. DRUT, University of North Carolina at Chapel Hill — We propose a coherent control scheme for multipartite entanglement of exciton states in optically driven quantum dot arrays (QDAs) coupled by charge tunneling and resonant energy transfer (RET) processes. An adiabatic manipulation of the entanglement dynamics is devised by pulse shaping and time-dependent electric field sweeps. By varying the inter-dot distance and number of quantum dots (QDs) comprising the QDA, the excitonic qubit manifolds are obtained by a Feshbach projection over the resulting multilevel exciton configurations. We identify regimes in which the dynamics is confined to decoherence-free excitonic qubit manifolds taking into account spontaneous recombination and non-Markovian effects introduced by a phonon bath. We present results for entanglement monotonies and measures such as the entanglement of formation and entanglement entropy for different QDA geometries and carrier injection conditions. Our results indicate that in spite of the effects of phonon-assisted relaxation, entanglement can be optimized and transferred between QDs by the controlled interplay of system geometry, pulse shaping, RET and carrier tunneling.

H1.00092 Anisotropic exchange coupling in a nanowire double quantum dot with strong spin-orbit coupling
- RUI LI, J.Q. YOU, Beijing Computational Science Research Center — A spin-orbit qubit is a hybrid qubit that contains both orbital and spin degrees of freedom of an electron in a quantum dot. Here we study the exchange coupling between two spin-orbit qubits in a nanowire double quantum dot (DQD) with strong spin-orbit coupling (SOC). We find that while the total tunneling in the DQD is irrelevant to the SOC, both the spin-conserved and spin-flipped tunnellings are SOC dependent and can compete with each other in the strong SOC regime. Moreover, the Coulomb repulsion between electrons can combine with the SOC-dependent tunnellings to yield an anisotropic exchange coupling between the two spin-orbit qubits. Also, we give an explicit physical mechanism for this anisotropic exchange coupling.

H1.00093 Spin decoherence of mobile impurity in a one dimensional spin bath
- TRITHEP DEVAKUL, ADRIAN FEIGUIN, Northeastern University — We study the spin decoherence of a mobile impurity interacting locally with a one dimensional spin bath. In contrast to the central spin model, where a single central spin interacts with the bath via long ranged interactions, our model considers only local exchange interactions, while allowing the impurity to move to neighboring sites via hopping t. We consider a spin-1/2 impurity, and study the decoherence, tracing over the position degree of freedom. In the large t limit, the delocalized impurity behaves identically to a localized spin interacting with the bath, same as a central spin. This model allows one to treat a spin problem – which inherently builds up long-range entanglement within the bath – instead as a Hamiltonian with only local interactions. Numerical calculations are done at various regimes of parameters, and comparison with the central spin model is discussed.

H1.00094 Finite-temperature reservoir engineering and entanglement dynamics
- SERGUEI FE-DORTCHENKO, Université Paris Diderot, ARNE KELLER, Université Paris-Sud 11, THOMAS COUDREAU, PEROLA MILMAN, Université Paris Diderot — We propose experimental methods to engineer reservoirs at arbitrary temperatures which are feasible with current technology. Our results generalize to mixed states the possibility of quantum state engineering through controlled decoherence. Finite-temperature engineered reservoirs can lead to the experimental observation of thermal entanglement—the appearance and increase of entanglement with temperature—to the study of the dependence of finite-time disentanglement and revival with temperature, quantum thermodynamical effects, and others, enlarging the comprehension of temperature-dependent entanglement properties. Our proposal is discussed in detail in two model systems, consisting of different modes of a single photon and a trapped-ion system.

H1.00095 Reproducing the D-Wave Entanglement Results in Candidate Models
- TAMEEM ALBASH, University of Southern California, ITAY HEN, FEDERICO SPEDALIERI, Information Science Institute, DANIEL LIDAR, University of Southern California — The demonstration of entanglement on the D-Wave devices [1] relies on the assumption that the populations derived from measurement correspond to energy eigenstate populations of the quantum Hamiltonian. We therefore ask whether leading model candidates for the D-Wave devices are able to reproduce this entanglement signature. We focus our work on a quantum adiabatic Markovian master equation (ME) [2] and a Monte Carlo rotor model (SSSV) [3]. We show that the ME reproduces both the energy spectrum and the thermal state populations of the quantum Hamiltonian extremely well, hence agreeing with the experimental results. SSSV on the other hand fails to reproduce either, a consequence of the absence of discrete energy states in this model.


H1.00096 Using the SLUG as a First Stage, Low Noise Microwave Amplifier for Superconducting Qubit Readout
- EDWARD LEONARD JR., TED THORBECK, SHAOJIANG ZHU, ROBERT MCDERMOTT, Univ of Wisconsin, Madison — The SLUG (Superconducting Low-inductance Undulators Galvonometer) microwave amplifier is a large bandwidth, high saturation power, high gain, and low noise microwave element designed as a first stage cryogenic amplifier for dispersive readout of superconducting qubits. High forward gain is paired with simultaneous high reverse isolation such that bulky, expensive cryogenic circulators and isolators might be eliminated from the microwave readout chain. Here we present recent experimental data on SLUG gain, noise, and reverse isolation. We achieve gain over 10 dB at 7 GHz across a band of several hundred MHz, with system added noise of order one photon. For appropriate flux bias of the device, reverse isolation is better than -20 dB. These qualities make the SLUG a very desirable first stage amplifier for a scalable superconducting qubit readout.
H1.00097 Dynamic nuclear polarization of nitrogen-vacancy centers in diamond. WEN-HUI HU, Beijing Computational Science Research Center, NAN ZHAO COLLABORATION — Single nitrogen-vacancy (NV) centers in diamond triggered the research for wild applications in quantum information processing and quantum metrology. One of the most important advantages of the NV centers is the long coherence time of the center electron spins. Dynamic nuclear polarization (DPN) has been introduced as an efficient method to protect the spin coherence. The coherence time $T_2^*$ should have been prolonged of two orders theoretically, nevertheless less than one order in experiments. In this work, we theoretically study the DNP process in a high-purity diamond, where the dipole-dipole hyperfine interaction between the center electron spins and the bath $^{13}$C nuclear spins is dominant. The simulations show that the saturated polarization of the nuclear bath depends on the spin-lock period and the efficiency of the initialization laser, accompanied with the magnitude of the external magnetic field. The polarization saturation comes from the capability of the polarization transfer and the equilibrium of probability distribution between the polarized and unpolarized states.

H1.00098 Phase noise of a cavity electromechanical oscillator at millikelvin temperatures. JUNHO SUH, SUNGWAN CHO, SANG GOON KIM, SEUNG-BO SHIM, Korea Research Institute of Standards and Science — The frequency stability of a mechanical resonator is an important factor in its application to quantum information technology. We investigate the phase noise in a self-oscillation of a micromechanical resonator, parametrically driven by a superconducting microwave resonator at millikelvin temperatures. Possible physical origins of the noise are also discussed.

H1.00099 Investigation of the thermal motion and mode coupling in a micromechanical resonator, SEUNG-BO SHIM, SUNGWAN CHO, SANG GOON KIM, Korea Research Institute of Standards and Science, SUNG UN CHO, YUN PARK, Seoul National University, JUNHO SUH, Korea Research Institute of Standards and Science — We have investigated the thermal motion and mode coupling in a micromechanical resonator. The mechanical resonator was designed for dielectric gradient force actuation scheme. The laser reflection measurement method enabled multi-mode detection of the thermal motion up to $5^{th}$ mode at room temperature. With these multi-modes, we could investigate the energy transfer between first and second mode by applying mechanical sideband signals. We have utilized the second mode as a phonon cavity and observed the coupling and interaction between two modes. Here, we will discuss about the room temperature mechanical mode detection method and mode coupling effect in the micromechanical resonator.

H1.00100 Construction of a Confocal Fluorescence Microscope to Image Nitrogen Vacancy Centers. JORDAN STROMAN, JAMES GRIFFIN, GARY HARRIS, Howard University — Long term atomic memory can be achieved using nitrogen vacancy centers (NV). Howard University is optimizing the process of creating nitrogen vacancy centers using hot filament chemical vapor deposition (HFCVD). In order to provide reliable feedback concerning the presence, concentration, and orientation of these color centers, an optical system capable of performing confocal laser scanning fluorescence microscopy has been constructed. This system consists of a 200mw laser that emits light with a wavelength of 532nm. This light is focused on a sample using a Nikon Oil Objective Lens with a numerical aperture of 1.3. The sample rest on a piezoelectric stage with a resolution of 20nm in the $x$, $y$ and $z$ direction. This optical system can confirm and locate NV centers with a resolution of 200nm.

1Supported by a grant from the National Science Foundation DMR-1231319

H1.00101 Digital quantum simulation of Heisenberg spin systems in circuit QED. MARKUS OPPLIGER, YVES SALATHE, MINTU MONDAL, JOHANNES HEINSOO, PHILIPP KURPIERS, ANTON PÓTOCNIK, STEFAN FILIPP, ANDREAS WALLRAFF, ETH Zurich, Switzerland, ANTONIO MEZZACAPA, URTZI LAS HÉRAS, LUCAS LAMATA, ENRIQUE SOLANO, University of the Basque Country, Bilbao, Spain — A Quantum simulator realized by a well-controlled quantum system allows to simulate a wide range of complex quantum systems that are very difficult to study with classical computing. We use a promising quantum simulator based on circuit quantum electrodynamics (QED) to digitally simulate the isotropic Heisenberg XXZ interaction between two spin 1/2 particles. Since the XYZ interaction does not occur directly in the Jaynes-Cummings Hamiltonian, the interaction is decomposed into a set of single- and two-qubit gates. The resulting quantum state is analyzed by state tomography for different interaction times after each step. As our approach can be generalized further, this experiment is a first step towards simulating large spin systems in a circuit QED architecture.

H1.00102 High-fidelity quantum memory utilizing inhomogeneous nuclear polarization in a quantum dot. WENKUI DING, ANQI SHI, Wuhan University, JIANGQING YU, Beijing Computational Science Research Center, WENXIAN ZHANG, Wuhan University — We numerically investigate the encoding and retrieval processes for a quantum memory realized in a semiconductor quantum dot, by focusing on the effect of inhomogeneously polarized nuclear spins whose polarization depends on the local hyperfine coupling strength. We find that the performance of the quantum memory is significantly improved by the inhomogeneous nuclear polarization, as compared to the homogeneous one. Moreover, the narrower the nuclear polarization distribution is, the better the performance of the quantum memory is. We ascribe the performance improvement to the full harnessing of the highly polarized and strongly coupled nuclear spins, by carefully studying the energy transfer processes. Our results shed new light on the implementation of a quantum memory in a quantum dot.

1The National Basic Research Program of China (Grant No. 2013CB922003 and 2014CB921401), the National Natural Science Foundation of China under Grant No. 11275139 and 91121015, the NSAF Grant No. U1330201.

H1.00103 A photon-photon quantum gate using a multilevel atomic system, YUUKI TOKUNAGA, NTT SC Labs. — We propose a method for a quantum gate between photons assisted by a multilevel atom system. The atomic system is supposed to be in a cavity or a one-dimensional waveguide. The system can transfer a quantum state between a photon and the atom, and also works as a quantum gate for consecutively input photons. This system could be used as a building block for a universal quantum computation. We also discuss the characteristics of such quantum gates with several different multilevel system.

H1.00104 Riemannium nucleus and quantum solution to the Riemann hypothesis (RH). CARLOS FIGUEROA-NAVARRO, Departamento de Ingeniería Industrial, Unidad Regional Centro, Universidad de Sonora, JULIO CAMPOS-GARCIA, Departamento de Ciencias de la Salud, Unidad Cajeme, Universidad de Sonora, MARTIN MOLIDAR-TABARES, Organismo de Cuenca Noroeste, Comisión Nacional del Agua, LAMBERTTO CASTRO-ARCE, Departamento de Física e Ingeniería, Unidad Regional Sur, Universidad de Sonora — Is there an energy spectrum according to the primes numbers? This raises the question whether physical systems whose spectrum is the Riemann zeta function; ie, is there a spectrum of resonances of a nucleus that are the zeros of the zeta function? The renowned HR is basically preceded by the Euclid principle, the Euler product and the Gauss theorem. The best mathematical interpretation is the one that threw Riemannian revolution. HR holds that the nontrivial zeros of the zeta function keep the harmony of primes, but this is not fully tested. There are two possibilities: The HR can be true, then the primes have harmony, but if false, they nest in the chaos. The idea of this is important for studying models of quantum chaos is getting stronger in the last decade. These investigations lead us to believe that a highly mathematical problem becomes a physical problem; because according to Hugh Montgomery and Michael Berry the variations of the zeros, with drums and quantum billiards, can provide a physical model for explain the primes. In this paper, we generate the Mount Riemann by using MATHEMATICA and we get the profile that relates the prime numbers with the zeros of the zeta function; also we explain how quantum helps to explain the famous old problem known as the conjecture of Riemann.
H1.00105 Distribution of quantum Fisher information in asymmetric cloning machines \(^1\), XING XIAO, YAO YAO, Beijing Computational Science Research Center, LEI-MING ZHOU, Key Laboratory of Quantum Information, University of Science and Technology of China, XIAOGUANG WANG, Zhejiang Institute of Modern Physics, Department of Physics, Zhejiang University — An unknown quantum state cannot be copied and broadcast freely due to the no-cloning theorem. Approximate cloning schemes have been proposed to achieve the optimal cloning characterized by the maximal fidelity between the original and its copies. Here, from the perspective of quantum Fisher information (QFI), we investigate the distribution of QFI in asymmetric cloning machines which produce two nondiagonal copies. As one might expect, improving the QFI of one copy results in decreasing the QFI of the other copy, roughly the same as that of fidelity. It is perhaps also unsurprising that asymmetric phase-covariant cloning outperforms universal cloning in distributing QFI since a priori information of the input state has been utilized. However, interesting results appear when we compare the distributabilities of fidelity (which quantifies the full information of quantum states), and QFI (which only captures the information of relevant parameters) in asymmetric cloning machines. Unlike the results of fidelity, where the distributability of symmetric cloning is always optimal for any d-dimensional cloning, we find that any asymmetric cloning outperforms symmetric cloning on the distribution of QFI for \(d \leq 18\), whereas some but not all asymmetric cloning strategies could be worse

\(^1\)supported by the NNSFC (Nos. 11247006, 11025527 and 11475146), the National 973 program(No. 2012CB921602)

H1.00106 Quantum Information in Biological Systems, SHANTILAL GORADIA, Retired — We can derive strong coupling and also recover Newtonian gravity with a quantum mechanical approach implicitly implying the variation of universal constant of gravity on a cosmic scale. Since constancy of \(G\) does not lead to cosmological constert, we derive 137 (described as the hand of God by Feynman) as a natural logarithm of the age of the universe in Planck times (10E60). Since we use Boltzmann equation on his tomb to do that, we describe that equation as the heart of God! Since otherwise, no theory including the string theory can so far come up with 137 mathematically. Maximum potential ON and OFF signals of interactions of 10E60 ever since the big bang could provide the fundamental basis of information system in the universe including in biology, implying the sperm of a man carries the genetic information of the male which when combined with the genetic information of a female egg decides the characteristics of the offspring. We may never know the exact language of nature. We speculate the string theory may be able to step in to show some deeper light in that direction.

H1.00107 Two-Slit Particle Experiment and the CMB, ALFRED PHILLIPS JR., Source Institute — Both Einstein and Feynman discussed the difficulty of understanding the two slit experiment for particles. We show a connection between this experiment and the Cosmic Microwave Background. We have not yet determined whether this new connection necessitates a modification of metrics such as that of Robertson-Walker or how much light this new connection sheds on the dark energy (cosmological constant) problem.

H1.00108 MATTER AT EXTREME CONDITIONS —

H1.00109 RKKY and Dzyaloshinsky-Moriya Interaction in the Electron Gas, MOHAMMAD MAHDI VALIZADEH, SASHI SATPATHY, Department of Physics & Astronomy, University of Missouri, Columbia, MO 65211, USA — We illustrate the origin of the Dzyaloshinsky-Moriya interaction \(S_1 \times S_2\) between two localized spins embedded in a solid by considering the example of the electron gas with spin-split bands, which serves as a simple pedagogical model for the understanding of this interaction. In this case, where symmetry is broken, the magnetic interaction acquires the Dzyaloshinsky-Moriya term in addition to the well-known RKKY interaction term \(S_1 \cdot S_2\), so that the net interaction has the form \(J = J_{\text{RKKY}} + J_{\text{DM}}\). For the standard electron gas with spin degenerate states, the DM term vanishes yielding the well known RKKY interaction results. Explicit expressions for the magnitudes of the interactions are obtained for the electron gas in two and three dimensions. This simple model serves as a pedagogical example for the origin of the Dzialoshinski-Moriya interaction in a system with broken time-reversal symmetry.

H1.00110 Chromium based Spinels under Compressions, YUEJIAN WANG, ILIAS EFTHIMIOPOULOS, Oakland University, THOMAS AHEARN, Oakland, VLADIMIR TSURKAN, JOACHIM DEISENHOFER, ALOIS LOIDL, University of Augsburg — The Chromium (Cr) based spinels, ACr2X4, represent a prototype system for the study of magnetism in solid [1]. More recently, multiferroicity has been found in members of this series [2]. However, the origin of the ferroic properties is not well understood; Given the strong interplay between structural and ferroic properties in this system, the structural evolution induced by pressure may shed light on the multiferroicity [3]. High-pressure X-ray diffraction and Raman spectroscopic studies have been conducted on ZnCr2Se4 and ZnCr2S4. The study elucidated the phase transformation of these spinels under high pressures by the X-ray data and the structural evolution induced by pressure may shed light on the multiferroic properties induced by the structural transitions were discussed.

H1.00111 SURFACES, INTERFACES AND THIN FILMS —

H1.00112 Directed Chemical Transport and Separation by Hydrogel Films containing Static and Dynamic Chemical Potential Gradients, TSUNG-HAN TSAI, CHUNJIE ZHANG, HYUNG-JUN KOO, PAUL V. BRAUN, University of Illinois at Urbana-Champaign — Materials that can manipulate the anisotropic molecular transport through built-in chemical potential gradients offer new opportunities to process chemical agents. Different from electrophoresis and microfluidics, here the chemical potential gradients, which provide the driving forces for molecular transport, are incorporated in the diffusion media. The autonomous systems can independently control the anisotropic flux of molecules and thus do not need external inputs such as electric fields and flowing carrier phases. As model systems, we used hydrogels containing static and dynamic built-in chemical potential gradients to direct molecular transport, concentrate dilute analyte and separate mixtures. The static gradients are based on electrostatic and supramolecular interactions which are specifically designed for the target molecules. The dynamic active chemical potential gradients triggered by reversible ion exchange process can alter the hydrophilicity gradually to transport or separate target molecules.

H1.00113 A density functional theory investigation of select transition metal dichalcogenides, RODRICK KUATE DEFO, Physics Department, Harvard University, GEORGIOS TRITSARI, SEAS, Harvard University, SHIANG FANG, EFTHIMIOS KAXIRAS, Physics Department, Harvard University — As a result of the extensive work done on graphene, leading to advances in sample preparation, optical detection, and transfer and manipulation of 2D materials, there has been a resurgence of interest in layered materials from which single sheets can be extracted, such as molybdenum disulfide. Particularly intriguing is the fact that layered MoS2 transitions from an indirect band gap in the bulk to a direct band gap in the monolayer opening up the possibility of optoelectronic applications. These results have been verified using density functional theory and, further, dependence of the band gap on lattice strain has been investigated. This dependence is crucial in understanding emergent properties of compounds consisting of MoS2 layered with other materials where there is a lattice mismatch. MoSe2, MoS2, WS2, WSe2 and WS2e have also been studied. Finally, dielectric functions have also been obtained for these compounds to explore the effect particularly of the asymmetric atom configurations on polarization of the material.
H1.00114 Monomer Adsorption on 6-Atoms Wide Zigzag (111) Terraces\textsuperscript{1}, ALAIN PARES, Villanova University, DAVID GRUMBINE, JR, St. Vincent College — We study monomer adsorption on six-atoms wide, zigzag (111) terraces, with first- (V), second- (W), and third-neighbor (U) interactions, specializing to repulsive first-neighbors. All possible crystallization patterns, or phases, that may exist are expected to occur at relatively low temperatures. Under these conditions, the energy phase diagram is three-dimensional and depends on the dimensionless variables, $v = U/W$, $u = U/V$, and $w = W/V$. The chemical potential energy of the monomers, $\mu$, in the medium to which the terrace is exposed depends on the pressure, if the medium is a gas, or the concentration if the medium is solution. There are 95 phases, or crystallization patterns, of the adsorbates with coverages ranging from 1/5 to 8/9. In particular, we find that there are 10 distinct 1/2, 2/3, and 4/9 coverage phases, and 9 distinct 1/3 coverage phases.

\textsuperscript{1}Work supported in part by NICS supercomputing grant # CHE040001.

H1.00115 Interplay between Self-Assembled Structures and Energy Level Alignment of Benzamidine on Au(111) Surfaces\textsuperscript{1}, GUI LI, Lawrence Berkeley Natl Lab, JEFFREY NEATON, Lawrence Berkeley Natl Lab; UC-Berkeley; Kavli Energy NanoSciences Institute at Berkeley — Using van der Waals-corrected density functional theory (DFT) calculations, we study the adsorption of benzene-diamine (BDA) molecules on Au(111) surfaces. We find that at low surface coverage, the adsorbed molecules prefer to stay isolated from each other in a monomer phase, due to the inter-molecular dipole-dipole repulsions. However, when the coverage rises above a critical value of 0.9nm², the adsorbed molecules aggregate into linear structures via hydrogen bonding between amine groups, consistent with recent experiments [Haxton, Zhou, Tamblyn, et al, Phys. Rev. Lett. 111, 265701 (2013)]. Moreover, we find that these linear structures at high density considerably reduces the Au work function (relative to a monomer phase). Due to reduced surface polarization effects, we estimate that the resonance energy of the highest occupied molecular orbital of the adsorbed BDA molecule relative to the Au Fermi level is significantly lower than the monomer phase by more than 0.5 eV, consistent with the experimental measurements [DellAngela, Kladnik, and Cossaro, et al, Nano Lett. 10, 2470 (2010)].

\textsuperscript{1}This work supported by DOE (the JCAP under Award number DE-SC000499 and the Molecular Foundry of LBNL), and computational resources provided by NERSC.

H1.00116 Benzene Derivatives Adsorbed to the Ag(111) Surface: A Binding Site Study \textsuperscript{1}, DANIEL MILLER, SCOTT SIMPSON, NINA TYMINSKA, EVA ZUREK, University at Buffalo, ZUREK GROUP TEAM — Dispersion corrected Density Functional Theory (DFT) calculations were employed to study the interaction of benzenes mono and disubstituted with functional groups encompassing a region of the activated/deactivated spectrum. Benzenes substituted with weak activating or deactivating groups like methyl and fluoro, respectively, do not have a strong site preference for adsorption to the Ag(111) surface. Strong activating (N(CH₃)₂) and deactivating (NO₂) groups, on the other hand, have a distinct site preference. The nitrogen in the former prefers to lie above a silver atom (top site), but in the latter an Hhcp site of the Ag(111) surface is favored. Benzenes derivatized with classic activating groups donate electron density from the highest occupied molecular orbital (HOMO) of the molecule to the surface, and those functionalized with deactivating groups withdraw electron density from the surface into orbitals that are unoccupied in the gas phase. In the case of disubstituted benzenes, the strong activating/deactivating groups control the site preference and other groups assume sites that are, to a large degree, dictated by their positions on the benzene ring. Surface adsorption alters the relative stabilities of the ortho, meta and para positional isomers of disubstituted benzenes.

\textsuperscript{1}A portion of this research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility

H1.00117 Quasi-1D States Confined in a Self-Assembled Organic Super-Lattice of TTF-TCNQ on Ag(111)\textsuperscript{1}, SEOKMIN JEON, Oak Ridge National Laboratory (ORNL), PANCHAPAKESAN GANESSH, BOBBY SUMPTER, ORNL, JORGE IRIBAS CERDÁ, Instituto de Ciencia de Materiales de Madrid, PETRO MAKSYMOVYCH, ORNL, CNMS TEAM, ICCM-CSIC TEAM — Organic charge transfer complexes (CTC) have drawn much attention due to their potential applications to conducting or semiconducting organic thin films and contacts in devices. TTF-TCNQ is a historic organic CTC with one of the highest conductivity values among numerous organic conductors. As a two-component molecular material, TTF-TCNQ in a low-dimension form on a surface naturally creates monolayer super-lattices with corrugated electrostatic potential and adsorbate-induced strain. Generally this will lead to strong confinement of the surface states, although the detailed response of the surface electronic structure remains to be understood. We investigated TTF-TCNQ monolayer films grown on Ag(111), Au(111) and Ag(100) surfaces using STM/STS at 4.3 K. Confinement of sp-derived surface states was indeed ubiquitous, including spontaneous formation of quantum dots and quasi-1D bands. The small periodicity of the lattice caused a complete depopulation of the surface states, with only 1 eV upshift of the band minimum — much stronger effect than normally observed in assemblies. This also allows us to infer the height of the confining potential using 1D Kronig-Penney model and critically assess the long-standing problem of molecule-surface charge transfer.

\textsuperscript{1}A portion of this research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility

H1.00118 Adsorption of pentacene on (100) vicinal surfaces: role of coordination, surface chemistry and vdWs effects\textsuperscript{1}, JERONIMO MATOS, ABDELKADER KARA, University of Central Florida — In contrast to low miller index surfaces, vicinal surfaces are characterized by steps and step edges that not only present an interesting atomic landscape for the adsorption organic molecules, but also a unique electronic structure resulting in part from the low coordinated atoms at the step edges. The adsorption of pentacene on the stepped (511), (711), (911) surfaces (respectively 3, 4 and 5-atom wide terraces) of Cu and Ag (coagined transition metals); Pt (reactive transition metal); and Ni (reactive, magnetic transition metal) are studied using density functional theory, in order to investigate the support effects arising from differing surface chemistry. We compare the adsorption energy, adsorption geometry and electronic structure predicted by the PBE functional with those obtained from one of the optimized vdW-DF methods: optB88-vdW.

\textsuperscript{1}Work supported by the U.S. Department of Energy Basic Energy Science under Contract No DE-FG02-11ER16243

H1.00119 Electron configuration and correlation effects in organometallic molecules from constraint density functional theory \textsuperscript{1}, KENJI NAWA, KOHIJ NAKAMURA, TORU AKIYAMA, TOMONORI ITO, Mie University, MICHAEL WEINERT, University of Wisconsin-Milwaukee — Interest in single organometallic molecule and that adsorbed on solid surfaces has rapidly increased because of possible novel applications. For molecules with transition metals (TMs), the d-electron configuration is an essential aspect of their electronic and magnetic properties, and correlation effects can be not excluded. Here, we investigate systematically the electron configuration and correlation effects for prototypical organometallic molecules of tridimensional metalloocene (TM Cp₂) and planer phthalocyanine (TMCp). Calculations were carried out based on the constraint density functional theory (DFT) by using the full-potential linearized augmented plane wave method that incorporates an on-site Coulomb interaction correction $U$. We find that these correlation effects play a key role in determining the ground state of the organometallic molecules. The calculated ground states of TMCp, where TM = Cr, Mn, Fe, Co, and Ni, obtained by constraint DFT with $+U$ reproduce the experimentally determined structures of $3E_{2g}$, $6A_{1g}$, $1A_{1g}$, $2E_{1g}$, and $3A_{2g}$, respectively. Results for the TMCp will be also presented.

H1.00120 MAGNETISM –
H1.00121 Structural and Magnetic Properties of Mn$_{1.5}$X$_{0.5}$Sn (X = Cr, Mn, Fe, Co) Melt-spin Ribbons

R. FUGLSBY, P. KHAREL, Department of Physics, South Dakota State University, Brookings, SD, W. ZHANG, S. VALLOPPILLY, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE, Y. HUH, Department of Physics, South Dakota State University, Brookings, SD, D.J. SELLMYER, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE — Mn$_{1.5}$X$_{0.5}$Sn (X = Cr, Mn, Fe, Co) nanomaterials in a hexagonal Ni$_2$In-type crystal structure have been prepared using arc-melting and melt spinning. All the samples show moderate saturation magnetization at 100 K with a highest value of 458 emu/cm$^3$ for Mn$_{1.5}$Fe$_{0.5}$Sn, but their Curie temperatures (Tc) are less than 300 K. The highest Tc is 206 K for the Fe containing sample. All samples except the Cr containing one show irreversibility between the zero-field-cooled and field-cooled measurements at the low temperature, showing a spin reorientation or spin-glass-like behavior. The magnetic anisotropy constants calculated at 100 K are on the order of 1 Merg/cm$^3$. The magnetic properties of these materials have substantially improved due to vacuum annealing, where the Tc for Mn$_3$Sn annealed at 450 °C has increased by about 75 K from 190 K to 265 K.

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H1.00122 Noncollinear ferromagnetic easy axes in spin valves induced by oblique deposition

ROBERTO RODRIGUEZ, Pontificia Universidad Católica de Chile, THIAGO BUENO, DANIEL PARREIRAS, Universidade Federal de Minas Gerais, Brazil, SEBASTIAN MICHEA, Pontificia Universidad Católica de Chile, MARIO ARAUJO, WALDEMAR MACEDO, Laboratório de Física Aplicada, Centro de Desenvolvimento da Tecnologia Nuclear, Belo Horizonte, MG, Brazil, KLAUS KRAMBROCK, ROBERTO PIANAGO, Universidade Federal de Minas Gerais, Brazil — In this work we investigate the magnetic properties of Py/Ru/FeCo/InMn spin valves grown by oblique magnetron sputtering. The in-plane angular dependence of the ferromagnetic resonance (FMR) was used to obtain the relevant magnetic anisotropies. As we show, the deposition geometry employed in the sample preparation setup can be used to induce noncollinear easy axes of the ferromagnetic (FM) layers of the spin valve. We could directly observe the non-collinearity on the symmetry shift of the angular dependence of the FMR resonances fields of the two FM layers. The observations of the present study suggest that, by combining oblique deposition and appropriate angles of incidence of the deposition flux, the uniaxial (and unidirectional) axes of individual FM layers can be precisely engineered in spin valve fabrication.

H1.00123 Temperature and size dependent magnetic hyperthermia studies of Dextran coated Fe$_3$O$_4$ and Co$_x$Fe$_{3-x}$O$_4$ ferrofluids

H. NEMALA, M. PALIHAWADANA ARACHCHIGE, G. LAWES, Department of Physics and Astronomy, Wayne State University, Detroit, Michigan, 48202, V.M. NAIK, Department of Natural Sciences, University of Michigan-Dearborn, Dearborn, Michigan, 48128, R. NAIK, Department of Physics and Astronomy, Wayne State University, Detroit, Michigan, 48202 — Magnetic hyperthermia (MHT) using magnetic nanoparticles (MNPs) is a promising technique for cancer therapy. The dominant mechanism of heat generation in MHT using superparamagnetic MNPs is the Néel relaxation in response to an applied ac magnetic field. The efficiency of heating depends on the particle size, particle size distribution and the intrinsic magnetic properties of the MNPs. In this study, we have prepared Fe$_3$O$_4$(8-14 nm) and Co$_x$Fe$_{3-x}$O$_4$ (10 nm) MNPs by the co-precipitation method and characterized using XRD, TEM, Zeta potential and DC magnetometry measurements. The MNPs are found to be polydisperse and form stable colloidal suspensions in weakly basic solutions (zeta potential −20 mV) with their hydrodynamic radii ranging from 80 to 120 nm. The specific power loss (SPL) was determined as a function of temperature using MHT measurements (140-235 °C and 188-375 kHz) by incorporating heat losses due to nonadiabatic sample conditions. The SPL values at 298 K measured with 235 °C and 375 kHz range from 20-95 W/g for the MNPs, and SPL monotonically decrease with increasing in temperature. The results are in agreement with the linear response theory. Details of the measurement and analyses will be presented.

H1.00124 First Successful Fabrication of Nanoparticles of magnetocaloric Gd$_5$Si$_2$Ge$_{1-x}$Si$_x$

RAVI L. HADIMANI, Iowa State Univ, SHALABH GUPTA, Ames Laboratory, US Dept. of Energy, SHANE M. HARSTAD, VITALIJ K. PECHARSKY, DAVID C. JILES, Iowa State Univ, IOWA STATE UNIVERSITY COLLABORATION, AMES LABORATORY, US DEPT. OF ENERGY COLLABORATION — The Gd$_5$(Si$_2$Ge$_{1-x}$)$_x$ system has been widely studied in bulk form due to its interesting properties at the phase transition. There are a few reports on the fabrication of thin films of this material but, there are no reports in the literature on synthesis and characterization of nanoparticles of this material. Unlike films, which are expected to have low refrigeration capacity due to low volume, nanoparticles have the potential to overcome the problem if a scalable and cost-effective method of nanoparticle fabrication can be developed. In this work, we have synthesized sub-micron particles of Gd$_5$Si$_2$ by high-energy ball-milling varying milling times and milling intensity. We have investigated their microstructure, crystal structure, composition and magnetic properties. We have determined the milling time beyond which the particles become non-crystalline and lose the long range ordering. We also show that the coercivity of the particles increases with increasing the milling time. Particles agglomerate at long milling times and the particles that are milled longer than 20 min no longer undergo magnetic phase transition close to 340 K, which is present in a bulk material.

1Work at Ames Laboratory was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering. Ames Laboratory is operated for DoE by Iowa State University under Contract No. DE-AC02-07CH11358.

H1.00125 Experimental Realization of Artificial Skyrmion Lattices

DUSTIN GILBERT, BRIAN MARANVILLE, NIST Center for Neutron Research, ANDREW L. BALK, Center for Nanoscience and Technology, NIST, BRIAN J. KIRBY, NIST Center for Neutron Research, PETER FISCHER, Advanced Light Source; University of California, Santa Cruz, DANIEL T. PIERCE, JOHN UNGURIS, Center for Nanoscale Science and Technology, NIST, JULIE A. BORCHERS, NIST Center for Neutron Research, KAII LII, University of California, Davis — Magnetic skyrmions exhibit topologically protected states, offering new mechanisms for high density/low dissipation information storage, and also exhibiting a host of unique topological phenomena. In bulk crystals, chiral spin textures are only found in certain systems and in limited regions in the temperature-magnetic field parameter space. We present experimental evidence of room-temperature artificially structured skyrmion lattices fabricated by carefully controlling the three dimensional anisotropy of a Co on/Pd hybrid structure. The hybrid structures were fabricated by patterning chirality controlled vortex-state Co nanodot arrays on top of a Co/Pd multilayer with perpendicular anisotropy, chirality control was confirmed by microscopy and magnetometry. The vortex polarity is set by an external magnetic field to manifest the skyrmion state, and confirmed by magnetometry measurements. The chiral structure of the nanodots is imprinted into the Co/Pd underlayer, as revealed by polarized neutron reflectometry and spin-transport studies. These artificial skyrmion lattices offer a convenient platform to explore skyrmion physics. This work has been supported by the NSF (DMR-1008791 and ECCS-1232275).
H1.00126 Anatomy of Dzyaloshinskii-Moriya Interaction at Co/Pt Interfaces. HONGXIN YANG, Spintec/INAC, Grenoble France. STANISLAS ROHART, ANDRE THIAVILLE. LPS, Universit Paris-Sud, CNRS UMR 8602, F-91405 Orsay, France. ALBERT FERT. Unit Mixte de Physique CNRS/Thales, 91767 Palaiseau and Universit Paris-Sud, 91405 Orsay, France. MAIRBEK CHISHIEV. Spintec/INAC, Grenoble France — Dzyaloshinskii-Moriya Interaction (DMI)[1] was recognized to play a crucial role at ferromagnetic (FM)/heavy metal (NM) interfaces to create magnetic skyrmions[2]. DMI also plays an essential role for fast domain wall dynamics driven by spin-orbit (SO) torques[3]. Here, we clarify the main features and microscopic mechanisms of DMI in Co/Pt bilayers by ab initio. We find that large anticlockwise DMI of the bilayers has a predominant contribution from DMI pair couplings between spins of interfacial Co layer. This DMI between interface Co spins is directly related to the change of SO energy in the adjacent Pt when Co spin chirality is reversed. DMI does not extend significantly into other Co layers and is very weak between the proximity-induced spins in Pt. It was suggested[4] that DMI at FM/NM interfaces is directly related to the proximity induced moment in NM. However, we find the opposite result; i.e. Pt moment reduction slightly increases the DMI[5]. [1] I. E. Dzialoshinskii, Sov. Phys. JETP 5, 1259 (1957); T. Moriya, Phys. Rev. 120, 91 (1960). [2] A. Fert et al. Nat. Nanotech. 8, 152 (2013). [3] A. Thiaville, et al, Europhys. Lett. 100, 57002 (2012). [4] K. Ryu et al, Nat. Nanotech. 8, 527 (2013). [5] H. Yang et al, submitted

H1.00127 Theory of damping for the standing spin waves. IRINA BARIAKHTAR, Boston College, USA, VICTOR BARIAKHTAR, Institute of Magnetism, Ukraine — It is well known, that the thin magnetic films exhibit dependency of the magnetic dispersion on the wave vector. This is due to the fact that in films with their thickness comparable to the exchange length, the wave vector of the spin waves becomes of the order of the exchange length because of the boundary conditions for magnetization. These kinds of thin films were studied at first by Kittel [1]. The standing spin waves are characterized by the fact, that under certain conditions they do not correlate to an alternating magnetic field within or outside the film [2]. The damping theory for the standing spin waves was not well studied yet. This problem appears interesting, since the distance between the neighboring standing spin waves increases with increasing number of frequency as n, and the attenuation increases with a mode number increase as n^4. In other words, high-frequency modes of the standing spin waves are not created if the exchange relaxation mechanism is valid. The standing spin waves properties are being well studied experimentally lately [3]. The authors would like to compare their theoretical results to the experimental data.


H1.00128 Controlling strain anisotropy in iron-palladium thin films using perovskite-oxide substrates. RENEW HARTON, VLADIMIR STOICA, ROY CLARKE. University of Michigan — In this study, iron-palladium (FePd) thin films were deposited on (100) barium-titanate (BaTiO_3) and (100) strontium-titanate (SrTiO_3) substrates. Both BaTiO_3 and SrTiO_3 have a perovskite crystal structure and exhibit similar structural phases, such as tetragonal and cubic, at various temperatures. In contrast to SrTiO_3, BaTiO_3 exhibits ferroelectric and piezoelectric behavior in all of its structural phases except the cubic phase. In the tetragonal phase, the strain anisotropy of BaTiO_3 is two-fold about the in-plane c-axis, while in the cubic phase the epitaxial strain in the substrate plane is four-fold. In this investigation, the effect of strain on the magnetism and structure of FePd/SrTiO_3 and FePd/BaTiO_3 heterostructures was studied using the Magneto-Optic Kerr Effect (MOKE), Atomic Force Microscopy (AFM) and X-Ray diffraction (XRD) analysis to investigate the correlation between the magnetic anisotropy, morphology and structure of the FePd films.

H1.00129 Synthesis of magnetic GdC_2 nanoparticles using cavitation plasma. RAKESH CHAUDHARY, ALI R. KOYMEN, Department of Physics, The University of Texas at Arlington — Gadolinium dicarbide (GdC_2) nanoparticles were synthesized using Gd electrodes in toluene. Gd nanoparticles are formed in plasma caused due to collapse of cavitation bubbles using ultrasonication in electric field between Gd wire electrodes. The presence of a single phase of GdC_2 nanocrystals have been determined by X-Ray Diffraction (XRD) and High Resolution Transmission Electron Microscopy (HRTEM). The GdC_2 nanoparticles have tetragonal crystal structure. Transmission Electron Microscopy (TEM) shows that the nanoparticles range in size of 4-45 nm in diameter. Magnetization measurements performed using a Superconducting Quantum Interference Device (SQUID) magnetometer shows GdC_2 nanoparticles are paramagnetic in nature. To the best of our knowledge, this is the first synthesis of GdC_2 in single phase form, allowing further characterization of physical properties.

H1.00130 Magnetic and Structural characterization of Co nanowires using advanced electron microscopy techniques. JESUS CANTU-VALLE, FRANCISCO RUIZ-ZEPEDA, JOHN EDER SANCHEZ, FERNANDO MENDOZA-SANTOYO, ARTURO PONCE, University of Texas at San Antonio, UTS TEAM — We report the magnetic imaging and crystalline structure of high aspect ratio cobalt nanowires. Experimental results of magnetization reversal in cobalt nanowires are presented to illustrate the functionality of the in situ magnetization process through the manipulation of the objective lens. By making use of this applicability, we measure the magnetization and show experimental evidence of the magnetic flux distribution in polycrystalline cobalt nanowires using off-axis electron holography. The retrieved phase map can distinguish the magnetic contribution from the crystalline contribution with high accuracy. To determine the size and orientation of the grains within the Co nanowires, PED-assisted orientation mapping was performed. Finally, the magnetic analysis performed at individual nanowires was correlated with the crystalline orientation map, obtained by PED-assisted crystal phase orientation mapping. The large shape anisotropy determines the major magnetization direction rather than the magneto-crystalline anisotropy in the studied nanowires. The combination of the two techniques allowed us to directly visualize the effects of the crystallographic texture on the magnetization of the nanowire.

1The authors would like to acknowledge Dr. B.J.H. Studler for providing the samples and financial support from NSF PREM #DMR 0934218, CONACYT, #215762 and Department of Defense #64756-RT-REP.

H1.00131 Magnetic properties of Ru-Ti doped Strontium hexaferrite nanocrystalline particles. ABDEL ALSMADI, Kuwait University, S. MAHMOOD, University of Jordan, I. BSOL, Al-Ibn University — We carried out a systematic study on the effect of the substitution of Ti^{2+} and Ru^{4+} ions for Fe^{3+} ions on the magnetic properties of the strontium ferrite SrFe_{12-x}Ru_xTi_{12}O_{39} nanoparticles with (0 ≤ x ≤ 1), using vibrating sample magnetometry, electrical resistivity, and Mössbauer spectroscopy. A clear irreversibility between the zero-field-cooled and field-cooled curves was observed below room temperature and the zero-field-cooled magnetization curves displayed a broad peak at a temperature T_M. These results were discussed within the framework of random particle assembly model and associated with the magnetic domain wall motion. The resistivity data show some kind of a transition from insulator to perfect insulator around \( T_M \). With Ru-Ti substitution at 5 K, the saturation magnetization showed small variations with x slightly increased up to x = 0.2 and then starts to decrease for x between 0.2 and 0.5, while the coercivity decreased monotonically, recording a reduction of about 93% at x = 0.4. These results were discussed in light of the single ion anisotropy model and the cationic distributions based on the results of the Mössbauer spectroscopy data.

3Thank ANR SOSPIN, ESPERADO and a CNRS postdoctoral fellowship.
H1.00132 Doping controlled spin reorientation in dysprosium-samarium orthoferrite single crystals

SHIXUN CAO, WEIYAO ZHAO, BAOJUAN KANG, JINCANG ZHANG, WEI REN, Shanghai University — As one of the most important phase transitions, spin reorientation (SR) in rare earth transition metal oxides draws much attention of emerging materials technologies. The origin of SR is the competition between different spin configurations which possess different free energy. We report the control of spin reorientation (SR) transition in perovskite rare earth orthoferrite Dy$_{1-x}$Sm$_x$Fe$_2$O$_4$, a whole family of single crystals grown by optical floating zone method from $x=0$ to 1. Temperature dependence of the magnetizations under zero-field-cooling (ZFC) and field-cooling (FC) processes are studied. We have found a remarkable linear change of SR transition temperature in Sm-rich samples for $x>0.2$, which covers an extremely wide temperature range including room temperature. The $\alpha$-axis magnetization curves under FC process bifurcate from and then jump down to that of warming process (ZFC and FCW curves) in single crystals when $x>0.5-0.9$, suggesting complicated 4f-3d electron interactions among Dy$^{3+}$, Sm$^{3+}$, Fe$^{3+}$, and Sm$^{3+}$-Fe$^{3+}$ sublattices of diverse magnetic configurations for materials physics and design. The magnetic properties and the doping effect on SR transition temperature in these single crystals might be useful in the spintronics device application.

3This work is supported by the National Key Basic Research Program of China (Grant No. 2015CB921600), and the National Natural Science Foundation of China (NSFC, Nos. 51372149, 50932003, 11274222)

H1.00133 Crystal structure and magnetic properties of 5d double perovskite oxide Sr$_2$EuOsO$_6$

JIANFENG HE, National Institute for Materials Science (NIMS), HAI L. FENG, Max Planck Institute for Chemical Physics of Solids, YAHUA YUAN, YOSHIHIRO TSUJIMOTO, KAZUNARI YAMURA, National Institute for Materials Science (NIMS), SUPERCONDUCTING PROPERTIES UNIT, NATIONAL INSTITUTE FOR MATERIALS SCIENCE TEAM, GRADUATE SCHOOL OF CHEMICAL SCIENCES AND ENGINEERING, HOKKAIDO UNIVERSITY TEAM, MATERIALS PROCESSING UNIT, NATIONAL INSTITUTE FOR MATERIALS SCIENCE TEAM — Polycrystalline Sr$_2$EuOsO$_6$ has been synthesized with high-pressures and temperatures. It crystallizes in a monoclinic double perovskite structure and shows an antiferromagnetic-like transition at 51 K in a magnetic susceptibility measurement. The transition has been further characterized by specific measurements and electrical resistivity measurements. The results are compared with the magnetic properties of Ba$_2$EuOsO$_6$ [1] and other double perovskite oxides containing Os(V) atom. We will discuss role of spin-orbit coupling and spin polarization on the gapped electronic structure of Sr$_2$EuOsO$_6$ and other related compounds.


H1.00134 Thermal fluctuations in novel artificial spin ice

HENRY STOPPEL, ERIK OSTMAN, UU, AARON STEIN, CFN, UNNAR ARNALS, UI, VASSILIOS KAPAKIS, BJORGVIN HJORVARSSON, UU, UU TEAM1, CFN COLLABORATION1, UI COLLABORATION1 — Artificial spin ice (ASI) is used as a model material to investigate frustrated systems. The square and kagome ASI has been extensively investigated since there discovery. Novel ASI structures like the Shakti lattice, have been proposed and already realized. In this structure what is not an adaption of natural magnetic materials the lattice topology leads to a high degree of degeneracy. We present here the results of Photoemission electron microscopy (using XMCD) to image the magnetization of nano-islands in a Shakti ASI. By using a three layer of Pd-Fe-Pd we can tune the Curie temperature of our magnetic material by varying the thickness of the Fe-layer. Beside a statistical analysis of the frozen-in ground state, we present also a temperature series, in which we could visualize the two energy levels of the small and large islands and due to this the different blocking temperatures for these islands. This comparison of these measurements with previous measurements on squared ASI give us a better understanding of the magnetic ordering and the thermal fluctuations in the novel Shakti ASI.

1Materials Physics, Department of Physics and Astronomy, Uppsala University, Sweden
2Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, USA
3Science Institute, University of Iceland, Reykjavik, Iceland

H1.00135 Negative magnetization and exchange bias in Y$_1-x$Pr$_x$CrO$_3$ with $(0>x>0.3)$

E. VERDIN, Departamento de Fisica, Universidad de Sonora, A. DURAN, Centro de Nanociencias y Nanotecnologia-UNAM, F. MORALES, E. ESCUDERO, Instituto de Investigaciones en Materiales-UNAM — Rare earth orthochromites compounds with perovskite structure have attracted great interest because its potential applications as data storage and spintronics. We report studies of the crystalline structure, thermal, and magnetic properties performed in the compound Y$_{1-x}$Pr$_x$CrO$_3$ with $0<x<0.3$. We found changes in the specific heat and in the magnetization when the Pr atoms are substituted into the compound. The antiferromagnetic transition, $T_N$, increases when the Pr atoms are substituted into the compound which is clearly observed by specific heat and magnetization measurements. We also found an exchange bias and magnetization reversal when the magnetization-temperature (M-T) curves were measured in field cooled mode (FC). All these changes are attributed to the influence of the Dzialoshinskii-Moriya indirect interaction that we related to the octahedral distortion, because the Pr substitution affecting the Cr-O bond lengths.

3This work was partially supported by DGAPA-UNAM, IN103213, IN10014, CONACyT-Mexico, project 129293, BISSNANO, and by the Institute of Sciences project PICCO 11-7, Distrito Federal, Mexico

H1.00136 Neutron diffraction study on the phase diagram in multiferroic DyFeO$_3$

JINCHEN WANG, JUANJUAN LIU, JIEMING SHENG, Remin Univ of China, ZHYING ZHAO, XIA ZHAO, XUEFENG SUN, University of Science and Technology of China, SERGEY DANILKIN, Australian Nuclear Science and Technology Organisation, WEI BAO, Remin Univ of China — The discovery of the multiferroic effect in perovskite DyFeO$_3$ has generated many interests due to a witnessed strong magnetoelectric coupling. In this low temperature and high magnetic-field study, the $\alpha$- and $\alpha$'-phase boundaries are determined by neutron diffraction studies. The multiferroic effect is observed only in the phase area where the applied magnetic field breaks the long-range order (LRO) AF order of the Dy ions into a short-range order (SRO). Our results suggest the mechanism of the remarkably strong multiferroic effect in the prototype rare-earth orthoferrite DyFeO$_3$ ought to be investigated through the interplay between the weak ferromagnetism of Fe and the antiferromagnetic SRO of Dy spins.

H1.00137 Engineering magnetic properties and microstructure of La$_2$CoMnO$_6$ thin films by tailoring the oxygen stoichiometry

BENJAMIN MARTINEZ, REGINA GALCERAN, CARLOS FRONTERA, LLUIS BACCELLS, JOSE CISNEROS-HERNÁNDEZ, ICMAB-CSIC, JAUME ROQUETA, JOSE SANTISO, ICN2-CSIC, ALBERTO POMAR, FELIP SANDIUMENGE, ICMAB-CSIC, ADVANCED MATERIALS CHARACTERIZATION TEAM, THIN FILMS GROWTH TEAM — We report on the magnetic and structural properties of ferromagnetic-insulating La$_2$CoMnO$_6$ thin films grown on top of (001) STO substrates by means of RF sputtering technique. Insulating ferromagnets are of interest because of the exchange splitting of the bands allowing obtaining tunnel barriers with different height for spin-up and spin-down carriers. Belonging to the perovskite family, this material can be easily integrated in spintronic devices, such as magnetic tunneling junctions and spin filters, with upgraded and distinctive functionalities.

An exhaustive structural analysis, by using synchrotron X-ray diffraction, allows identifying a close correlation between the film composition and their magnetic properties. Both Curie temperature and the features of the hysteresis loops turn out to be dependent on the oxygen stoichiometry. In situ annealing conditions confirm the insulating character of the films.

3We acknowledge financial support from the Spanish MINECO (MAT2012-33207).
H1.00138 Magnetic and thermoelectric properties of Fe\(_{3-x}\)Co\(_x\)O\(_4\) thin films and CoFe\(_2\)O\(_4/\)Fe\(_3\)O\(_4\) superlattices. QUANG NGUYEN VAN, University of Ulsan, Korea. M. JUAN CHRISTIAN, Institute of Physics and Chemistry for Materials of Strasbourg, Unif 7504 UDS-CNRS, Strasbourg, France. ANH TUYAN DUC, VOOLEM SHIN, RHM. S. H, MINH NHI NGUYEN THI, SUNGLAE CHO, University of Ulsan, Korea — Microcrystalline ferrites are used as a medium for the magnetic recording and storage of information. Magnetite, Fe\(_3\)O\(_4\), is a ferrimagnet with a cubic inverse spinel structure and exhibits a metal-insulator, Verwey, transition at about 120 K. It is predicted to possess as half-metallic nature, ~100% spin polarization, and high TC 2850 K. Cobalt ferrite, Co\(_x\)O\(_4\), is one of the most important members of the ferrite family, which is characterized by its high H\(_c\), moderate magnetization and very high magnetocrystalline anisotropy. Here we report on the magnetic and thermoelectric properties of Fe\(_{3-x}\)Co\(_x\)O\(_4\) (x = 0 to 1) thin films and CoFe\(_2\)O\(_4/\)Fe\(_3\)O\(_4\) superlattices grown on MgO (100) by MBE. XRD and RHEED patterns confirmed the inverse spinel structure of the Fe\(_3\)O\(_4\) films. Magnetic properties of the Fe\(_{3-x}\)Co\(_x\)O\(_4\) films are markedly sensitive to the Co content. The Verwey transition was disappeared in Co-doped films. A negative MR curve with butterfly shape was observed with low Co content but disappeared for the samples with x = 0.8 and 1. Seebeck coefficients increased with Co concentration: -70 \(\mu\)V/K for x=0 and -220 \(\mu\)V/K for x=1. We will also discuss on the relationship between magnetic and thermoelectric characteristics in CoFe\(_2\)O\(_4/\)Fe\(_3\)O\(_4\) superlattices with the modulations of 5, 10, and 20 nm.

H1.00139 Magnetic and electrical properties on possible room temperature hybrid multiferroic BaTiO\(_3/\)La\(_{2/3}\)Sr\(_{1/3}\)MnO\(_3\). JOHN EDWARD ORDOÑEZ, MARIA ELENA GOMEZ, WILSON LOPERA MUÑOZ, Universidad del Valle, Cali, Colombia. PEDRO ANTONIO PRIETO, Center for Excellence on Novel Materials — CENM, Cali, Colombia. THIN FILM GROUP TEAM, CENTER OF EXCELLENCE ON NOVEL MATERIALS — CENM, Cali, Colombia. THIN FILM GROUP TEAM. — We addressed to deposit the ferromagnetic phase of the La\(_{1-x}\)Sr\(_x\)MnO\(_3\) and the ferroelectric BaTiO\(_3\) for possible hybrid multiferroic heterostructure. We have optimized the growth parameters for depositing BaTiO\(_3\) (BTO) / La\(_{2/3}\)Sr\(_{1/3}\)MnO\(_3\) (LMO) / (001) SrTiO\(_3\) by sputtering RF and DC, respectively, in pure oxygen atmosphere and a substrate temperature of 830°C. Keeping fixed the magnetic layer thickness (t\(_{\text{M}}\) = 40 nm) and varying the thickness of the ferroelectric layer (t\(_{\text{BTO}}\) = 20, 40, 80, 100 nm). We want to point out the influence of the thicknesses ratio (t\(_{\text{BTO}}\)/t\(_{\text{SMO}}\)) on electrical and magnetic properties. From x-ray diffraction (XRD) analysis, we found the bragg peaks for LSMO maintain its position but BTO peak shift to lower Bragg angle indicating a strained BTO film. Magnetization and polarization measurements indicate a possible multiferroic behavior in the bilayers. Hysteresis loop measurements of bilayers show ferromagnetic behavior.

1 Authors thank Instituto de Nanociencia de Aragón, Zaragoza, Spain. Work partially supported by COLCIENCIAS-UNIVALLE Project 110656933104 contract No.2013-0002, CI 7917 and CI 7978.

H1.00140 Magnetization fluctuation in FeB nanomagnets under asymmetric magnetization-potential. SHINJI MIWA, Osaka Univ. HITOSHI KUBOTA, KAY YAKUSHIJI, AIIST, SHOTA ISHIBASHI, AKIO FUKUSHIMA, SHINJI YUASA, AIIST, YOSHISHIGE SUZUKI, Osaka Univ. — Thermal fluctuation of magnetizations gives understandings of physics in magnetic materials and noise in magnetic devices. It is theoretically calculated using the Fokker-Planck equation and the fluctuation-dissipation theorem, [1] and is experimentally characterized using magnetoresistive devices [2]. In the present study, the magnetization-fluctuation under asymmetric magnetization potential has been investigated. Magnetic tunnel junctions (MTJs) [CoFeB (3 nm)/ MgO (1 nm)/ FeB (2 nm)] were employed to conduct the study. The FeB layer (120 nm in a diameter) is a magnetic free layer whose magnetic anisotropies are 8 mT (in-plane) and 97 mT (perpendicular). The asymmetric magnetization-potential was prepared using magnetic field application (110 mT) tilted from the film normal (10 deg.). [3] Unlike the first-order response to the thermal fluctuation, [2] the second-order response is identified as a Lorentzian power spectrum whose peak appears at 0 Hz. To derive the analytic formula, fourth-order moments were calculated using the quasi-normality hypothesis \(\langle AB \rangle \langle CD \rangle = \langle AB \rangle \langle CD \rangle + \langle AC \rangle \langle BD \rangle + \langle AD \rangle \langle BC \rangle \). As a results, the obtained formula quantitatively reproduces the experiment.


1 This work was supported by JSPS KAKENHI (No. 23260001).

H1.00141 Exchange interaction reduction as a precursor to laser-induced demagnetization in ferromagnets. GUOPING ZHANG, YIHUA BAI, Indiana State University. THOMAS F. GEORGE, University of Missouri-St. Louis — Laser-induced femtosecond demagnetization in a ferromagnet presents an opportunity to develop all-optical ultrafast magnetic storage devices, but its underlying mechanism is under intense debate. The controversy has been on the first several hundred femtoseconds, where the spin moment is reduced sharply up to 50% or higher, but the optically accessible electrons are very few. This apparent contradiction is puzzling. Here we show that a small number of excited electrons is enough to trigger a strong band structure relaxation. In all of the three 3d ferromagnets investigated here, this band relaxation sharply reduces the exchange splitting and spin moment. For fcc Ni, for every electron excited, the spin moment can be reduced by 0.23 \(\mu\)B or more. Our first-principles calculation, free of fitting parameters of any kind, finally explains the experimental findings and presents a paradigm for future experiments.

1 Solely supported by the U.S. Department of Energy under Contract No. DE-FG02-06ER46304. The work was done on Indiana State University’s quantum cluster and high-performance computers and used resources of NERSC at BNL.

H1.00142 A mechanical analogy for spin currents and torques. YAROSLAW BAZALIY, University of South Carolina — We map the problem of spin-transfer torques in nanostructures with diffusive spin currents on a mechanical problem involving elastic strings connecting points of attachment that slide along the fixed straight rails. The obtained mechanical analogy provides a qualitative understanding of the effects of spin relaxation on spin torques, and of the phenomenon of sign-changing angular dependence \([1-3]\) of the efficiency factor \(g(\theta)\).


1 Supported by NSF grant DMR-0847159.
H1.00143 Ultra Low Energy Switching of Ferromagnet with Perpendicular Anisotropy on Topological Insulator by Voltage Controlled Magnetic Anisotropy

BAHMIMAN GHOSH, TANMOY PRAMANIK, RIK DEY, ÜRMİMALA ROY, LEONARD REGISTER, SANJAY BANERJEE, Microelectronics Research Center, Univ of Texas at Austin — We propose and demonstrate, through simulation, an ultra low energy memory device on a topological insulator thin film. The device consists of a thin layer of Fe deposited on the surface of a topological insulator, Bi$_2$Se$_3$. The top surface of Fe is covered with MgO so that the ferromagnetic layer has perpendicular anisotropy. Current is passed on the surface of the topological insulator which switches the magnetization of the Fe ferromagnet through strong exchange interaction, between electrons contributing to the surface current on the Bi$_2$Se$_3$, and the d electrons in the ferromagnet, and spin transfer torque due to shunting of current through the ferromagnet. Voltage controlled magnetic anisotropy enables ultra low energy switching. Our micromagnetic simulations, predict switching time of the order of 2.4 ns and switching energy of the order of 0.16 fJ for a ferromagnetic bit with thermal stability of 90 k$_B$T. The proposed structure combines the advantages of both large spin torque from topological insulators and those of perpendicular anisotropy materials.

This work is supported by NRI SWAN and NSF NASCENT Center.

H1.00144 Capturing the Magnetic and Structural Phase Transition of Feruh by Extreme Ultraviolet Light

DMITRIY ZUSIN, PATRIK GRYCHTOL, CHRISTIAN GENTRY, MARGARET MURNANE, HENRY KAPTEYN, JILA, University of Colorado, Boulder, CO 80309, SOPHIE CANTON, Max-Lab, Lund University, SE-223 63 Lund, Sweden, RONNY KNUT, JUSTIN SHAW, HANS NEMBACH, THOMAS SILVA, Electromagnetics Division, National Institute of Standards and Technology, Boulder, CO 80305, ALEJANDRO CEBALLOS, CATHERINE BORDEL, PETER FISCHER, FRANCES HELLMAN, University of California, Berkeley, CA 94720 — The temperature dependent transition from the anti-ferromagnetic to the ferromagnetic phase in FeRh is accompanied by a modification of its crystal lattice. The interplay between the magnetic and the structural transition is a matter of strong debate. It is important to better understand the mechanism(s) of the transition since it can be induced by femtosecond laser pulses and, unlike slower (nano-second) magnetic phase transitions, does not seem to be limited by heat transfer. In this work, we use extreme ultraviolet light generated by a tabletop high harmonics source to perform element-selective investigations of the temperature-dependent magneto-optical response of a thin film FeRh sample. We study the optically induced phase transition using two ultrafast pump-probe spectroscopy approaches: by monitoring the time-resolved transversal mageto-optical Kerr effect (T-MOKE) and the transient change in reflectivity.

PF acknowledges support from BES MSD DOE # DE-AC02-05-CH11231 and LFRIR program (# 2012K1A4A305565) through NRF Korea funded by MEST, and JILA from DOE # DE-FG02-09ER4665.

H1.00145 The effects of shape anisotropy and exchange coupling on spin precession frequencies in exchange coupled Co/Cu/Pt trilayers

SAM KERAMATI, UDAY SINGH, SETH KURFMAN, CH. BINEK, S. ADENWALLA, Univ of Nebraska - Lincoln — Ultrafast high-power laser systems have successfully opened up the field of magnetization dynamics, studying subpicosecond laser-induced spin precession dynamics, demagnetization processes and magnetization reorientation. Here we investigate laser-induced magnetization dynamics in a series of photolithographically patterned microstructures of exchange coupled trilayers of Co/Cu/Pt grown on Si substrates. The microstructures have different shape anisotropies as well as different exchange coupling parameters. The latter determines the magnetization state, varying from ferromagnetically to anti-ferromagnetically coupled. We explore how the different spin precession frequencies of the constituent exchange coupled magnetic layers with unequal relaxation times can trade-off with the differing shape anisotropies. The key physical point is that the precession frequency of ferromagnetic materials and their damping parameter vary with the effective field which depends on both the shape anisotropy, and exchange coupling, while their corresponding effects can be modulated through the action of the intense pump beam. Precession frequency maps of the behavior of the exchange coupling parameter of the samples with respect to their shape anisotropy and their laser-induced modulated precession frequencies will be generated through a pump-probe experiment to address the above-mentioned objective of our work.

This work is supported by NSF Grant No. 1409622 and MRSEC DMR-0820521.

H1.00146 Electron Irradiation Induced Modification of Ferromagnetism in (Ga,Mn)As

JIA LUO, GANG XIANG, Department of Physics and Key Laboratory for Radiation Physics and Technology of Ministry of Education, Sichuan University — The ferromagnetism properties of diluted magnetic semiconductor (Ga,Mn)As firstly improved by energetic electron irradiation, through a sequence of irradiation doses. We did a systematic study of magnetization as a function of temperature and additional magnetic field. SQUID measurements demonstrate the T$_C$ of all (Ga,Mn)As film increased from 40K to 60K after irradiation. At the same time, electron irradiation improved the crystal quality and electric properties. The irradiation process decreases the resistance by a factor of 1/2 in the range of 10K to 50K, and transforms (Ga,Mn)As samples from insulator behavior to metallic behavior. SIMS and transport measurements confirm that the rearrangement of Mn interstitials plays a key role in the improvement of ferromagnetism properties. We infer that electron irradiation paves a new path to room-temperature ferromagnetism of (Ga,Mn)As.

This work is supported by NRI SWAN and NSF NASCENT Center.

H1.00147 ABSTRACT WITHDRAWN

H1.00148 Dynamics of bright and dark localized excitonic magnetic polarons in CdMnTe spin glass compound

YURIY GNATENKO, PETRO BUKIVSKIJ, YURIY PIRYATINSKI, Institute of Physics of National Academy of Science of Ukraine — The measurements of the magnetic properties of spin glass (SG) system indicate that the magnetic relaxation is characterized by a broad range of times below T$_f$. Here, for the first time, we have investigated time-resolved photoluminescence spectra of Cd$_{1-x}$Mn$_x$Te SG compound at the temperature below the freezing temperature T$_f$. This enables us to study the dynamics of different localized excitonic magnetic polarons (LEMPs) at T =0.7T$_f$ excited in the crystal regions where various microscopic magnetic spin states (MMSSs) are formed. It was found that there is a broad distribution of the lifetimes of the LEMPs which have different lifetimes but same energies. It was shown that the presence of the long-lived LEMPs is caused by the admixture of the optically active bright exciton states to the dark exciton states as a result of the local magnetic fields formation. The lifetimes of these dark LEMPs correspond to hundreds of nanoseconds. It was also found that the decay process of the PL exciton band intensity is described by the Kohlrusch–Williams–Watts stretched exponential function which describes the relaxation processes which correspond to the emission of the LEMPs formed in the crystal region of the finite clusters as well as the infinite cluster. These complex dynamical phenomena, observed for Cd$_{1-x}$Mn$_x$Te at low temperatures, reflect the spatially heterogeneous dynamics in the SG system which is due to the presence of different MMSSs below T$_f$. 

Natural Science Foundation of China (NSFC) Grant Nos. 11041411004142, and 11174212

H1.00149 ABSTRACT WITHDRAWN

H1.00150 Dynamics of bright and dark localized excitonic magnetic polarons in CdMnTe spin glass compound

YURIY GNATENKO, PETRO BUKIVSKIJ, YURIY PIRYATINSKI, Institute of Physics of National Academy of Science of Ukraine — The measurements of the magnetic properties of spin glass (SG) system indicate that the magnetic relaxation is characterized by a broad range of times below T$_f$. Here, for the first time, we have investigated time-resolved photoluminescence spectra of Cd$_{1-x}$Mn$_x$Te SG compound at the temperature below the freezing temperature T$_f$. This enables us to study the dynamics of different localized excitonic magnetic polarons (LEMPs) at T =0.7T$_f$ excited in the crystal regions where various microscopic magnetic spin states (MMSSs) are formed. It was found that there is a broad distribution of the lifetimes of the LEMPs which have different lifetimes but same energies. It was shown that the presence of the long-lived LEMPs is caused by the admixture of the optically active bright exciton states to the dark exciton states as a result of the local magnetic fields formation. The lifetimes of these dark LEMPs correspond to hundreds of nanoseconds. It was also found that the decay process of the PL exciton band intensity is described by the Kohlrusch–Williams–Watts stretched exponential function which describes the relaxation processes which correspond to the emission of the LEMPs formed in the crystal region of the finite clusters as well as the infinite cluster. These complex dynamical phenomena, observed for Cd$_{1-x}$Mn$_x$Te at low temperatures, reflect the spatially heterogeneous dynamics in the SG system which is due to the presence of different MMSSs below T$_f$. 

Natural Science Foundation of China (NSFC) Grant Nos. 11041411004142, and 11174212
H1.00149 Ferruquadrupolar phase of the Heisenberg model with bilinear and biquadratic interactions. ANTONIO PIRES, Universidade Federal de Minas Gerais — The Heisenberg antiferromagnet with bilinear and biquadratic exchange interactions has been studied using several techniques. In contrast to bilinear interactions models, quantum spin models with biquadratic interactions present a phase diagram qualitatively different from their classical counterparts, as for instance nonmagnetic phases such as the quadrupolar phase. In this work I study the ferruquadrupolar phase of the $S = 1$ Heisenberg model with bilinear and biquadratic exchange interactions on the square lattice using a SU(3) Schwinger boson formalism in a mean field approximation. This nonmagnetic phase is characterized by a finite quadrupole moment. I will calculate the quadrupole moment and the static spin structure factor for several values of the parameters involved in the model. The results obtained will also be compared with the ones obtained from other theories.  

1 I acknowledge support from CNPQ.

H1.00150 Effect of Zn substitution on the magnetic properties of Skyrmion Cu$_2$OSeO$_3$. TIEN-YU WEI, HUNG-CHENG WU, KAKARLA DEVI CHANDRASEKHAR, HUNG-DUEN YANG, Natl Sun Yat Sen Univ, NATIONAL SUN YAT-SEN UNIVERSITY TEAM — There is a considerable interest in the new magnetic state, the “Skyrmion state (A-phase),” whose magnetic properties have a remarkable characteristic as a vortex-like spin orientation. The polycrystalline (Cu$_{1-x}$Zn$_x$)$_2$OSeO$_3$ ($x = 0.0$ to $0.20$) samples were synthesized using solid state reaction method and studied by X-ray diffraction, X-ray absorption spectra and magnetic measurements. Variation of lattice constant with Zn doping follows the Vegard’s law which signifies the successful substitution of Zn in place of Cu up to $x$ less than 0.20. The Cu L$_{2,3}$ spectra show 2+ valence state for all samples. The Curie temperature decrease with Zn doping indicate the ferrimagnetic ordering is gradually suppressed. Moreover, we have noticed another magnetic phase for the doping level $x$ between 0.05 and 0.2, whose magnetic transition also shifted to low temperature for higher Zn doping. The H-T magnetic phase diagrams of the samples from ac susceptibility have been established with increasing Zn doping. The explanations for the observations of doping effects on the A-phase of Skyrmion Cu$_2$OSeO$_3$ will be discussed.

H1.00151 Effect of Ni substitution on the magnetic properties of Skyrmion Cu$_2$OSeO$_3$. CHUNG-LUN HUANG, HUNG-CHENG WU, KAKARLA DEVI CHANDRASEKHAR, HUNG-DUEN YANG, Natl Sun Yat Sen Univ, NATIONAL SUN YAT-SEN UNIVERSITY TEAM — Chiral magnetic lattice shows many exotic physical properties such as spin ice/spin liquid order, topological insulators and magneto-electric coupling. The chiral magnetic lattice of Cu$_2$OSeO$_3$ exhibits such kind of unique magnetic ordering where spins form the vortex like ordering called as Skyrmion. In this poster, the effects of isovalent ion doping on the Skyrmion phase of Cu$_2$OSeO$_3$ were presented. Polycrystalline (Cu$_{1-x}$Ni$_x$)$_2$OSeO$_3$ ($x = 0.0$ to $0.1$) samples were prepared by standard solid-state methods. Temperature and magnetic field dependent AC and DC magnetic measurements were performed. The Curie temperature decreases obviously with increasing Ni concentration by using ac susceptibility $(\chi_{ac})^{-1}$. Systematic H-T phase diagrams indicating the effects of Ni doping are established and will be discussed.

H1.00152 High pressure and doping effect on the magnetic properties of CaMn$_2$O$_4$. KUN-JU HSIEH, HONG-CHENG WU, KAKARLA D. CHANDRASEKHAR, HUNG-DUEN YANG, Natl Sun Yat Sen Univ, NATIONAL SUN YAT-SEN UNIVERSITY TEAM — Polycrystalline Ca$_{1-x}$Sr$_x$Mn$_2$O$_4$ ($x = 0.05, 0.10, 0.15, 0.20$) compounds were synthesized using solid state reaction method. Samples were characterized by X-ray diffraction and magnetization measurements. The lattice constants (a, b, c) determined by Rietveld refinement increases with Sr substitution. CaMn$_2$O$_4$ shows antiferromagnetic transition $T_N$ near 220 K due to the Mn(III)-O-Mn(III) superexchange interaction. High-pressure effect on the $T_N$ of CaMn$_2$O$_4$ has been investigated by piston-cylinder type high pressure apparatus designed for MPMS-XLT magnetometer. It is found that the $T_N$ increases with applying pressure up to 17.7 kbar at a rate of 0.487(22) K/kbar and decreases with higher Sr content.

H1.00153 Exact Diagonalization of a Quantum Ising Model with Long-Range Interactions. SHANNA MUEHE, THOMAS GUNN, Univ of West Florida, C.C.-JOSEPH WANG, None, CHRISTOPHER VARNEY, Univ of West Florida — Due to the rapid advance of quantum spin simulators in ultra-cold ions, the varying interaction for spin models in two-dimensional lattices have become feasible for experimental exploration for exotic states of collective states of multiple spins. It is particularly interesting for the case of a triangular lattice with antiferromagnetic interaction between spins. When the Ising spin-spin interaction is uniform and restricted between nearest neighbors, the spins are geometrically frustrated. When the system interaction becomes long ranged, the geometric frustration is lost but the spins are frustrated by the long-range interaction. In the latter case, the underlying orders present in the ground state are unclear and understanding these states in finite spin systems is crucial for the benchmarking of experimental observations. Here, we investigate the quantum dipolar Ising model with exact diagonalization to analyze the ground state, order parameters, and excitations and provide a baseline for comparison with experiments.

H1.00154 Exchange interaction between J-multiplets. NAOYA IWAWARA, LIVIU CHIBOTARU, Theory of Nanomaterials Group, Katholieke Universiteit Leuven — The crystal-field levels in lanthanides and other metal complexes with unquenched orbital momentum originate from the ground atomic $J$-multiplet. It was long believed that the exchange interaction between $J$-multiplets is basically described by Heisenberg form, $J_1$ - $J_2$. In this work, Anderson’s superexchange model is applied for analytical derivation of exchange interaction between arbitrary $J_1$ and $J_2$ multiplets [1]. The structure and the energy spectrum of the obtained exchange Hamiltonian are significantly different from those of a Heisenberg Hamiltonian. Besides, it is also found that the 1/$U$ approximation [2] is not applicable for the description of exchange spectrum, since it gives qualitatively different predictions compared to the present treatment. Similar results are obtained for the exchange interaction between $J$-multiplet ($J_1$) and isotropic magnetic center ($S_2$).


H1.00155 The origin of magnetic ordering in quasi-two-dimensional quantum magnets Cu$_{tn}$Cl$_2$ and Cu(en)(H$_2$O)$_2$SO$_4$. ALZBETA ORENDACOVA, P.J. Safarik University, Park Angelinum 9, 041 54 Kosice, Slovakia, LUCIA BARANOVA, Technical University of Kosice, Vysokeškolska 4, 042 00 Kosice, Slovakia, ROBERT TARASENKO, MARTIN ORENDAC, ALEXANDER FEHER, P.J. Safarik University, Park Angelinum 9, 041 54 Kosice, Slovakia, RUDOLF SYKORA, DOMINIK LEGUT, VSB-Technical University of Ostrava, 17. listopadu 15, Ostrava 70833, Czech Republic — A comparative analysis of magnetic properties of Cu(en)(H$_2$O)$_2$SO$_4$ (en = C$_5$H$_7$N$_2$) (1) and Cu(tn)Cl$_2$ (tn = C$_5$H$_7$N$_2$) (2) has been performed to search for the origin of magnetic ordering observed in (1) at $T_c = 0.9$ K while hidden in (2). Previously, both materials were approximated by a quasi-two-dimensional (2d) spin 1/2 Heisenberg model on the square lattice with effective intralayer and interlayer coupling $J/K_B = 3$ and $J'/K_B = 10^{-14}$, respectively. The first principles calculations revealed in (1) a spatial anisotropy of exchange coupling within a layer, $J_1/J_2 = 0.15$, in accordance with a proposed data to toy behavior. Considering only effect of interlayer coupling, $T_c = 0.8$ K was evaluated, while $T_c = 0.85$ K when a weak Ising-like spin anisotropy, $\Delta = 0.015$ was introduced into Heisenberg layers. The effects of spin and spatial anisotropy on the ordering of (1) and the absence of a phase transition in (2) are discussed.

1 Supported by CFNT MVEP, ITMS2622012005, APVV 0132-11, SK-CZ-2013-0083, CZ.1.07/2.3.00/30.0055, and CZ.1.05/1.1.00/02.0070.
H1.00156 Thermodynamic properties of a layered $S = 7/2$ Heisenberg magnet Gd(OH)CO$_3$.1

MARTIN ORENDAČ, MARTIN ULICNY, ERIK CIZMAR, ALZBETA ORENDAČOVA, P. J. Safarik University, Park Angelinum 9, 040 01 Kosice, Slovakia, YUN-CONG CHEN, ZHAO-SHA MENG, MING-LIANG TONG, Sun Yat-Sen University, Guangzhou, 510275, P. R. China. — Thermodynamic quantities and ESR spectra of Gd(OH)CO$_3$ (I) are reported. The material may be considered to consist of weakly coupled layers with potentially triangular arrangement of exchange paths within each layer. Different bridging groups and distances among Gd$^{3+}$ ions may be responsible for spatial anisotropy of magnetic coupling. Preliminary analysis of magnetic susceptibility using Curie-Weiss law yielded $\theta = -1.05$ K indicating weak antiferromagnetic coupling and consequently, spin frustration in (I). More detailed simultaneous analysis of specific heat, susceptibility and magnetization studied down to nominally 0.45 K revealed non-negligible role of single-ion anisotropy. Using the model of weakly interacting $S = 7/2$ trimers, the gross features of measured data may be explained while assuming single-ion anisotropy $D/k_B \approx 0.6$ K and effective intratramer magnetic coupling $|J/k_B| \approx 0.3$ K. The obtained $D$ value reasonably reproduces the position and shape of ESR line. The performed analysis suggests that magnetism in (I) is governed predominantly by crystal field effects and frustration plays a minor role.

1Supported by ITMS26220120005 and VEGA 1/0143/13.

H1.00157 The structural, electronic and magnetic properties of Ga$_8$-xMn$_x$As$_8$ clusters.1 GANXU GU, GANG XIANG, College of Physical Science and Technology, Sichuan University — We systematically investigate the ground-state magnetic properties of Ga$_8$-xMn$_x$As$_8$ clusters ($x = 0, 2, 4, 6, 8$) within the framework of density functional theory (DFT) using a strategy that successively adopts the particle swarm optimization (CALYPSO) code and fixed spin-moment (FSM) method. The results show that for Ga$_8$-xMn$_x$As$_8$ in the ground states or low-lying isomers, Mn atoms tend to assemble at the core of the clusters and the ferrimagnetic Mn-Mn couplings are identified for Ga$_8$-xMn$_x$As$_8$ ($x = 4, 6$, and $8$), while GaMn$_8$ and Ga$_6$Mn$_2$As$_8$ are nonmagnetic. The possibility of multiple ground states of Ga$_8$-xMn$_x$As$_8$ ($x = 4, 6$, and $8$) is also demonstrated. The binding energy and LUMO-HOMO gap analysis show that Ga$_8$-xMn$_x$As$_8$ clusters with large $x$ are more likely synthesized and exhibit stronger chemical reactivity.

1The Natural Science Foundation of China (NSFC) Grant No. 11174212

H1.00158 Quantum oscillations of the mechanical forces in rotating molecular magnets. GWANG-HEE KIM, Sejong University — We study a rotating nanomagnet that exhibits beat structure of the quantum forces. We show that such forces are originated from tunneling between two entangled states of spin and mechanical angular momentum. They can be observed in the presence of a static magnetic field gradient with ac magnetic field and disappear on increasing total angular momentum and parameter which depends on the moment of inertia and the tunnel splitting.

H1.00159 Uniaxial-pressure dependence of the magnetization dynamics in the high-symmetry single-molecule magnet Mn$_{12}$-MeOH. JAMES H. ATKINSON, Dept. of Physics, University of Central Florida, Orlando, FL, and the Dept. of Physics, Amherst College, Amherst, MA, LAXMI BHASKARAN, STEPHEN HILL, National High Magnetic Field Laboratory and Dept. of Physics, Florida State University, Tallahassee, FL, YURI MYASOEDOV, ELI ZELDOV, Dept. of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel, IRAN FOTOH, Dept. of Physics, University of Central Florida, Orlando, FL, JOHNathan BesNel, B. K. CELESTE, G. K. GORDON, J. A. KAspin, J. P. PIZZETTI, I. ZILCH, Dept. of Physics, Amherst College, Amherst, MA, ADeline FORNUET, GEORGE CHRISTIOU, Dept. of Chemistry, University of Florida, Gainesville, FL — The single-molecule magnet [Mn$_{12}$O$_{12}$(OC$_2$H$_5$)$_{16}$(CH$_3$OH)$_4$]CH$_3$OH ("Mn$_{12}$-MeOH") is a high-symmetry sibling of the Mn$_{12}$-Acetate SMM that offers a prime opportunity to explore the consequences of molecular symmetry. A previous study [1] has shown that applied pressure induced changes in the Mn$_{12}$-Acetate's anisotropy parameters. Here we present the results of a study in which uniaxial pressure was applied to a crystalline sample of Mn$_{12}$-MeOH in order to examine how the pressure affects the quantum tunneling of magnetization at low temperature. We find that the pressure induces an increase in the resonant tunneling rate manifested as a change in the height of the tunneling steps in the magnetic hysteresis. These results suggest that pressure is altering symmetry-breaking terms in the molecule’s spin Hamiltonian, giving rise to increased tunneling.


H1.00160 Phase transitions of a quantum chain with four-spin interactions in longitudinal and transverse magnetic fields. B. BOECHAT, J. FLORECIO, A. SAGUIA, Universidade Federal Fluminense, O. F. DE ALCANTARA BONFIM, University of Portland — We study the ground-state properties of a spin-1/2 model on a chain containing four-spin Ising-like interactions in the presence of both transverse and longitudinal magnetic fields. We use entanglement entropy and finite-size scaling methods to obtain the phase diagrams of the model. Our numerical calculations reveal a rich variety of phases and the existence of multi-critical points in the system. We identify phases with both ferromagnetic and anti-ferromagnetic orderings. We also find periodically modulated orderings formed by a cluster of like-spins followed by another cluster of opposite like-spins. The quantum phases in the model are found to be separated by either first or second order transition lines.

H1.00161 Quantum criticality in a magnetic chain with two- and four-spin interactions in a transverse field. O. F. DE ALCANTARA BONFIM, University of Portland, A. SAGUIA, B. BOECHAT, J. FLORECIO, Universidade Federal Fluminense — We use entanglement entropy and finite-size scaling methods to investigate the ground-state properties of a spin-1/2 Ising chain with two-spin ($J_1$) and four-spin ($J_2$) interactions in a transverse magnetic field ($B$). We concentrate our study on the unexplored critical region $B = 1$ and obtain the phase diagram of the model in the ($J_1$, $J_2$) plane. The phases found include ferromagnetic (F), antiferromagnetic (AF), as well as more complex phases involving spin configurations with multiple periodicity. The system presents both first and second order transitions separated by tricritical points. We find an unusual phase boundary on the semi-infinite segment ($J_4 < -1$, $J_2 = 0$) separating the F and AF phases.

H1.00162 Unusual Phase Transitions in Single Crystals of Gd$_{3}$Si$_{1-x}$Ge$_{2}$ and Gd$_{3}$Si$_{1-x}$Ge$_{2}$6.1 R.L. HADIMANI, Iowa State Univ, Y. MELIKHOV, Polish Academy of Science, D.L. SCHLAGEL, T.A. LOGRASSO, K.W. DENNIS, R.W. MCCALLUM, Ames Laboratory, US Dept. of Energy, D.C. JILES, Iowa State Univ, IOWA STATE UNIVERSITY COLLABORATION, POLISH ACADEMY OF SCIENCE COLLABORATION, AMES LABORATORY, US DEPT. OF ENERGY COLLABORATION — Gd$_{3}(Si_{1-x}Ge_{x})$ has been widely studied over the composition range 0.41 $< x <$ 0.51 where the coupled magnetic and structural first order phase transitions occur close to room temperature. It has a mixed phase region in the phase diagram with both orthorhombic I and orthorhobic II phases for compositions 0.32 $< x <$ 0.41. Previously we have used modified Arrott plots to determine the second order phase transition temperature when it is suppressed by the first order phase transition in samples with compositions $x < 0.51$. We also used these modified Arrott plots on the mixed phase composition of Gd$_{3}Si_{1-x}Ge_{2}$ ($x = 0.375$) to determine the second order phase temperatures of both the monoclinic and the orthorhobic II phases. We have now investigated two more single crystals of Gd$_{3}Si_{1-x}Ge_{2}$ and Gd$_{3}Si_{1-x}Ge_{2}$6, whose compositions fall in the mixed phase region of orthorhombic I and orthorhobic II phases. The temperature above which the low temperature quantum oscillations of the samples were estimated to be 383 K for Gd$_{3}Si_{1-x}Ge_{2}$ and 365 K for Gd$_{3}Si_{1-x}Ge_{2}$6. These temperatures are much higher than the expected second order phase transition temperature of orthorhobic II phase (280 K). This may be due to the presence of the orthorhombic I phase in larger volume fraction.
H1.00163 Evidence for a magnetic metallic R phase in Vanadium dioxide VO$_2$, HUI XING, PAYAM TAHERI, PEIHONG ZHANG, HAO ZENG, Department of Physics, The State University of New York at Buffalo — Vanadium dioxide VO$_2$ has garnered extensive research interests for over decades due to its metal-insulator transition (MIT) around 340 K (Ref. 1). Much is known for the physics behind the MIT (including a correlated structural transition and the involvement of several intermediate states). On the other hand, the magnetic property across the MIT is much less known. Although there are no fundamental arguments against the possibility of forming local magnetic moments in VO$_2$. So far, only the M2 phase has been confirmed to possess local magnetic moments. However, our temperature-dependent magnetic susceptibility measurements of VO$_2$ show a sudden jump at the MIT. This jump cannot be attributed to a simple Pauli susceptibility from conducting electrons. In a recent paper, we pointed out local magnetic moments may form in the metallic R phase. The formation of local moment would naturally explain the extremely high magnetic susceptibility of VO$_2$ above the phase transition temperature. We further discuss the magnetoresistance (MR) measured across the MIT, which shows different magnitude and field dependence in M1 and R phase, including the MR in the metallic phase suppressed to lower temperature in a VO$_2$ electric double layer transistor device using ionic liquid as gate dielectrics. 1. F. J. Morin, Phys. Rev. Lett. 3, 34 (1959). 2. Xun Yuan et al., Phys. Rev. B 86, 235103 (2012).

H1.00164 Control of proliferation rate of N27 dopaminergic neurons using Transcranial Magnetic Stimulation orientation, YIWEI MENG, RAVI HADIMANI, VELLAREDDY ANANTHARAM, ANUMANATA KANTHASAYAM, DAVID JILES, None — Transcranial magnetic stimulation (TMS) has been used to investigate possible treatments for a variety of neurological disorders. However, the effect that magnetic fields have on neurons has not been well documented in the literature. We have investigated the effect of different orientation of magnetic field generated by TMS coils with a monophasic stimulator on the proliferation rate of N27 neuronal cells cultured in flasks and multi-well plates. The proliferation rate of neurons would increase by exposed horizontally adherent N27 cells to a magnetic field pointing upward through the neuronal proliferation layer compared with the control group. On the other hand, proliferation rate would decrease in cells exposed to a magnetic field pointing downward through the neuronal growth layer compared with the control group. We confirmed results obtained from the Trypan-blue and automatic cell counting methods with those from the CyQuant and MTS cell viability assays. Our findings could have important implications for the preclinical development of TMS treatments of neurological disorders and represents a new method to control the proliferation rate of neuronal cells.

H1.00165 Accurate projected augmented wave (PAW) datasets for rare-earth elements (RE=La-Lu), MEHMET TOPSAKAL, RENATA WENTZCOVITCH, Univ of Minn - Minneapolis — We provide accurate projected augmented wave (PAW) datasets for rare-earth (RE) elements with some suggested Hubbard U values allowing efficient plane-wave calculations. Solid state tests of generated datasets were performed on rare-earth nitrdes. Through density of state (DOS) and equation of state (EoS) comparisons, generated datasets were shown to yield excellent results comparable to highly accurate all-electron full-potential linearized augmented plane-wave+local orbital (FLAPW+LO) calculations. Hubbard U values for trivalent RE ions are determined according to hybrid functional calculations. We believe that these new and open-source PAW datasets will allow further studies on rare-earth materials.

H1.00166 Half-metallic magnetism and the search for better spin valves, KARIN EVERSCHOR-SITTE, MATTHIAS SITTE, ALLAN MACDONALD, Univ of Texas, Austin — We propose a simple formula for the temperature dependence of tunneling magnetoresistance to shed light on ongoing efforts to optimize spin valves. It captures a mechanism in which spin valve performance at finite temperatures is limited by uncorrelated thermal fluctuations of magnetization orientations on opposite sides of a tunnel junction. Furthermore, it directly reveals the advantages for spin-valve optimization by using materials with a high spin polarization of Fermi-level tunneling electrons, and by using materials with high ferromagnetic transition temperatures. We show that our theory is in good agreement with recent experimental studies of the temperature-dependent magnetoresistance of high-quality tunnel junctions with MgO barriers. We conclude that half-metallic ferromagnets can yield better spin-value performance than current elemental transition metal ferromagnet/MgO systems only if their ferromagnetic transition temperatures exceed ~ 900 K.

H1.00167 Nonlinear damping effects in spin torque dynamics of magnetic tunnel junctions, IGOR BARSUKOV, YU-JIN CHEN, HAN KYU LEE, University of California, Irvine, ALEXANDRE CONGALVES, CBPF, Rio de Janeiro, Brazil, JORDAN KATINE, HGST, San Jose, CA, RODRIGO ARIAS, Universidad de Chile, Santiago, Chile, BORIS IVANOV, Academy of Sciences, Kiev, Ukraine, ILYA KRIVOROTOV, University of California, Irvine — Performance of nanoscale spin torque devices such as memory (STT-MRAM) and oscillators critically depends on magnetic relaxation. It is commonly assumed that magnetization dynamics in the presence of spin torque can be understood as simple competition between antidamping arising from spin torque and Gilbert damping of the free layer. However, we have performed nonlocal spin torque measurements in magnetic tunnel junctions (MTJ) and found that the spin torque driven dynamics can strongly depend on the nature of the MTJ nanopillars, for example, whether they are patterned or not. We have performed nonlocal spin torque measurements in magnetic tunnel junctions (MTJ) with in-plane magnetiizations of the free layer and SAF layers by spin torque ferromagnetic resonance. We find an excitation spectrum associated with standing spin waves of the free layer. By varying the external field, the energy of a higher-order spin wave mode increases twice the energy of the main mode. This opens up a nonlinear, resonant relaxation channel, giving rise to a damping increase of approximately 20%. With increasing spin torque provided by a DC bias current, we find that this relaxation channel competes with antidamping in a nonlinear manner, increasingly contributing to and even dominating the relaxation at subcritical currents.

H1.00168 Generation of Spin and Orbital Current in Carbon Nanotubes by Spin-rotation Coupling, MASATO HAMADA, SHUICHI MURAKAMI, Tokyo Institute of Technology — Spin-rotation coupling represents a coupling between the electron spins and mechanical rotations, and may be used for generation of spin currents by mechanical rotation. In our presentation we consider carbon nanotubes, and use one of the phonon modes called a twist mode. This mode gives rise to a rotation around the tube axis and eventually an effective Zeeman field parallel to the axis is generated by spin-rotation coupling. We calculate this generated spin current by solving the spin diffusion equation. We hypothesize that effective orbital magnetic field in the radial direction is generated by the radial magnetic field, and discuss the generated orbital current.

H1.00169 Spin Torque Driven Anti-vortex Dynamics in Patterned Nanomagnets, MUSTAFA METE, AHMET COSKUNER, ALI TAH A HABIBOGlu, VEDET KARAKAS, YELIHA BILAL KALYONCU, AISHA GOKCE, OZHAN OZATAY, Bogazici University, ANNA GIORDANO, MARIO CARPENTIERI, University of Calabria, GIOVANNI FINOCCHIO, University of Messina, FEDERICA CELEGATO, CNR-Institute of Materials for Electronics and Magnetism, PAOLA TIBERTO, Istituto Nazionale di Ricerca Metrologica — Recent studies have shown that unconventional spin configurations in patterned nanomagnets like vortices are potentially applicable to ultrafast memory, rf oscillators and detectors utilizing the static and dynamic response of these structures under external magnetic field and current bias. Due to the difficulties of stabilizing an isolated anti-vortex, there is still much to be explored about the stability and dynamics of this structure. In this study, we report on our investigation of stable anti-vortex formation conditions and the subsequent magnetic field/dc current driven excitations. Permalloy based asteroid geometry devices exhibit anti-vortex nucleation at the center with the application of an in-plane AC demagnetizing field and an out of plane magnetic field. Changes in the stable localization of the spins immediately motivates the characterization of the dynamic response to the application of spin torque from a spin-polarized current as sensed using the anisotropic magnetoresistance effect (AMR). We will present the field and current dependence of the anti-vortex gyration frequency, the bandwidth and power in the asteroid devices. This work allows the evaluation of anti-vortex structures to be utilized in practical on-chip microwave oscillators.
Molecular beam epitaxy (MBE) grown (001)-oriented Cr intriguing compounds in chromium chalcogenides family because of its unusual magnetic and magneto-transport properties. Here we have presented studies of [2] J. Lee et al., Nanotechnology 25, 045604 (2014); T. Tanaka et al., IEEE Transactions on Magnetics 150, 3000503 (2014).

This mechanism behind an unusually large thermal hysteresis ($\Delta T \approx 200$ K) in In$_{1-x}$Mn$_x$Se, which extends up to room temperature, is not completely understood at this time. Typically, thermal hysteresis in most materials has a $\Delta T \approx 20$ K occurring well below room temperature. The host III-V semiconductors themselves are among the best non-linear optical materials.

**H1.00170 Magnetic properties of layered III-VI Diluted Magnetic Semiconductors (DMS)**

**H1.00171 Computational Aspects of Anisotropy Calculations**

**H1.00172 Terbium-Aluminum (TbAl$_2$) Binary Alloy as High Magnetostrictive Material**

**H1.00173 Cold plasma cleaning of SmCo$_5$ nano-flakes prepared by surfactant-assisted Ball-milling**

**H1.00174 Magnetic and magneto-transport studies of MBE grown Cr$_2$Te$_3$ thin films with perpendicular magnetic anisotropy**

**H1.00175 Influence of the magnetic properties and repetitions on the energy product in layered thin film hard soft magnetic nanocomposites**

1. This research was supported by the UNF Terry Presidential Professorship, the Florida Space Grant Consortium, A Purdue U. Academic Reinvestment Program, and by NSF Grant Nos. DMR-07-06593 and DMR-14-29428.

2. Supported by grant # NS-DMR1105380.

3. This work is funded by NRI-SWAN.
Hard magnetic phase evolution in nanocrystalline mechanically milled amorphous Pr$_x$Co$_{2-y}$B powder. CAJETAN NLEBEDIM, Ames Laboratory, U.S. Department of Energy, HUSEYIN UCAR, PARANS PARANTHAMAN, Oak Ridge National Laboratory, U.S. Department of Energy, HUSEYIN UCAR, PARANS PARANTHAMAN, Oak Ridge National Laboratory, U.S. Department of Energy — In this work, the evolution of the structural and magnetic properties of Pr$_x$Co$_{2-y}$B with mechanical milling and heat-treatment is presented. Understanding the phase evolution of magnetic properties in hard magnetic materials is crucial for developing high performance permanent magnets. Mechanical alloying/milling offers a traditional and easily deployable approach to synthesizing nanostructured materials. Nevertheless, such can result in amorphization due to high defect density leading to disorder in atomic arrangement. The crystalline phase can be thermally recovered but requires the understanding of how the properties evolve with temperature, in order to achieve useful hard magnetic properties desired for developing permanent magnets. This work shows how properties such as energy product, coercivity, remanent magnetization, saturation magnetization and Curie temperature evolve when PrCoB alloy transitions from amorphous to crystalline phase. The presentation will also include how different levels of amorphization affect the magnetic properties.

Effect of 3d-metal doping on magnetic properties of Fe$_3$Se$_4$. RENAT SABIRIANOV, NABIL AL-AQTA$SH$, Univ of Nebraska - Omaha, DEBASISH SENGUPTA, CFDRC — Fe$_3$Se$_4$ exhibits large magnetocrystalline anisotropy (MAE) and coercivity up 40kOe. The large anisotropy of Fe$_3$Se$_4$ should be accompanied by large magnetization for permanent magnet applications. The magnetization of Fe$_3$Se$_4$ suffers from antiferromagnetic (AFM) superexchange coupling of Fe across the Se planes. We present density functional theory study of the magnetic properties of Fe$_3$Se$_4$ doped with TM (Co, Cr, Ni and Mn). TM ions doped in Fe sites, Fe$_x$M$_{1-x}$(TM)$_y$Se$_4$ (x = 0.5), to examine a potential increase of the magnetization and Curie temperature of Fe$_3$Se$_4$. We performed screening of the exchange interactions and magnetization modifications upon the substitution of Fe by 3d-transition metals at various Fe sites in the Fe$_3$Se$_4$. We find that the doping of Fe$_3$Se$_4$ with 3d-elements does not remove AFM coupling across layers. The increase in the strength of exchange interactions on doping with Cr should increase the Curie temperature of the system. We compare the results of doped alloy with the ones for Fe$_3$Se$_4$ and the theoretical calculations for Fe$_3$Se$_4$. Cr$_3$Te$_4$ has ferromagnetic coupling and magnetization larger than one possible in Fe$_3$Se$_4$. Magnetization per unit cell is 18.24$\mu_B$. MAE of this material is large (MAE = 1.67 MJ/m$^3$).

Effects of TiN buffer layer on microstructure and magnetic anisotropy of FePt thin films. ZHAOGUO QIU, Department of Physics, University of Texas at Arlington; School of Materials Science and Engineering, South China University of Technology, GUANGBING HAN, Department of Physics, University of Texas at Arlington, DECHANG ZENG, School of Materials Science and Engineering, South China University of Technology, J. PING LIU, Department of Physics, University of Texas at Arlington, UNIVERSITY OF TEXAS AT ARLINGTON COLLABORATION, SOUTH CHINA UNIVERSITY OF TECHNOLOGY COLLABORATION — FePt films were deposited at room temperature on TiN buffer layer followed by annealing. The effects of thickness of the TiN layer on the microstructure and magnetic properties of FePt films were investigated. It was found that TiN layer has significant effects on the magnetic anisotropy of the FePt films. The L1$_0$ phase transformation of the FePt films with TiN layer was more completely than that without a TiN layer. The FePt film with TiN (111) layer of 30nm thickness exhibited out-of-plane anisotropy and enhanced ordering parameter. When the thickness of TiN (111) layer further increased, the coercivity tended to decrease. The anisotropy gradually switched from out-of-plane to in-plane when the annealing temperature was increased to 700 degree. The in-plane coercivity was increased to 9.6 kOe when the thickness of randomly oriented TiN layer was 80nm. The high in-plane coercivity may come from the smooth surface morphology of FePt films induced by the small relaxation of internal stress of the thick TiN layer.

Transient Reflectivity of a Low-Dimensional Quantum Magnet. MICHAEL BISHOP, Natl High Magnetic Field Lab, HAIDONG ZOU, University of Tennessee Knoxville, STEPHEN MCGILL, Natl High Magnetic Field Lab — Frustrated, low-dimensional spin systems have drawn wide interest due to their ability to exhibit novel quantum phenomena such as superconductivity, spin-liquid phases, and gapped spin excitations (e.g. Haldane, Spin-Peierls, etc.). SrCu$_2$BO$_2$$_2$, a close experimental realization of the Shastry-Sutherland model, is a one such quantum system in which the singlet ground state is separated from the excited triplet state by an energy gap (35 K) that can be closed by high magnetic fields (>20 T). Furthermore, high magnetic field magnetization measurements reveal an unusual series of plateaus which occur when the magnetic field-tuned density of states becomes commensurate with the lattice periodicity. We have investigated the coupling of singlet and triplet pairing in SCBO to changes in its electronic structure using transient near-infrared reflectivity measurements. We investigated the temperature and magnetic field dependences of the transient reflectivity, and we will discuss these behaviors and their correlation with dimer spin excitations.

Strong effect of low-dimensional Fe-doped cobalt niobate on a strongly ferrimagnetic system. CAJETAN NLEBEDIM, Ames Laboratory, U.S. Department of Energy, DAVID JILES, Department of Electrical and Computer Engineering, Iowa State University — In this work, the first investigation of the effect of Fe-doped cobalt niobate (CoNb$_2$O$_6$) imbedded in the matrix of a strongly ferrimagnetic cobalt-iron oxide, is presented. The temperature dependence of the magnetic properties and how they change with variations in the concentration of CoNb$_2$O$_6$ is also presented. CoNb$_2$O$_6$ is a prototypical low-dimensional material belonging to the pyrochlore-type AB$_2$O$_6$ systems. Its low-dimensional magnetic characteristics can help in understanding the magnetic properties of higher order systems. It has been investigated for applications in resonators and capacitors. This work shows that the magnetization of the ferrimagnetic phase is strongly affected by the concentration of Co ions in the low-dimensional phase, below 15 K but changes in coercivity with temperature were predominantly due to the ferrimagnetic phase. The systematic variation in the concentration of both phases and the cation ratio in each phase, enable us to understand the variation of the magnetic properties with temperature. This work provides useful insights into tuning the magnetism in strongly magnetic materials with transition metal AB$_2$O$_6$ systems imbedded in their matrices.

Crystallization behavior and recoilless fraction determination of amorphous and nanocrystalline Fe$_{56}$Co$_{24}$Nb$_{14}$Si$_{3}$Cu$_{1}$ system. MONICA SORESCU, JULIA LIMONGELLI, CHRISTOPHER STROH, Duquesne University, KEVIN BYERLY, Spang — Amorphous ferrimagnetic alloy with the composition Fe$_{56}$Co$_{24}$Nb$_{14}$Si$_{3}$Cu$_{1}$ was obtained by rapid quenching from the melt. Samples cut from the ribbons were annealed at 450, 550, 650 and 750 C in a vacuum furnace. 57Fe Mossbauer spectroscopy was used to identify the phases formed based on the refined values of the hyperfine parameters. The as-quenched specimen was analyzed with a hyperfine magnetic field distribution and corresponded to an in-plane orientation of the magnetic moment directions. The sample annealed at 450 C was found to be in a nanocrystalline state due to observation of the (FeCo)-Si alloy with the DO3 structure. The balance of the composition was represented by a metalloid-enriched amorphous grain boundary phase. In contradistinction to this, the samples annealed at 550-750 C were totally crystallized, but the new phases formed were alpha-(FeCo), (FeCo)$_2$(BSi) and (FeCo)$_3$(BSi). The f factor value dropped from 0.6 to 0.37 for the sample annealed at 450 C, consistent with the onset of nanocrystallization in the system. For the completely crystallized specimens, the f factor maintained values close to 0.5. This indicates that the presence of quenched-in stresses may play a role in the ability of samples to undergo recoilless emission and absorption of gamma rays.
H1.00182 Scaling and memory effects in the reentrant spin glass phase of nanostructured Mn$_2$TaS$_5$. **PAUL SHAND, JOHN DANKER, XUN XIAO, TIM KIDD, LAURA STRAUSS**, University of Northern Iowa — We have investigated the nature of the reentrant spin glass phase of nanostructured Mn-intercalated Ta$_2$S$_5$. The sample consisted of bundles of nanoscale fibers with an average atomic concentration of intercalated Mn of 22%. The sample exhibits a ferromagnetic transition at 74 K and a transition to a cluster glass state at 40 K. The ac susceptibility measured in small dc bias fields near the cluster glass transition exhibited scaling behavior, indicating a magnetic-field dependent crossover to glassy dynamics. At temperatures below the cluster-glass transition, the nature of the dynamics was probed by ac susceptibility and zero-field cooled (ZFC) magnetization measurements. Aging and memory effects were observed, consistent with the non-equilibrium dynamics exhibited by glassy magnetic systems. In particular, we probed the ZFC magnetization memory effect as a function of cooling rate, aging time and magnetic field. The behavior is explained in terms of domain growth within the framework of droplet theory.

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H1.00183 Enhanced Tunneling Magneto-resistance in Voltage-controlled CoFeB/MgO Junctions. **HAMD ALMASI, MENG XIU, CHRISTIAN GENTRY, DI YU, TY NEWHOUSE-ILLIGE**, Department of Physics, University of Arizona, Tucson, Arizona 85721, USA, Y.H. LIU, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA, J.W. FREELAND, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA, S.G.E. TE VELTHUIS, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA, WEIGANG WANG, Department of Physics, University of Arizona, Tucson, Arizona 85721, USA — Perpendicular magnetic anisotropy (PMA) at the CoFeB/MgO interface originates from the hybridization of d orbitals of Fe and Co and the Pz orbital of Oxygen. Due to different electronic band structures, the hybridization of the d orbitals of Fe and Co is likely different, therefore contributing unequally to the total PMA. This difference has been probed by an X-ray magnetic circular dichroism (XMCD). The orbital moment of Fe was found to be much larger than that of Co by XMCD. These results demonstrated that Fe contributes most to the PMA at the interface. MTJs with Fe-rich electrodes were fabricated and a substantially larger PMA was achieved. With further optimization in post-growth thermal annealing, we have achieved over 150% TMR in these voltage-controllable CoFeB/MgO MTJs.

3This work was supported in part by NSF (ECCS-1310338) and by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA. Work at ANL was supported by the DOE-BES, MSE and SURF.

H1.00184 Fermi level tuning of highly spin-polarized complex Heusler alloys via materials genome. **SUDIP PANDEY, ABDIEL QUETZ, ANIL ARYAL, MICHAEL FRALAIDE**, Southern IL Univ-Carbondale, TAPAS SAMANTA, Louisiana State University, Baton Rouge, KAMRAN MUNIRA, WILLIAM BUTLER, University of Alabama, Tuscaloosa, IGOR DUBENKO, Southern IL Univ-Carbondale, DIPANJAN MAZUMDAR, SHANE STADLER, Louisiana State University, Baton Rouge, NAUSHAD ALI, Southern IL Univ-Carbondale — Heusler alloys are the largest family of half-metals (100% spin-polarized at the Fermi level) and most promising for spintronic device applications. Many half-metallic full-Heusler alloys are predicted from *ab-initio* calculations, but may or may not be experimentally realizable. Here, we present a novel strategy to utilize these predicted materials to tune the Fermi level of well-known, highly spin-polarized Heusler alloys. We start with the test sample of [Co$_x$MnSi]$_{1-x}$[Co$_x$CrGe]$_{1-x}$, and, by controlling the ratio of these materials, we are able to shift the Fermi level of Co$_x$MnSi. Experimentally, we study the structural and magnetic properties of such Heusler alloys by room temperature X-ray diffraction (XRD) and taking magnetization measurements. It was found that these complex combinations of materials are single phase even though some components (Co$_x$CrGe for example) might not be stable in bulk form alone.

2This work was supported by the Office of Basic Energy Sciences, Material Science Division of the U.S. Department of Energy (DOE Grant No. DE-FG02-06ER46291 and DE-FG02-13ER46946).

H1.00185 Phase Transitions and Magnetocaloric Effects in GdNi$_2$Mn$_x$. **ANIL ARYAL, ABDIEL QUETZ, SUDIP PANDEY**, Southern IL Univ-Carbondale, TAPAS SAMANTA, Louisiana State University, ICOR DUBENKO, Southern IL Univ-Carbondale, SHANE STADLER, Louisiana State University, NAUSHAD ALI, Southern IL Univ-Carbondale — The structural and magnetic properties of the GdNi$_2$Mn$_x$ system (for $x = 0.5, 0.6, 0.8, 1.0, 1.2, 1.4, 1.5$) have been studied by x-ray diffraction and magnetization measurements. A rhombohedral Pn$\overline{3}$m-type structure was observed in the XRD data. A second order magnetic phase transition from ferromagnetic (FM) to paramagnetic (PM) was found, characterized by a long-range exchange interaction as predicted by mean field theory. A magnetic entropy change of $\Delta S_{M} = 3.1$ J/kg K and 2.9 J/kg K for $\Delta H = 5$ T was observed in the vicinity of the Curie temperature ($T_C$) for GdNi$_2$Mn$_{0.8}$ and GdNi$_2$Mn$_{1.4}$ respectively. In spite of the low values of $\Delta S_{M}$, the relative cooling power (RCP) was found to be 176 J/kg for the GdNi$_2$Mn$_{0.8}$ compound.

2This work was supported by the Office of Basic Energy Sciences, Material Science and Engineering Division of the U.S. Department of Energy (USDOE-DE-FG02-06ER46291 and DE-FG02-13ER46946).

H1.00186 Influence of Ga content on structure and anomalous Hall effect of Fe$_{1-x}$Ga$_x$ thin films on GaSb(100). **THI MINH HAI NGUYEN, ANH TUAN DUONG, YOOLEEMI SHIN, VAN QUANG NGUYEN, SUNGLAE CHO**, Univ of Ulsan, Korea — The Fe-Ga alloys have recently attracted great interests because they exhibited ferromagnetic properties with high Curie temperature, high saturation magnetization and unique magnetoresistive properties which are promising to real applications such as actuators, acoustic sensors, torque sensors, and positioning devices in particular for nano and nanoelectromechanical systems and the integrated magnetostriective devices. Recently, electrical spin injection from Fe$_x$Ga$_{0.5}$ produces an electron spin polarization above 70% on GaAs(001). However, the out-of-plane saturation field and magnetization decrease rapidly with Ga content. The Fe$_{1-x}$Ga$_x$ thin films ($x=0.4, 0.5$) have been grown on GaSb(100) substrate using MBE. An epitaxial film with bcc $\alpha$-Fe crystal structure (A2) was observed in Fe$_{0.5}$Ga$_{0.5}$ film, while an impure Fe$_x$Ga phase with DO$_2$ structure appeared in Fe$_{0.3}$Ga$_{0.7}$ film. The saturated magnetizations are $570$emu/cm$^3$ and $180$emu/cm$^3$ and the coercivities are $170$ and $364$Oe at room temperature for Fe$_{0.5}$Ga$_{0.4}$ and Fe$_{0.5}$Ga$_{0.5}$, respectively. A hysteresis trend in Hall resistance vs. magnetic field was observed for Fe$_{0.5}$Ga$_{0.5}$ film. However, there is a weak hysteresis in Fe$_{0.5}$Ga$_{0.6}$ film.
H1.00187 Magnetic Properties of MnFe2Ga Heusler Alloys — AHMED A. ELGENDY, MOHAMMAD SALEHI-FASHAMI, University of Delaware, DAVID SELLMYER, University of Nebraska, GEORGE HADJIPANAYIS, University of Delaware — Recently, MnFe2Ga Heusler alloys have attracted significant attention due to their interesting physical properties such as large magnetic-field-induced strain, giant magnetocaloric effects, large magnetoresistance, and exchange bias behavior [1-2]. These properties make them promising candidates for various practical applications in the field of smart materials, magnetic refrigeration and spintronics. In this work, we prepared MnFe2Ga alloys by melt-spinning and sputtering and studied the structural and magnetic properties. The melt-spun ribbons were prepared with a wheel speed of 30 m/s. The ribbons were annealed at different temperatures for 1 hour and ground to make fine powders. The ground powders were used to make the target that is used in the cluster gun for the fabrication of MnFe2Ga nanoparticles. The structure of the as-made, annealed ribbons, and powders displayed a face-centered-cubic structure. The microstructure of the as-made ribbons showed equiaxed grains with an average size of 3-5 µm while the annealed ribbons showed bigger grains with small particles covering homogeneously their surface. The magnetic properties show an enhancement of magnetization while coercivity remains the same with values M(3T) and HC of 85 emu/g and 150 Oe, respectively. Transmission electron microscopy with elemental mapping is currently underway to determine the structure and composition of the surface nanoparticles. The work was supported by DOE-BES-DMSE (Grant No. DE-FG02-04ER4612).


H1.00188 Growth and Structural Study of Epitaxial NaMnF3 Thin Films on SrTiO3 — AMIT KC, TRENT JOHNSON, PAVEL BORISOV, DAVID LEDERMAN, WWU — Perovskite fluorides (ABF3) exhibit many interesting phenomena, e.g. dipolar and magnetic long-range order superconductivity, as well as magnetoelastic coupling. Recently, G. C. Garcia-Castro et al. predicted that orthorhombically distorted Pnma NaMnF3 perovskite should have a particularly soft ferroelectric mode, and is expected to demonstrate ferroelectric order regardless of elastic strain, despite the competing antiferrodistortive instability. Thus, in combination with weak ferromagnetic order, this material is expected to be multiferroic. Here, we report the growth of epitaxial NaMnF3 thin films on SrTiO3(100) single crystal substrates via Molecular Beam Epitaxy (MBE). Structural qualities of the films were studied as a function of the substrate temperature and film thickness by the techniques of X-ray diffraction (XRD), in-situ reflection high-energy electron diffraction (RHEED), and atomic force microscopy (AFM). The best films were smooth single phase NaMnF3, grown with four in-plane and two out-of-plane twin domains.

H1.00189 Developing Nuclear Magnetic Resonance Force Microscopy (NMRFM) as an Electronic Probe of Nanoscale Condensed Matter Systems — JEREMY W. PASTER, DANIEL M. TENNANT, SHIRIN MOZAF-FARI, JOHN T. MARKERT, Department of Physics, The University of Texas at Austin — The investigation of NMR via magnetic force coupling in a large field gradient has led to vast improvements in spatial resolution over the conventional inductive method. It has been demonstrated that nanoscale force sensors could be scaled to distinguish a single nuclear spin, assuming experimental noise can be minimized and other specious force signatures stifled. Accordingly, there are many efforts aimed at repurposing NMR for 3D imaging on the atomic scale [1]. In addition to proof-of-concept experiments aimed at separately resolving some of the eventual experimental barriers to atomic resolution, some of us have directed our attention to using NMR to probe the electronic environment in larger condensed matter systems which are not well suited for other scanning probe microscopy techniques and which are prohibitively small for inductive NMR detection. Previously, we proposed using NMRFM to probe superconducting transitions in microcrystals. In parallel, we rewound our investigation of thin films [2] to explore two-dimensional conducting interfaces between oxide interfaces. Presented here is a survey of the technical impediments as well as current strategies for unlocking this exciting potential for NMRFM, as a tool to investigate sub-surface electronic transport in microscale and nanoscale condensed matter systems.


H1.00190 Competition between itinerant ferromagnetism and spin-density wave antiferromagnetism in FeGa — YAN WU, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, 70803, HUIBO CAO, Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, 37831, GREGORY MCCANDLES, JULIA CHAN, Department of Chemistry, The University of Texas at Dallas, Richardson, 75080, AMAR KARKI, RONGYING JIN, JOHN DITUSA, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, 70803 — The metallic magnetFeGa displays a rich magnetic behavior that includes transitions between a FM ground state to an AFM intermediate state above 360 K as well as incommensurate spin density wave order between these temperatures. Our refinement of the diffraction data has uncovered the existence of a small non-coplanar moment which may be the origin of our previously discovered topological Hall Effect. Presented here is a survey of the technical impediments as well as current strategies for unlocking this exciting potential for NMRFM, as a tool to investigate sub-surface electronic transport in microscale and nanoscale condensed matter systems.

H1.00191 COMPLEX STRUCTURED MATERIALS INCLUDING GRAPHENE —

H1.00192 Thickness dependence of mechanical properties of free-standing graphene oxide papers — TAO GONG, Advanced Institute of Nano Technology (SAIN), Sungkyunkwan University, DO VAN LAM, Nano Mechatronics, Korea University of Science and Technology, SEJEONG WON, Korea Advanced Institute of Science & Technology, RENLONG LIU, School of Mechanical Engineering, SKKU, HWANGBO YUN, Korea Institute of Machinery & Materials, SANGHYUK Kwon, JINSEONG KIM, School of Mechanical Engineering, SKKU, KE SUN, SANGHYUK Kwon, JINSEONG KIM, School of Mechanical Engineering, SKKU, KE SUN, SAIN, SAIMOON LEE, Nano-Mechanical Systems Research Division, KIMM, CHANGGU LEE, Advanced Institute of Nano Technology, and School of Mechanical Engineering, Sungkyunkwan University, GRAPHENE ENGINEERING LAB TEAM, NANOMECHANICS LAB COLLABORATION — We have characterized thickness dependence of mechanical properties, such as Young's modulus, fracture strength, fracture strain and toughness, of graphene oxide papers using tensile and bulge test methods. The GO papers were made from Hummer's method and the fabricated GO paper's thickness varied from 0.1 ~ 100 µm. The measured Young's modulus and fracture strength decreased with increasing thickness ranging from 44.6 ~ 8.5 GPa and 170.2 ~ 40MPa respectively. Through TEM, SEM and AFM characterization, the inner structure and surface morphology such as crack formation and roughness change are the keys to the variation of mechanical properties in the GO papers by the thickness. The thicker GO papers are weaker because it has more manufacturing voids in it that cause it to fail easily and less stiff. Surface wrinkle and residual stress are the mechanism of terraced fracture strain.

H1.00193 ABSTRACT WITHDRAWN —
H1.00194 Transition metals-graphene interaction: the role of the screened van der Waals energy. ALBERTO AMBROSETTI, PIER LUIGI SILVESTRELLI, Università degli Studi di Padova — The interaction of graphene with transition metals is of particular interest for practical applications, which include for instance the efficient production of high-quality graphene. The accurate theoretical description of transition metals-graphene interfaces, however, is a particularly challenging problem due to the complex interplay between van der Waals (vdW) and hybridization effects. Here we apply the DFT/vdW-WF2s method [1], which allows to augment semi-local Density Functional Theory through the introduction of screened vdw interactions. Notably, we find that a reliable modeling of the van der Waals interaction should account for complex metal screening effects, that are due to the combined contributions of the p- and s-like quasi-free electrons, and the more localized d-states. The resulting geometry and energetic properties are in good agreement with experimental data and sophisticates theoretical calculations. Moreover, the Maximally Localized Wannier Functions underlying the DFT/vdW-WF2s method allow for an intuitive understanding of the complex binding mechanism.


H1.00195 Synthesis of carbon nano-structures using organic-molecule intercalated taeniolite layered silicates. TAKAAKI MAEZUMI, NOBORU WADA, Toyo University, Japan — By calcining organic-molecule intercalated taeniolite layered silicates, carbon nano-structures were made between the 2:1 layered silicate sheets. Raman scattering, XRD, TGA and SEM were used to characterize the samples. Large taeniolite crystals (NaLiMg2Si2O10(F) were first prepared by melting appropriate chemicals at high temperatures using a platinum crucible. Then, the taeniolite crystals made were cation-exchanged with Li\textsuperscript{+}, K\textsuperscript{+}, NH\textsubscript{4}\textsuperscript{+}, Ca\textsuperscript{2+} and Mg\textsuperscript{2+} in salt solution. Finally, various organic molecules such as ethylene glycol, pyridine and so on were intercalated into the taeniolite crystals, and calcinated under a N\textsubscript{2} atmosphere at about 1000K. The resulting crystals are usually gray or black. X-ray (001) diffraction spectra which exhibited a sharp G-band peak with a high G-band/D-band ratio indicated that the carbon structures were relatively well crystallized. Cation and organic-molecule dependence on the carbon structures will be discussed. In addition, evidence for stage-2 taeniolite will be presented.

H1.00196 A first principles study on CVD graphene growth on copper surfaces: C-C bonding reactions at graphene edges. NOBUO TAJIMA, TOMOAKI KANEKO, JUN NARA, National Institute for Materials Science, Materials Research Consortium for Energy Efficient Electronic Devices (MARCEED), OHNO TAKAHISA, National Institute for Materials Science, Materials Research Consortium for Energy Efficient Electronic Devices (MARCEED). University of Tokyo — Graphene has attracted considerable research interest owing to its potential applications in electronics and photonics. Here, molecular dynamics simulations are performed to study frictional behaviors of atomic force microscope tip and substrate on graphene. The sub-peaks (i.e., low and high frequency components) in the Raman spectrum of graphene substituted with B, N and BN. The dielectric function and hence the absorption spectrum of single layer graphene sheet have been calculated. Ab-initio calculations based on density functional theory (DFT) have been performed to study the changes in the absorption spectrum of graphene substituted with B, N and BN. The dielectric function and hence the absorption spectrum of single layer graphene sheet have been calculated. The present study can be concluded as, the individual B and N doping does not significantly affect the imaginary dielectric function and hence the absorption spectrum. However, red shift in the absorption towards visible range of the radiation at high doping is found to occur in case of B/N co-doping at high doping concentration. It can be inferred that the graphene can alter the optical properties of graphene to make it reflect in the visible region.

H1.00199 Molecular dynamics simulation of graphene friction: the interplay of tip, graphene and substrate. MINWOONG JOE, CHANGGU LEE, Sungkyunkwan Univ — Graphene is a promising future platform material that could be harnessed in wealth of new applications by virtue of its superior electronic and mechanical properties. Also, atomically thin graphene provides an ideal testbed for investigating fundamental aspects of nanoscale friction. Here, molecular dynamics simulations are performed to study frictional behaviors of atomic force microscope tip on graphene. The effects of tip crystallinity, scan direction (or graphene orientation), and graphene thickness are examined. Puckering hypothesis is revisited with comparison by rigid-supported/suspended graphene cases. Our studies provide broader perspectives into the friction mechanism on graphene.

H1.00200 Effect of Ar Overpressure Ratio on the Growth of Graphene on Cu(111)\textsuperscript{2}. HEIKE GEISLER, SEAMUS MURRAY, SUNY College at Oneonta, ENG WEN ONG, TYLER MOWLL, University at Albany-SUNY, PARUL TYAGI, Global Foundaries, CARL A. VENTRICE, JR., SUNY Polytechnic Institute — A graphene growth study was performed on Cu(111) in a UHV chamber by CVD using ethylene. The sample holder consisted of an oxygen series button heater with Ta heat shields to allow annealing the crystal to 900 °C at pressures as high as 100 mTorr. The crystal structure of the surface was determined using LEED. Growth attempts on the clean Cu(111) surface at ethylene pressures as high as 5 mTorr only resulted in broad diffraction arcs out of phase with the substrate. Therefore, the carbon deposition rate, which depends on the ethylene partial pressure, was increased by using an Ar atmosphere at about 1000K. The resulting crystals were first prepared by melting appropriate chemicals at high temperatures using a platinum crucible. Growth attempts on the clean Cu(111) surface at ethylene pressures as high as 5 mTorr only resulted in broad diffraction arcs out of phase with the substrate. At 50 mTorr of ethylene and no Ar overpressure, broad diffraction arcs were observed in LEED that were ±15° out of phase with the substrate. The carbon deposition rate, which depends on the ethylene partial pressure, has a large effect on the quality of the graphene film.

\textsuperscript{2} This research was supported by the NSF (DMR-1006411).

H1.00201 Origin of the 2450 cm\textsuperscript{-1} peak (G* band) in the Raman spectrum of graphene. RAKRISHNA PODILA, Clemson University, RAHUL RAO, Honda Research Institute US, MEHMET KARAKAYA, JINGYI ZHU, APPARAO RAO, Clemson University, DEPARTMENT OF PHYSICS AND ASTRONOMY, CLEMSON NANOMATERIALS CENTER, CLEMSON UNIVERSITY TEAM, HONDA RESEARCH INSTITUTE TEAM — Here, we report the Raman studies of mechanically exfoliated and chemical vapor deposited (CVD) pristine, ionirradiated, and N-doped graphene (SLG, BLG, and FLG), which identify the origin of the so-called G*-band in graphene ~ 2450 cm\textsuperscript{-1}. Our results show that the asymmetry of the G*-band clearly increases with interlayer stacking, with the high frequency peak exhibiting more sensitivity to intralayer defects compared to the lower component. The sub-peaks (i.e., low and high frequency components) in the G*band were observed to merge with increasing excitation energy and could be understood in terms of the energy dependent scattering rates of photo-excited carriers.
Force-displacement measurements will be presented for these samples. We checked the resistivity values of the graphene sheet which varies with growth conditions. Furthermore, Raman, atomic force microscopy (AFM), I-V and light emitting diodes (OLED) were efforts in progress to replace brittle indium tin oxide (ITO) electrode with a flexible graphene electrode because ITO raw materials are becoming increasingly expensive, and its brittle nature makes it unsuitable for flexible devices. In this work, we grow graphene on Pt and Cu substrates using chemical vapour deposition (CVD) and transferred it to a polymer material (PVA) using lamination technique. We used hydrogen bubbling method for separating graphene from Pt and Cu catalyst to reuse the substrates many times. After successful transfer of graphene on polymer samples, we checked the resistivity values of the graphene sheet which varies with growth conditions. Furthermore, Raman, atomic force microscopy (AFM), I-V and Force-displacement measurements will be presented for these samples.

Non-covalent interactions in the colloidal graphene dispersions, DORSA PARVIZ, Texas A&M Univ, ZINU YU, SRiya DAS, FAHMIDA IRIN, RONALD HEDDEN, Texas Tech Univ, MICAH GREEN, Texas A&M Univ — We have studied stabilization mechanisms in colloidal dispersions of pristine graphene. Electrostatic and steric stabilization in presence of pyrene derivative as dispersants depends on the dispersant concentration, functional groups and the solution pH. The graphene/dispersant yield obtained by pyrene derivatives was considerably higher compared to conventional dispersants. Pyrene-graphene π-π interactions were combined with a designer functional group (polydimethylsiloxane (PDMS)) to synthesize a polymer with dual functionality as dispersant and polymer matrix. The same strategy was applied to produce graphene/polymer and graphene/ PS films. Controllable crumbling of graphene nanosheets was induced through rapid evaporation of dispersion droplets within a spray dryer. Dimensional transition of 2D nanosheets to 3D crumpled particles was directly observed. Multi-faced dimpled morphology of pristine graphene was different than highly wrinkled morphology of crumpled graphene oxide. Changing the compressive forces during drying allowed for controllable folding of the nanosheets, while the unfolding of the redispersed crumpled particles was controlled by the solvent choice.

Surface plasmons in doped graphene excited by the Attenuated Total Reflection technique in the THz regime, F. RAMOS-MENDIETA, Departamento de Investigacion en Fisica, Universidad de Sonora, Hermosillo, Sonora, Mexico., J.A. HERNANDEZ-LOPEZ, M. PALOMINO-OVANDO, Facultad de Ciencias Fisico-Matematicas, Benemerita Universidad Autonoma de Puebla, Puebla, Mexico — Surface plasmons of transverse electric (TE) and transverse magnetic (TM) polarization in doped free-standing graphene are numerically investigated at THz frequencies. For detecting these modes sufficient sensitivity of the prism-based Otto configuration is demonstrated. Complete agreement with the TM dispersion relation is found in doped graphene of Fermi level μ = 0.8 eV, perfect absorption due to wave interference is also observed. On the other hand, TE surface plasmons are special surface vibrations without induced surface charge; they are self-sustained oscillations (unique of graphene) that arise in frequency ranges where the imaginary part of the graphene dynamical conductivity is negative. We found that TE plasmons are excited for angles of incidence very close to the critical angle between prism and air, as predicted from their dispersion relation. Reflection profiles and field intensities of these waves are presented for μ = 0.2, 0.3 eV. This work was supported by SESIC Mexico, Promep Grant FOFM-2008 and by CONACyT, Mexico.

Hetero epitaxial graphene on various substrates, GARY HARRIS, HNF-Howard University, GURPREET KAUT, CRAWFORD TAYLOR, Howard University — Large-scale production of graphene is pivotal for the development of graphene-based electronics. These results focus on the synthesis and characterization of graphene layers. Two methods were used to grow graphene films. First, graphene films were epitaxially grown on silicon carbide substrates by thermal decomposition of SiC at high temperature and low pressure. In-house built reactor consisting of induction furnace was used to form epitaxial graphene for electronic applications. Second, chemical vapor deposition method was used for direct graphene synthesis on 3C-SiC with the use of copper as a catalyst. In thermal CVD process, hydrogen and methane gases were used as precursors. Methane acts as a carbon source and annealing and cooling were done hydrogen environment. Different polytypes of silicon carbide (6H-SiC and 3C-SiC) and their crystal orientations were exploited as substrates to form epitaxial graphene. Hetero epitaxial 3C-SiC epilayer was first deposited on Si substrate using chemical vapor deposition technique in cold wall, low pressure, and horizontal CVD reactor. The reactor temperature, argon pressure, flow rate, temperature of the growth substances (propane, silane, hydrogen and argon) was investigated to control the growth of 3C-SiC and silicon sublimation rate. The resulting graphene films were confirmed using Raman spectroscopy. Further, graphene films have been characterized with the tools of atomic force microscopy (AFM) and scanning electron microscopy (SEM). Mobility, electrical resistivity and carrier density measurements were taken using hall measurements.

Graphene oxide membrane for liquid phase organic molecular separation, RENLONG LIU, GIRISH ARABALE, JINSEON KIM, KE SUN, YONGWOON LEE, CHANGKOOK RYU, CHANGGU LEE, Sungkyunkwan Univ — The selective permeation of organic solvents and water through graphene oxide (GO) membranes has been demonstrated. Water was found to permeate through GO membranes faster than various alcohols. The permeation rates of propanol are about 80 times lower than that of water. Taking advantage of the differences in the permeation rates, we separated water from the alcohol and obtained alcohols with high purity. For ethanol and 1-propanol, binary solutions of the alcohol and water were filtered efficiently to produce alcohols with concentration of about 97%. However, the selectivity of the filtration of methanol is significantly lower than those of the other alcohols. To understand the mechanism we followed the structural changes in the GO membranes by X-Ray diffraction analysis. From the X-ray diffraction results we speculate that the selectivity of the permeation of water and alcohols is closely related to the molecular sizes of the solvents and their polarity. In order to demonstrate the potential applications of this process for the selective removal of water from aqueous organic mixtures, we performed the separation of water from a bio-oil containing 73% of water. The majority of the water was filtered out resulting in a higher purity bio-oil.

Magneto-electronic and optical properties of transition metal dicalcogenide monolayers, YEN-HUNG HO, Physics, National Tsing Hua University, Taiwan, CHIH-WEI CHIU, MING-FA LIN, Physics, National Cheng Kung University, Taiwan, WU-PEI SU, Physics and Texas Center for Superconductivity, University of Houston, TX — A generalized tight-binding model is utilized to study the Landau level spectra of various transition metal dicalcogenide monolayers. The intrinsic spin-orbit coupling effectively gives rise to multiple splitting of Landau levels. With a close inspection of wavefunction characteristics, these levels can be classified into specific groups in terms of their orbital, spin and valley signatures. In the calculation of magneto-absorption spectra, the physical origins of optical selection rules are clearly resolved. Compounds are different from one another in terms of transition energies and appearance of twin peaks. Our numerical results clearly demonstrate the magnetic control of spin and valley charge carriers and provide a basis for future experiments.
H1.00208 Understanding the optical and electronic properties of Ga-doped graphene\textsuperscript{1}. N. C. CREANGE, C. CONSTANTIN, Department of Physics and Astronomy, James Madison University, J.-X. ZHU, Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, A.V. BALATSKY, Institute for Materials Science, Los Alamos National Laboratory, J. T. HARALDSEN, Department of Physics and Astronomy, James Madison University — We simulate the optical and electrical responses in gallium-doped graphene, using density functional theory with a local density approximation. We show the effects of impurity doping (0-3.91\%) in the graphene sheet and for each doping percentage the change in electron density, refractive index, and optical conductivity are reported. Here, gallium atoms are placed randomly (using a 5-point average) throughout a 128-atom sheet of graphene. These calculations demonstrate the effects of hole doping due to direct atomic substitution, where we find a disruption in the electron density for small doping levels, which is due to impurity scattering of the electrons. However, there seems to be a doping percentage, above which we have calculated, at which the system transitions to produce metallic or semi-metallic behavior. These calculations are compared to a purely theoretical 100\% sheet for comparison of conductivity. Furthermore, we examine the change in the electronic band structure and density of states, where the introduction of gallium electronic bands produces a shift in the electron bands and dissolves the characteristic Dirac cone within graphene.

\textsuperscript{1}We acknowledge support from the Center for Integrated Nanotechnologies User Program and the Institute for Materials Science.

H1.00209 Van der Waals Epitaxy of Two-Dimensional $\alpha$-MoO$_3$ Nanosheets using Mica as Grown Templates\textsuperscript{1}. WANG DI, ZHOU YU, WANG MU, PENG RUWEN, XIONG XIANG, Nanjing University — The orthorhombic Molybdenum trioxide, $\alpha$-MoO$_3$, is one kind of graphene-like layered materials. Since the great promise for future electronic and optoelectronic application, this molybdenum-based two-dimensional (2D) layer material has recently attracted much attention. In this work, we report a Van der Waals epitaxy of $\alpha$-MoO$_3$ nanosheets on mica substrate under ambient pressure. This simple physical vapor-phase deposition process is proposed to mediate through the weak Van der Waals interaction between layered $\alpha$-MoO$_3$ and mica substrate. As a result, the grown $\alpha$-MoO$_3$ nanosheets, whose lateral dimension is up to 0.1mm and thickness less than 2.8 nm (about bilayer MoO$_3$ octahedral structure), exhibit defined lattice orientation. From bulk to bilayer, Raman spectra of $\alpha$-MoO$_3$ nanosheets show independent with layered number, which unlike to MoO$_3$ nanosheets. The measurement of electric resistances at room temperature shows the conductance of original $\alpha$-MoO$_3$ nanosheets is already high, moreover, which can be greatly improved by hydrogen doping. Our works indicate that VDWE with mica templates is a simple and feasible strategy to grow high-quality ultrathin $\alpha$-MoO$_3$ nanosheets, which have superiorities for investigating its novel physical properties and potential application in future.

\textsuperscript{1}National Natural Science Foundation of China (Grant Nos. 15132268); National Natural Science Foundation of China (Grant Nos. 15472123)

H1.00210 Photoluminescence Quenching in Single-Layer MoS$_2$ via Oxygen Plasma Treatment, NARAE KANG, HARI P. PAUDEL, MICHAEL N. LEUENBERGER, LAURENE TETARD, SAIFUL I. KHONDAKER, NanoScience and Technology Center and Department of Physics, University of Central Florida — Ultrathin two-dimensional (2D) layer transition dichalcogenides (TMDs) families have emerged as a new class of semiconducting candidates due to its intrinsic bandgap. The ability to control the properties of 2D TMDs will become a key in the development of future electronic and optoelectronic applications; however, altering the properties via creating and manipulating defects through external control is not fully investigated yet. In this work, we studied tunable optical properties of single-layer (SL) MoS$_2$, by applying time-dependent oxygen plasma exposure. As the exposure time increased, the strong photoluminescence (PL) of SL MoS$_2$ changed to complete quenching accompanied by clear changes in Raman spectra with gradual reduction of MoS$_2$ peaks as well as an appearance of oxidation-induced peak of Mo-O bonds formation. Using band structure calculations, we found that the creation of Mo-O$_x$ disordered-domains led to plasma-induced direct-to-indirect bandgap transition in defected SL MoS$_2$, resulting in PL quenching with lattice distortion. Our results suggest new opportunities of tailoring and understanding the properties of 2D TMDs.

H1.00211 Scanning Photocurrent Microscopy on Single-Layer CVD MoS$_2$, MoSe$_2$, and Alloys, EDWIN PRECIADO, VELVEL KLEE, DAVID BARROSO, Univ of California - Riverside, KRISTOPHER ERICKSON, Sandia NL, MARK TRIPLETT, Univ of California - Davis, ARIANA NGUYEN, CHRIS LEE, HSU LU, SARAH BOBEK, JOHN MANN, Univ of California - Riverside, ALEC TALIN, FRANCOIS LEONARD, Sandia NL, LUDWIG BARTELS, Univ of California - Riverside — We report scanning photocurrent measurements on CVD-grown single-layer films of MoS$_2$, MoSe$_2$, and MoS$_2$-(1-x)Se$_x$. Measurements of electric resistances at room temperature shows the conductance of original $\alpha$-MoO$_3$ nanosheets is already high, moreover, which can be greatly improved by hydrogen doping. Our works indicate that VDWE with mica templates is a simple and feasible strategy to grow high-quality ultrathin $\alpha$-MoO$_3$ nanosheets, which have superiorities for investigating its novel physical properties and potential application in future.

H1.00212 Lateral hydrogenated graphene/h-BN Tunneling Magnetoresistance Devices, SHAYAN HEMMATIYAN, CRISTIAN CERNOV, ARTEM ABANOV, Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA, MARCO POLINI, NEST, Istituto Nanoscience - CNR and Scuola Normale Superiore, I-56126 Pisa, Italy, ALLAN H. MACDONALD, Department of Physics, University of Texas at Austin, Austin, Texas 78712-1081, USA, JAIRIO SINOVA, Institut für Physik, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Germany — Based upon first principle calculations, we propose a practical heterostructure of hydrogenated graphene on the top of hexagonal-boron nitride, which exhibits ferromagnetic properties and relatively large spin orbit coupling. We propose to use this functional substrate for the lateral spin valve systems.

H1.00213 The Optical Properties of Germanane, PATRICK ODENTHAL, WALID AMAMOU, DANTE O’HARA, Univ of California - Riverside, LUYI YANG, W. D. RICE, SCOTT CROOKER, National Magnetic Field Laboratory, Los Alamos National Laboratory, ROLAND KAWAKAMI, Univ of California - Riverside, The Ohio State University — Hydrogenated 2D germanium, known as germanane (GeH), is predicted to be a direct bandgap semiconductor with high electron mobility (\$10^4$ cm$^2$/Vs) and circularly polarized optical selection rules. However, very little experimental work on the optical properties of germanane has been reported to date. Here, we present temperature-dependent photoluminescence (PL) and photoluminescence excitation spectroscopy (PLE) data on several-layer germanane grown by Molecular Beam Epitaxy (MBE). We observe a broad PL band that is Stokes-shifted by hundreds of meV below the predicted direct bandgap of 1.53 eV. The PL intensity increases by several orders of magnitude upon decreasing the temperature from room temperature to 4K.

H1.00214 Adsorption of Fluorine on single layer MoS$_2$: a first principles study\textsuperscript{1}. CONRAD TROHA, DUY LE, TALAT S. RAHMAN, Department of Physics, University of Central Florida — One of the effective methods for tuning properties of single layer MoS$_2$ is to impose interactions with adsorbates. Using density functional theory, with the optB88-vdW exchange correlation functional, we have studied the adsorption of fluorine atoms on a single layer MoS$_2$. We find that fluorine atoms prefer to adsorb on top of sulfur atoms in $(2 \times 2)$, $(3 \times 3)$, and $(4 \times 4)$ overlayer structures and that at 1/9 ML or smaller coverage, the interactions between fluorine atoms are small and can be ignored. The band structures of the considered overlayer structures suggest that the adsorption of fluorine atoms introduces defect state inside the band-gap of MoS$_2$. This state disperses near the Fermi level in the $(2 \times 2)$ overlayer structure and is dispersionless in the $(3 \times 3)$ or larger overlayer structures.

\textsuperscript{1}Work supported in part by DOE Grant DE-FG02-07ER15842.
Carrier lifetimes are measured at different pump fluences, from which we propose possible carrier relaxation mechanisms. In suspended bulk MoS\textsubscript{2} pressure for different pump fluences. Both a fast and a slow carrier lifetime are acquired in monolayer MoS\textsubscript{2} which makes it a promising candidate for future photonic and field-effect transistor (FET) applications. Our ultrafast measurement utilizes optical 400nm-pump acoustic phonons with a peak frequency around 38GHz are observed. Phonon lifetime and amplitude at different pump fluences have also been investigated.

H1.00223 Hydrogen Molecule Adsorption on a Borophene-Titanium System.

GREGORIO RUIZ-CHAVARRIA, Universidad Autonoma Chapingo — From the synthesis of graphene have developed a wide range of researchs on their use, both theoretical and experimental. So there have been research on graphene-based electronics, but also on issues of energy, particularly hydrogen adsorption on graphene-based systems. Given the potential represented by these structures is very natural to wonder about similar structures, but based in elements near carbon. One of the lines developed very recently consider the boron as the element to build graphene-like structures. Different studies, both theoretical and experimental have been made where the studied structures are graphene type or fullerene, where boron is used in place of carbon. We will use as a starting point the proposed structures by Xiaoao[1] and Tang[2]. This structure is known as the borophene, which in first place will be decorated with titanium and then, this system interact with hydrogen molecule. In our calculation we use functional density theory, atomic pseudopotentials, Born approximation and molecular dynamic.


H1.00224 Transport Properties Across Misoriented Bilayer MoS2 using Ab-initio Calculations.

KUAN ZHOU, SUPENG GE, DARSHANA WICKRAMARATNE, ROGER LAKE, Univ of California - Riverside — Fabrication of electrical and opto-electronic devices with vertically stacked transition metal dichalcogenides (TMDCs), leads to interfaces that are misoriented. Prior experimental and theoretical studies of misorientation in graphene bilayers demonstrated that a few degrees of misorientation is sufficient to decouple the low energy states of the individual layers. Experimental and ab-initio calculations have shown the bandgap of misoriented bilayer MoSremains indirect. The transport properties across the misoriented interface of the bilayer TMDCs is currently unknown. The coherent interlayer transmission across two stacks of MoSis calculated for unrotated and rotated MoSbilateral layers using ab-initio calculations. The energy dependence of the interlayer transmission is analyzed.

H1.00225 Fluorinated graphene as an efficient diffusion barrier in Ge semiconductor devices.

WEI REN, HENG GAO, Shanghai University — We evaluate the efficient diffusion barrier effects of the fluorinated graphene from the first principles. By taking its advantage of impermeability, we discover such monoatomic layer can suppress the formation of the unstable interfacial oxide in Ge-based semiconductor devices. To elucidate the physical mechanism governing this shielding functionality, nudged elastic band method is adopted to calculate the barrier height of one oxygen or one germanium atom penetrating the pristine graphene and fluorinated graphene. The energy of the adsorbed O or Ge atom on different sites of the graphene is calculated, namely three positions on the honeycomb lattice, bridge, hollow, and top. Our results reveal that both the O and Ge atoms adsorbed on the graphene are most stable on the bridge site, followed by the top and hollow sites with higher energies. Different penetration paths of O and Ge atoms are considered, and the calculated values of the energy barriers for both graphene and fluorinated graphene exhibit superior impermeability and hence to hinder diffusion of O and Ge atoms across the graphene and fluorinated graphene. This latter insulating structure is expected to expedite the implementation of germanium as channel materials in next-generation nanoelectronic devices.

H1.00226 Fabrication of graphene field-effect transistor on top of ferroelectric single-crystal substrate.

NAHEE PARK, HAEYONG KANG, YOURACK LEE, JEONG-CYUN KIM, JOONG-CYU KIM, YOOJOO YUN, JEONGMIN PARK, TAESOO KIM, JUNG HO KIM, YOUNG SEON SHIN, YOUNG HEE LEE, DONGSEOK SUH, Center for Integrated Nanostructure Physics (CINAP/IBS) and Dept. of Energy Science (DOES), Sungkyunkwan University — In the analysis of Graphene field-effect transistor, the substrate material which has the direct contact with Graphene layer plays an important in the device performance. In this presentation, we have tested PMN-PT(1-x)Pb(Mg1/3Nb2/3)O3-xPbTiO3 substrate as a gate dielectric of Graphene field-effect transistor. Unlike the case of previously used substrates such as silicon oxide or hexagonal Boron-Nitride(h-BN), the PMN-PT substrate can induce giant amount of surface charge that is directly injected to the attached Graphene layer due to its ferroelectric property. And the hysteresis of polarization versus electric field of PMN-PT can cause the device to show the ferroelectric nonvolatile memory. This latter insulating structure is expected to expedite the implementation of graphene-based devices. To elucidate the physical mechanism governing this shielding functionality, nudged elastic band method is adopted to calculate the barrier height of one oxygen or one germanium atom penetrating the pristine graphene and fluorinated graphene. The energy of the adsorbed O or Ge atom on different sites of the graphene is calculated, namely three positions on the honeycomb lattice, bridge, hollow, and top. Our results reveal that both the O and Ge atoms adsorbed on the graphene are most stable on the bridge site, followed by the top and hollow sites with higher energies. Different penetration paths of O and Ge atoms are considered, and the calculated values of the energy barriers for both graphene and fluorinated graphene exhibit superior impermeability and hence to hinder diffusion of O and Ge atoms across the graphene and fluorinated graphene. This latter insulating structure is expected to expedite the implementation of graphene-based devices. To elucidate the physical mechanism governing this shielding functionality, nudged elastic band method is adopted to calculate the barrier height of one oxygen or one germanium atom penetrating the pristine graphene and fluorinated graphene. The energy of the adsorbed O or Ge atom on different sites of the graphene is calculated, namely three positions on the honeycomb lattice, bridge, hollow, and top. Our results reveal that both the O and Ge atoms adsorbed on the graphene are most stable on the bridge site, followed by the top and hollow sites with higher energies. Different penetration paths of O and Ge atoms are considered, and the calculated values of the energy barriers for both graphene and fluorinated graphene exhibit superior impermeability and hence to hinder diffusion of O and Ge atoms across the graphene and fluorinated graphene. This latter insulating structure is expected to expedite the implementation of graphene-based devices. To elucidate the physical mechanism governing this shielding functionality, nudged elastic band method is adopted to calculate the barrier height of one oxygen or one germanium atom penetrating the pristine graphene and fluorinated graphene. The energy of the adsorbed O or Ge atom on different sites of the graphene is calculated, namely three positions on the honeycomb lattice, bridge, hollow, and top. Our results reveal that both the O and Ge atoms adsorbed on the graphene are most stable on the bridge site, followed by the top and hollow sites with higher energies. Different penetration paths of O and Ge atoms are considered, and the calculated values of the energy barriers for both graphene and fluorinated graphene exhibit superior impermeability and hence to hinder diffusion of O and Ge atoms across the graphene and fluorinated graphene. This latter insulating structure is expected to expedite the implementation of graphene-based devices.

H1.00227 Study of quantum capacitance in N doped few layer graphene.

MEHMET KARAKAYA, JINGYI ZHU, RAMAKRISHNA PODILA, Clemson University, ANURAG SRIVASTAVA, IIITM- Gwalior, Madhya Pradesh, India, APPARAO RAO, Clemson University, DEPARTMENT OF PHYSICS AND ASTRONOMY, CLEMSON NANOMATERIALS CENTER, CLEMSON UNIVERSITY TEAM, IIITM- GWALIOR, MADHYA PRADESH, INDIA TEAM — The intrinsically small density of states at the Fermi level in graphene results in a small serial quantum capacitance CQ, which diminishes the total device capacitance value (Curat) in supercapacitors. In this work, we studied CQ of N doped graphene in pyrrolic(N1), graphitic (N2) and pyridinic (N3) configurations. The observed CQ value for sample N1 was significantly different from samples N2 and N3, as predicted by DFT calculations, thus implying that precisely engineered dopant configurations, rather than concentration, can enhance CQ. Such approaches are pivotal for alleviating the existing bottlenecks in both graphene-based device scaling and supercapacitor electrode limitations.

1NSF-1124733

H1.00228 Effect of adsorbed gases on the G and D’ peaks of the Raman spectrum of graphene.

GINA GREENIDGE, JOSHUA HALPERN, Department of Chemistry, Howard University, Washington, DC 20059 — The ability of graphene to function as a gas sensor for polar molecules has been widely investigated by monitoring the conductivity of graphene near the Dirac point. Here we demonstrate that Raman spectroscopy can also monitor the interaction of these molecules with graphene. Using a Raman microscope we observe measureable changes in the width and position of the G peak, and the intensity of the D’ prime peak upon exposure to water vapor (H2O and D2O). The changes are reversible. Baking the material at 350 °C restores the graphene spectrum to its original state. We are investigating the effects of additional gases as well as the relationship of these shifts to the conductivity and the gas-graphene interaction.

1Funding for this research was provided by the Partnership for Reduced Dimensional Materials (PRDM), an NSF Partnership for Research and Education in Materials (PREM) (Award Number DMR-1205608).
H1.00220 Effect of Al$_2$O$_3$ deposition on electronic Transport in Graphene: DFT-NEGF study. TOMOAKI KANEKO, TAKAHIRO OHNO, National Institute for Materials Science, MATERIALS RESEARCH CONSORTIUM FOR EFFICIENT ELECTRONIC DEVICES TEAM, UNIVERSITY OF TOKYO TEAM — In order to screen the charged impurities and to prevent the adsorption of contaminant on graphene, the deposition of high-k materials such as Al$_2$O$_3$ on graphene surface is important issue for graphene device application. Since the interfacial structure of graphene and high-k materials are not identified, theoretical study on the interfacial structure dependence on electronic transport is highly demanded. In this paper, we performed the electronic transport simulation in graphene under Al$_2$O$_3$ based on the density functional theories (DFT) and nonequilibrium Green’s function method (NEGF). We investigated the effect of Al$_2$O$_3$ surface termination on the electronic transport properties. According to the calculation of stability of interfaces and electronic structures, the graphene’s linear band structure is preserved in O$_2$ deficient condition. In O$_2$ rich condition, on the other hand, the graphene’s unique electronic structure is disturbed. These properties are important for the electronic transport in graphene under Al$_2$O$_3$. Graphene shows relatively good transport properties in O$_2$ deficient condition, but transport is considerably suppressed in O$_2$ rich condition. Our results suggest O$_2$ deficient condition is desirable for the device application.

A portion of this research was supported by the grant for “Strategic Programs for Innovative Research” Field No. 4: Industrial Innovations.

H1.00230 Asymmetric capacitance and ambipolar metal insulator transition in black phosphorus. YU SAIITO, YOSHIHIRO IWASA, Quantum-Phase Electronics Center (QPEC) and Department of Applied Physics, The University of Tokyo, Japan — Black phosphorus is a van der Waals type semiconducting layered material with a puckered honeycomb structure where each phosphorus atom is covalently bonded with three adjacent phosphorus atoms and has a direct band gap of 0.3 (bulk) - 2 (monolayer) depending on the number of layers [1], which can be promising material for optoelectronics such as photodetectors. In this presentation, by using ionic liquid gating method, we report the ambipolar transistor operation and the field effect controlled ambipolar metal-insulator transition in black phosphorus thin flake. We observed a large modulation of the sheet resistance by more than 4 orders of magnitude in both electron channel and hole channel. These results suggest black phosphorus will be a key material not only for understanding the physics of the conduction channel produced by ionic gating, but also potential functions including formation of p-n junction and therefore lateral tunnel diode utilizing intrinsic narrow band gap.


H1.00231 Graphene/GaN diodes for ultraviolet and visible photodetectors. FANG LIN, SHAOWEN CHEN, JIE MENG, GEOFFREY TSE, XUEWEN FU, FUJUN XU, BO SHEN, ZHIMIN LIAO, DAPENG YU, Peking Univ, NANOLAB TEAM — The Schottky diodes based on graphene/GaAs interface are fabricated and demonstrated for the dual-wavelength photodetection of ultraviolet (UV) and green lights. The physical mechanisms of the photoelectric response of the diodes with different light wavelengths are different. For UV illumination, the photo-generated carriers lower the Schottky barrier and increase the photocurrent. For green light illumination, as the photon energy is smaller than the bandgap of GaN, the hot electrons are accelerated and contribute to the photoresponse leading up to 0.5 A/W photoresponsivities and high external quantum efficiencies of up to ∼90%. Also, these transistors display fast photoresponsive transient times of several ms, providing an alternative route toward multi-wavelength photodetectors.

H1.00232 Exciton Radiative Lifetimes in Layered Transition Metal Dichalcogenides. MAURIZIA PALUMMO, Department of Physics, University of California, Berkeley, CA 94720, USA, MARCO BENARDI, Department of Physics, University of Rome Tor Vergata, Italy, JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology, MA 02139, USA — Light emission in two-dimensional (2D) transition metal dichalcogenides (TMDs) changes significantly with the number of layers and stacking sequence. While the electronic structure and optical absorption are well understood in 2D-TMDs, much less is known about exciton dynamics and radiative recombination. In this talk, we show first-principles calculations of intrinsic exciton radiative lifetimes at low temperature (4 K) and room temperature (300 K) in TMD monolayers with different chemical formula MX2 (M=W or Mo and X=S or Se), bilayer and bulk MoS2, and in two MX2 hetero-bilayers. Our results elucidate the time scale and microscopic origin of light emission in TMDs, which have been the subjects of recent intense investigation. We find radiative lifetimes of a few ps at low temperature and a few ns at room temperature in the monolayers, and slower radiative recombination in bulk and bilayer than in monolayer MoS2. The MoS2/WS2 and MoSe2/WS2 hetero-bilayers exhibit long-lived (~30 ns at room temperature) inter-layer excitons constituted by electrons localized on the Mo-based and holes on the W-based monolayer; this finding agrees with recent ultrafast spectroscopy experiments. We discuss how the radiative lifetime tunability can be employed to manipulate excitons in 2D-TMDs.

H1.00233 ABSTRACT WITHDRAWN

H1.00234 Photoconductivity spectroscopy of epitaxial germanane devices. ELIZABETH BUSHONG, YUNQIU KELLY LUO, The Ohio State University, JEREMIAH VAN BAREN, WALID AMAMOU, PATRICK O'DENTHAL, DANTE O'HARA, University of California, Riverside, IGOR PINCHUK, JYOTI KATOCH, ADAM AHMED, The Ohio State University, ROLAND KAWAKAMI, The Ohio State University; University of California, Riverside — Germanene, a 2D sheet of hydrogen terminated germanium atoms, has recently generated a great deal of interest. Unlike graphene, which has been the focus of 2D materials for almost a decade, germanene has a direct band gap (~1.5 eV) and strong spin-orbit coupling. Additionally, it is predicted that changing the surface functionalization of germanene will allow tuning of the band gap, which makes it promising for electronic and optoelectronic applications. Here, we investigate wavelength dependent absorption and transport properties of optically excited carriers via photoconductivity on germanane. Samples with thicknesses ranging from several atomic layers up to 250 nm have been studied. We observe an absorption edge as a function of wavelength, as expected for a semiconducting material. There appears to be a small shift to shorter wavelengths for thinner samples. The dependence on intensity and temperature are also investigated, as well as the bias dependence. These results have implications for the use of germanane in future applications.

H1.00235 Planar Nanoscale Capacitors from Laterally Stacked Graphene - Boron Nitride Layers. V. OUNG OZCELİK, ENGIN DURGUN, SALIM CIRACI, Bilkent University — We propose a nanoscale planar capacitor model consisting of laterally stacked two-dimensional insulating BN layers placed between two commensurate and metallic graphene layers. First-principles calculations of structure optimized total energy and self-consistent field potential performed on these nanoscale capacitors for different levels of charging and different number of BN layers indicate the photo-electrical response is not from the area surrounding the electrical contacts. It was found that the three-layer WSe2 FETs display a strong photoresponse, providing an alternative route toward multi-wavelength photodetectors. Using graphene as a transparent electrode, the diodes show a ~ mS photoresponse, using an alternative route toward multi-wavelength photodetectors.

H1.00236 High Photoresponsivity and Extrinsic Quantum Efficiency in Tri-Layer Tunsten Diselenide Phototransistors. ZHENGUANG LU, YOHAN PRADHAN, KOMALAVALLI THIRUVAVUKRASU, JONATHAN LUDWIG, DANIEL RHODES, DMITRY SMIRNOV, LUIS BALICAS, National High Magnetic Field Lab, Florida State University, 1800 E. Paul Dirac Dr. Tallahassee, FL 32310 — We report on the photoresponse properties of three-layer tungsten diselenide field-effect transistors (FETs) fabricated by mechanical exfoliation of bulk crystals on SiO2/substrate connected with Au/Ti contacts. These devices exhibit two-terminal field-effect hole mobilities of about 350 cm2/Vs at 300K increasing up to 500 cm2/Vs at T<50 K. The photoresponse properties were carried out at room temperature using various excitation wavelengths (405nm, 532nm, 670nm). In addition, we mapped photocurrent of this device with a laser spot size considerably smaller than the area of the conducting channel which indicate the photo-electrical response is not from the area surrounding the electrical contacts. It was found that the three-layer WS2 FETs display a strong photocurrent response leading up to 0.5 A/W photoresponsivities and high external quantum efficiencies of up to ~90%. Also, these transistors display fast photoresponsive transient times of several ms.
Study of Charge Density Wave Modulations in the Extended Hubbard Model

SAUMYA BISWAS, ROGER LAKE, University of California Riverside — Charge density wave (CDW) modulations in a two-dimensional lattice are modeled in the mean field approximation using the extended Hubbard Hamiltonian. The electron phonon coupling is included with an on-site interaction term. The effect of coupling strength and Fermi level on the CDW wavelength and amplitude is examined. Periodic and closed boundary conditions are considered. The effect of potential modulation by electrostatic gating on the CDW phase and wavelength is calculated.

Magneto-photoconductivity of atomically thin transition metal dichalcogenides

M. EGÍNGLIGIL, C. ZOU, N. PEIMYÜO, B. CAO, X. SHEN, J. SHANG, C. CONG, T. YU, Nanyang Technological University — Photoinduced effects of two-dimensional (2D) transition metal dichalcogenides (TMDs) are of great interest since the bandgap of these materials corresponds to visible range of spectrum. For instance, in molybdenum disulphide (MoS$_2$) — a 2D semiconductor TMD and a non-centrosymmetric crystal, inherent broken inversion symmetry in monolayers leads to a large spin-orbit interaction which splits the valence band (VB) by 160 meV and gives rise to strong excitonic transitions due to the direct band gap at low energy K and $\bar{K}$ valleys. The same broken inversion symmetry together with time reversal symmetry is responsible for spin-valley coupling in monolayer MoS$_2$ and similar TMDs (such as tungsten disulphide, WS$_2$). Spin-valley coupled band edges in TMDs result in different localization behaviors for different scattering mechanisms. In this work, we present our magneto-photoconductivity studies of mono- and bilayer field-effect transistor devices of MoS$_2$ and WS$_2$, and discuss our results in terms of localization effects.

Lateral MoS$_2$ p-n junctions formed by chemical doping method

WON JONG YOO, MIN SUP CHOI, DESHUN QU, DAELYONG LEE, XIAOCHI LIU, YOUNGDAE JANG, CHANGSI KIM, JUNGJIN RYU, Sungkyunkwan Univ — Interests on transition metal dichalcogenides, especially MoS$_2$, are growing immensely due to its semiconducting nature with visible light range bandgap and strong light absorption property, which can pave the way to replace Si-based electronics and realize flexible and transparent electronics. For more versatile applications and industrialization, however, a proper doping process is required because various devices such as photonics and tunneling devices are composed of p-n junctions. Here, we demonstrated the formation of lateral MoS$_2$ p-n junction by using partially stacked of HBN and p-doping with AuCl$_3$ solution. The fabricated devices showed an ideal rectifying behavior with ideality factor about 1. Under the exposure of monochromatic light, it revealed the properties of conventional p-n diode and also highly efficient photonic properties, showing feasibility to be applied for photovoltaic cells and photodetectors. Furthermore, we fabricated novel tunneling devices with similar device structure where local gates are located under MoS$_2$. Its Fermi level can be effectively controlled by local gate modulation, so that the tunneling current can flow by band-to-band tunneling. This study provides an effective way to realize the practical devices such as photonics and tun

Carbon nanotube networks grown on varios carbon nanostructures: SWCNT, MWCNT and Graphene

YOUNGWOON Kwon, ANVAR ZAKHIDOV, Univ of Texas, Dallas, ALAN G. MACDIARMID NANOTECH INSTITUTE TEAM — Secondary growth of carbon nanotubes (CNT) on the various nanoscale substrates has been performed by using chemical vapor deposition (CVD). Spinnable CNT yarns, single wall CNT sheets and graphene flakes, in NMP have been used as scaffolds for such secondary networks. The CNT yarn drawn from spinnable CNT forest is one of the promising applications of the CNT. However, orientation of the yarn and comparatively high sheet resistance make them harder for applications. Processing secondary CVD grows CNTs on the CNT yarn without any orientation of the secondary grown CNTs. Thus, this decreases the effect of the orientation of the CNT yarn and also decreases sheet resistance since the yarn have more contact each other. This after-treating will make more application possible. Furthermore, since CNT yarn does not make perfect surface and have gap between each bundle, arranging yarns to certain directions allows to growth CNT forest with specific pattern such as check pattern. Also it is possible not to make vertical CNT forest to the substrate by stack multi-layer of CNT yarn so that make felt-like-sheet of CNTs. The secondary growth of CNTs on CNTs, Its Fermi level can be effectively controlled by local gate modulation, so that the tunneling current can flow by band-to-band tunneling. This study provides an effective way to realize the practical devices such as photonics and tun

Structural transition and chemical properties of one dimensional boron ribbons and chains from first principles

MINGJIE LIU, VASILI I. ARTYUKHOV, BORIS I. YAKOBSON, Department of Materials Science and NanoEngineering, Rice University, Houston, TX — The past decade has brought great progress in fabrication and characterization of single-atom chains of carbon (carbyne). Very recently novel atomic chain compositions such as BN and CsI were reported. The extreme and unusual properties of such 1D materials motivate the search for other possible compositions with interesting behaviors. We use first-principles calculations to uncover the rich structural and mechanical properties of 1D boron. While the ground state structure of linear boron is a two-atoms-wide ribbon, tension can unravel it into a single-atom string structure. We analyze the mechanical and electronic properties of these two “phases” and study the thermodynamics and kinetics of transition between them using static first-principles calculations and semiempirical (DFTB) molecular dynamics. The interesting properties of 1D boron nanostructures make them an attractive system for experimental investigations.

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4H1.00237 Study of Charge Density Wave Modulations in the Extended Hubbard Model

H1.00238 Magneto-photoconductivity of atomically thin transition metal dichalcogenides

H1.00239 Lateral MoS$_2$ p-n junctions formed by chemical doping method

H1.00240 ABSTRACT WITHDRAWN

H1.00241 Magneto-resistance of multiwall carbon nanotube Fermat yarn and coil yarn

H1.00242 ABSTRACT WITHDRAWN

H1.00243 Carbon nanotube networks grown on varios carbon nanostructures: SWCNT, MWCNT and Graphene

H1.00244 Structural transition and chemical properties of one dimensional boron ribbons and chains from first principles

1M. Liu et al., ACS Nano 7, 10075 (2013)

H1.00245 Non-covalent functionalization of single wall carbon nanotubes and graphene by a conjugated polymer

JILLIJI JIWIJU, KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia, AYJAMAL ABDURAHMAN, OĞUZ GÜLSEREN, Department of Physics, Bilkent University, 06800 Ankara, Turkey, UDO SCHWINGENSCHÖGL, KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia — We report first-principles calculations on the binding of poly[(9,9-bis-(6-bromohexyl)fluorene-2,7-diy1-co-(benzene-1,4-diy1)] to a (8,0) single wall carbon nanotube (SWCNT) and to graphene. Considering different relative orientations of the subsystems, we find for the generalized gradient approximation (GGA) a non-binding state, whereas the local density approximation (LDA) predicts reasonable binding energies. The results coincide after inclusion of van der Waals (vdW) corrections, which demonstrates a weak interaction between the polymer and SWCNT/graphene, mostly of van der Waals type. Accordingly, the density of states shows essentially no hybridization. The physisorption mechanism explains recent experimental observations and suggests that the conjugated polymer can be used for non-covalent functionalization. (Reference: Appl. Phys. Lett. 105, 013103, 2014)

H1.00246 Design of Inorganic Electrides

YUNWEI ZHANG, HUI WANG, YANCHAO WANG, YANMING MA, State Key Lab of Superhard Materials, Jilin University — Electrides, in which all of or part of the valence electrons occupy interstitial regions in the crystal and behave as anions, have been synthesized at ambient or high-pressure conditions [1]. Their loosely bound anionic electrons make electrides good candidates for electro-active materials. Here, we report a developed methodology to systematically design electrides for given chemical systems. The new approach is based on the swarm-intelligence CALYPSO algorithm on structure prediction [2] and requires only the chemical compositions to predict the electrode phases. In contrast to the traditional ground state structure prediction method where the total energy was solely used as the fitness function, we adopted a new fitness function in combination with the first-principles calculation to select the optimal solutions for a description of given chemical systems. The experimentally known electrides have been successfully reproduced. The results suggested that our approach is reliable and can be widely applied into prediction of new electrodes.


H1.00247 Monte Carlo(MC) simulation study on ammonia anchored TON zeolite for carbon dioxide capture

HANSOL WEE, WONBO LEE, Sogang Univ — If zeolites are modified by ammonia, the electronic effect in ammonia resulted in different surface basicity of the zeolite materials. So, ammonia anchored materials show better adsorption rate of CO2 than pure materials at low pressure. MC simulations for CO2 adsorption were performed at 298K. The results show that, at pressure 1000 kpa CO2 loading is 1.404 mol/kg at ammonia anchored TON, and 0.529 mol/kg at pure TON. However, at high pressure, the ammonia effect becomes marginal. Ammonia anchored TON structures may be used to adsorb CO2 more effective than normal TON structure.

H1.00248 Anisotropic mechanical properties of hexagonal SiC sheet: a molecular dynamics study

MING YU, Univ of Louisville, EMILY LIU, duPont Manual High School, CONGYAN ZHANG, Univ of Louisville — The anisotropic mechanical properties of hexagonal SiC sheet have been studied using an efficient quantum mechanics molecular dynamics scheme based on a robust semi-empirical Hamiltonian (referred as SCED-LCAO) [PRB 74, 15540; PHYSE 42, 2]. It was found that the SiC sheet could sustain the heavy load up to about 20 %. In particular, it was found that the SiC sheet also shows large difference in the strain direction. It will quickly crack after 20 % of strain in armchair the direction, but it will be slowly destroyed after 30% in the zigzag direction, indicating the anisotropic nature of the mechanical properties of the SiC sheet. The nominal and 2D membrane stresses will be analyzed, from which we will obtain the 2D Young’s modulus at infinitesimal strain and the third-order (effective nonlinear) elastic modulus for the SiC sheet. The detail results and discussions will be reported in the presentation.

H1.00249 Towards first-principles based prediction of highly accurate electrochemical Pourbaix diagrams

ZHENHUA ZENG, Purdue University, MARIA CHAN, Argonne National Laboratory, JEFF GREELEY, Purdue University — Electrochemical Pourbaix diagrams lie at the heart of aqueous electrochemical processes and are central to the identification of stable phases of metals for processes ranging from electrocatalysis to corrosion. Even though standard DFT calculations are potentially powerful tools for the prediction of such Pourbaix diagrams, inherent errors in the description of strongly-correlated transition metal (hydr)oxides, together with neglect of weak van der Waals (vdW) interactions, has limited the reliability of the predictions for even the simplest bulk systems; corresponding predictions for more complex alloy or surface structures are even more challenging.

Through introduction of a Hubbard U correction, employment of a state-of-the-art van der Waals functional, and use of pure water as a reference state for the calculations, Pourbaix diagrams are systematically calculated. The strong performance is illustrated on a series of bulk transition metal (Mn, Fe, Co and Ni) hydroxide, oxyhydroxide, binary and ternary oxides where the corresponding thermodynamics of oxidation and reduction can be accurately described with standard errors of less than 0.04 eV in comparison with experiment.

H1.00250 Preferential adsorption positions for an adsorbed Li atom on the layered black phosphorus structures

CONGYAN ZHANG, MING YU, University of Louisville — The preferential adsorption positions for an adsorbed Li atom on the layered black phosphorus were determined by mapping out the total energy as a function of its positions on the layered black phosphorus using the density functional theory based method (referred as VASP) [Phys. Rev. B 48, 13115 (1993)]. Various possible adsorption positions including the top of the bridge, the valley, and the interstitial positions of the puckered layers have been studied. It is found that the adsorption energy strongly depends on these positions with different environment. In particular, the most preferential adsorption positions for an adsorbed Li atom are found at the valleys and the interstitials of the puckered layers. The analysis of structural and electronic properties of the black phosphorus layer with the adsorbed Li atom will be discussed.

H1.00251 Ab initio NMR Confirmed Evolutionary Structure Prediction for Organic Molecular Crystals

CONG-HUY PHAM, International School for Advanced Studies (SISSA), Trieste (Italy), EMINE KUCUKBENLI, Ecole Polytechnique federale de Lausanne (EPFL), Lausanne (Switzerland), STEFANO DE GIRONCOLI, International School for Advanced Studies (SISSA), Trieste (Italy) — Ab initio crystal structure prediction, molecular flexibility and difficulties in addressing the dispersion interaction from first principles [1]. We recently implemented vdW-aware density functionals and demonstrated their success in energy ordering of aminoaicid crystals [2]. In this work, we combine this development with the evolutionary structure prediction method where the total energy is selected as the fitness function, we adopted a new fitness function in combination with the first-principles calculation to select the optimal solutions for a description of organic molecular crystals. We thoroughly assess the applicability of evolutionary structure prediction to address such real world problems. We validate the newly predicted structures with ab initio NMR chemical shift data using second-order referencing for an improved comparison with experiments [4].

H1.00252 Exceptional Optoelectronic Properties of Si-related compounds. Bing Huang, Houlong Zhuang, Min Yoong, ORNL, SU-Huai Wei, NREL, Bobby Sumpter, ORNL — The search of new silicon-related functional compounds are of great interests but still very chalenging. In the last few decades, researchers have heavily studied the structural and electronic properties of silicon in order to improve its optical absorption in the visible light range using analyses of metastable silicon phases, silicon-based alloys, and silicon-based superlattices. In this talk, I will present our recent theoretical efforts on searching and designing new silicon phases, from bulk to two-dimensional (2D) silicon, with exceptional optoelectronic properties. Especially, we find that chemically functionalized 2D silicon and silicon alloys could be the best candidates to create efficient thin-film solar absorbers and silicon-based, white-light-emitting diodes, paving the way for new “green” energy applications.

H1.00253 Maximizing the bandgap of BCN nanoribbons. Raissi Baldez, Paulao Piquini, Alex Schmidt, Universidade Federal de Santa Maria, Marcelo Kuroda, Auburn University — Carbon and boron-nitride based compounds share many electronic and structural features. This fact permits mixed carbon-boron-nitride catalysts to be easily synthesized without significant structural changes. Further, the partially ionic character of the boron-nitrogen bonds allow to modulate the electronics of carbon based materials, introducing a variability that can be used to tune the electronic properties according to the boron and nitrogen contents. Graphene and graphene nanoribbons have emerged as promising materials for electronic applications, due to the high mobility of charge carriers. In this work we use the genetic algorithm approach to search for configurations with variable B, C and N contents that maximize the band gap of BCN nanoribbons. Different stoichiometries are analyzed and the structural patterns that lead to the maximal band gaps are presented.

H1.00254 Pd/W(110) as a highly CO tolerant electrocatalyst for hydrogen oxidation: insight from first principles. Nagendra Dhakal, Sergey Stolbov. University of Central Florida — Platinum perfectly catalyzes hydrogen oxidation reaction on the hydrogen fuel cell anodes. However, it has at least two drawbacks: a) it is too expensive; b) it has a low tolerance to CO poisoning. Pt-Ru bi-functional catalysts are more tolerant to CO, but they are still very expensive. In this work, we performed first-principle studies of stability reactivity of M/W(110) structures, where M=Pd,Ru, Au monolayers. All three systems are found to be stable: formation energy of MLs is significantly higher than cohesive energy of the M-elements. The calculated binding energies of H, H2, OH, CO, and H2O were used to obtain the reaction free energies. Analysis of the free energies suggest that Au-W bonding does not activate sufficiently Au monolayer, whereas Ru/W(110) is still too reactive for the CO removal. Meanwhile, Pd/W(110) is found to catalyze hydrogen oxidation and at the same time to be highly tolerant to the CO poisoning. The latter finding is explained by the fact that CO binds much weaker to Pd on W(110) than to Pt, while the OH binding energy is strong enough to ensure CO oxidation. The obtained results are traced to the electronic structure of the systems.

H1.00255 Electronic and vibrational properties of monolayer and bilayer TaSe2. Mack Adrian Dela Cruz, Jia-an Yan, Department of Physics, Astronomy, Geosciences, Towson University — Distinct from MoS2, two-dimensional atomic crystal of tantalum diselenide (TaSe2) is metallic and exhibits charge-density wave (CDW) transitions. Using density-functional theory, we present a first-principles study of the electronic and vibrational properties of monolayer and bilayer TaSe2 without including the CDW-induced structural distortions. For monolayer 1T-TaSe2, the frequencies of the Raman active modes are 159 cm^-1 (E1g) and 226 cm^-1 (A1g), while the Raman-active modes for monolayer 2H-TaSe2 are at 138 cm^-1 (E1g), 214 cm^-1 (E2g), and 241 cm^-1 (A1g). For bilayer TaSe2, different stackings of monolayer 2H-TaSe2 and 1T-TaSe2 phases have been calculated. Electronic band structures and vibrational properties of four energetically favorable configurations will be presented. Finally, the spin-orbit coupling on the structural and electronic properties will also be discussed.

H1.00256 Density Functional Theory Studies of Li-ion interaction with defected group 14 heteronanotubes and nanosheets. Tichakunda Pasipanodya, Prabath Wanaguru, Raymond Atta-Fynn. University of Texas at Arlington — Nanomaterials show significant promise in enhancing Lithium ion (Li-ion) battery properties. Using density functional theory, we study the binding and diffusion of Li on defected nanotubes and nanosheets of silicon carbide (SiC) and silicon germanium (SiGe). Point and extended defects are considered to fully evaluate the influence of defects on the adsorption and diffusion properties. The trends in the adsorption-induced changes in the geometric and electronic properties will be presented. Furthermore, room temperature ab initio molecular dynamics simulations will be carried out to investigate finite temperature effects on the binding mechanisms and electronic structure.

H1.00257 Ferromagnetism in SrTiO3 Single Crystals Induced by Laser irradiation. Srinivasa Rao Singamaneni, Y.F. Lee, J.T. Prater, A.I. Smirnov, J. Narayan, North Carolina State University — SrTiO3 (STO) is diamagnetic in pristine state, important in emerging field of complex oxide electronics. No attention has been paid to explore the magnetic properties of STO crystal upon laser irradiation/annealing. In this presentation, we demonstrate [1-2] that STO single crystals show ferromagnetic order up to 400 K upon KrF (248 nm) laser irradiation. The high resolution x-ray photo emission spectroscopy (XPS) measurements reveal a strong shift of Sr-, Ti- and O-related peaks. X-ray diffraction (XRD) of laser annealed STO does not reveal a signature of either secondary magnetic or amorphous phases. 300 K X-band (∼ 8.95 GHz) angle-dependent electron paramagnetic resonance (EPR) measurements showed no evidence of additional magnetic peaks up on laser irradiation. XPS and EPR data did not provide a strong evidence of Ti3+ formation upon laser annealing. No differences in the visible 300 K Raman spectra of pristine and laser annealed STO are noticed. Interestingly, the magnetic moment is decreased by almost 10-fold upon oxygen annealing of laser annealed STO, inferring that oxygen vacancies play an important role in establishing the observed ferromagnetism.

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2 Undergraduate

H1.00258 Cross-over from antiferromagnetic to ferromagnetic interface exchange coupling in epitaxial ferromagnetic oxides. Srinivasa Rao Singamaneni, North Carolina State University, John T. Prater, Army Research Office, Jay Narayan, North Carolina State University — Interface magnetism in La0.7Sr0.3MnO3/SrRuO3 (LSMO/SRO) bilayer (BL) has been the subject of great interest in the recent past owing to interesting physics and potential applications. Through a novel approach [1-3], LSMO (131nm)/SRO (45nm) and LSMO (33nm)/SRO (45nm) bilayers have been epitaxially integrated with Si (100). Notably, in the former sample, positive exchange bias is observed –indication of antiferromagnetic exchange coupling and is found to be absent in the later. Interestingly, in the former sample, the cross-over from antiferromagnetic to ferromagnetic interface coupling is noticed by varying the cooling field. We have verified that the coupling is of magnetic origin, not due to electrostatic interaction by inserting a thin (∼ 10nm) SrTiO3 layer between LSMO and SRO. We believe that the formation of interface domain walls and strong interplay among Zeeman, dipole and exchange energies could play a dominant role. Our results would have important implications for the physics of magnetic exchange coupled systems.

H1.00259 Exchange bias study of epitaxial LSMO/Cr2O3 thin film heterostructures integrated on Si(100) 1. SANDHYARANI PUNUGUAPATI, FRANK HUNTE, JAGDISH NARAYAN, North Carolina State University — FM/AFM exchange bias continues to be an interesting phenomenon from both a fundamental physics and an applications point of view. Recent studies of multiferroic materials have also seen a revival of interest in the magnetoelectric (ME) and antiferromagnetic (AFM) material Cr2O3. The study of exchange bias in heterostructures consisting of ferromagnet (FM) and ME thin films provides an additional mechanism of switching the magnetization of the FM by the application of an electric field. La0.75Sr0.3MnO3 (LSMO) is a FM material with TC above room temperature and shows colossal magnetoresistance. We have studied exchange bias in epitaxial thin film heterostructures of LSMO/Cr2O3 grown on C-YSZ/Si(100) by the PLD technique. We present a detailed structural characterization of the films by XRD (20 and 0) and TEM which confirm that the films were grown epitaxially. The heterostructures exhibited exchange bias as measured by SQUID magnetometry. The effects of LSMO deposition conditions, crystal orientation, temperature, and cooling field on the exchange bias will be discussed.

1Part of this research is supported by the National Science Foundation and the Army Research Office

H1.00260 Probing defect ordering in the Curie-Weiss metallic phase of NaxCoO2 1, BEN-LI YOUNG, P.-Y. CHU, J.Y. JUANG, Dept. of Electrophysics, Natl Chiao Tung Univ., G.I. SHU, F.C. CHOU, Center for Condensed Matter Sciences, National Taiwan Univ. — Single crystals of Na2/3CoO2, Na2/9CoO3, and Na2/7CoO2, which are metallic Curie-Weiss paramagnets, have been investigated by nuclear magnetic resonance (NMR) techniques, in order to clarify the Na atomic ordering among these samples. By analyzing the 23Na and 59Co NMR spectra, we confirm that the Na vacancies arrange orderly in Na2/3CoO1.96 and Na2/7CoO2, so that a superlattice structure is formed due to such Na ordering. In addition, the oxygen vacancies in Na2/3CoO1.98 can be located by the NMR spectra. As for the Na2/3CoO2 single crystal, a long-range Na order is not observed.

1This work was supported by NSC 102-2112-M-009-008 and NSC 101-2112-M-009-015-MY2.

H1.00261 Extended X-ray Absorption Fine Structure (EXAFS) Analysis of Vitreous Rare Earth Sodium Phosphates, CHANGHEYON OYO, KANISHKA MARASINGHE, Department of Physics and Astrophysics, University of North Dakota, Grand Forks, ND 58202, CARLO SEGREG, TOMOHIRO SHIBATA, Department of Physics & Center for Synchrotron Radiation Research and Instrumentation, Illinois Institute of Technology, Chicago, IL 60616 — The local structure around rare-earth ions (RE3+) in rare-earth ultraphosphate (REUP) glasses has been studied using RE Li/Na edge (RE = Nd, Er, Dy, and Eu) and K edge (RE = Nd, Pr, Dy, and Eu) extended X-ray absorption fine structure (EXAFS) spectroscopy. (RE2O3)1/3(Na2O)x(P2O5)1-x-y glasses in the compositional range 0<x<0.14 and y+0.3=0.4 were studied. RE-oxygen (RE-O) coordination number decreases from ~10 to ~7.5 with increasing RE-content for Nd, Pr, Eu, and Dy. For Er, RE-O coordination number increases from ~8.7 to ~10 with increasing RE-content. For the first oxygen shell, the RE-O distance ranges between 2.41-2.43 Å, 2.44-2.46 Å, 2.24-2.36 Å, 2.28-2.32 Å, and 2.32-2.36 Å for Nd, Pr, Er, Dy, and EU glasses, respectively. Second shell around RE ions consists of phosphorus atoms, with RE-P distance about 3.0-3.5 Å and coordination number ranging from 1 to 3. The third shell primarily contains oxygen and is at a distance about 4.0-4.1 Å from RE ions.

H1.00262 Extended X-ray Absorption Fine Structure (EXAFS) Analysis of Zirconium-Doped Lithium Silicate / Borate Glass-Ceramics 1, CHANGHEYON OYO, KANISHKA MARASINGHE, Department of Physics and Astrophysics, University of North Dakota, Grand Forks, ND 58202, CARLO SEGREG, Department of Physics & Center for Synchrotron Radiation Research and Instrumentation, Illinois Institute of Technology, Chicago, RICHARD K. BROWN, Materials Science & Engineering, Missouri University of Science & Technology, Rolla, MO 65409 — Results of Zr K-edge Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy analysis of a series of Zr-doped (~3-10 mol% Zr and atomic ratio Li/Si ~0.8) lithium silicate glass ceramics (ZLS) and their parent glasses and a series of Zr-doped (~2-6 mol% Zr and atomic ratio Li/B ~0.25-0.18) lithium borate (ZLB) glasses are presented. Immediate coordination environment of all ZLS samples, i.e. the parent glasses and glass ceramics prepared via two different techniques, are remarkably similar. This observation suggests that zirconium ions may remain in the glass phase during nucleation and crystallization process. In contrast, immediate coordination environment of ZLB glasses appear to change markedly with the Zr concentration. These results also suggest that the structural role of Zr ions in ZLS and ZLB glasses may be significantly different. Details of analysis and results will be presented.

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H1.00263 Direct Calculation of Modal Contributions to Thermal Conductivity via Green-Kubo Modal Analysis, WEI LV, ASEGUEN HENRY, Georgia Inst of Tech — In studying the physics of thermal conductivity, tremendous progress has been made over the last 20 years toward understanding lattice thermal conductivity in crystalline solids. However, most of the existing methods are based on “phonon gas model”, which is the dominant paradigm. It essentially treats vibrations as gas particles, which scatter with each other. This analogy works well for crystals, but it hinges on the assumption that particle velocity being well defined. Because amorphous materials and molecules lack periodicity, it is difficult to define the phonon velocity. We used molecular dynamics simulations and a new formalism for calculating the modal contributions to thermal conductivity to study the amorphous materials, a-Si and a-SiO2. It is the first method that is able to obtain the modal details of phonon transport in amorphous materials including full anharmonicity. This method offers a different perspective on phonon-phonon interactions and allows for direct calculation of phonon contributions to thermal conductivity, which will advance our understanding of the phonon transport mechanism and facilitate heat transfer applications in disordered solids and polymers.

H1.00264 Effect of electron-electron interaction on the conductance plateaus of a quantum wire, YONATAN ABRANYOS, GODFREY GUMBS, Hunter College of the City University of New York, MICHAEL PEPPER, Department of Electronic and Electrical Engineering, University College London, DANHONG HUANG, Air Force Research Laboratory, Space Vehicles Directorate, Kirtland Air Force Base — We present a model which is employed to explain recent experimental results for the conductance in a channel within GaAs/AlGaAs heterostructures.

H1.00265 Direct Calculation of Modal Contributions to Thermal Conductivity via Green-Kubo Modal Analysis
H1.00265 Study of optical properties of titania nanotube arrays by FDTD Method. OOMMAN VARGHESE1, PAWANJIIT KAUR2. University of Houston — Finite Difference Time Domain (FDTD) method is a powerful tool for understanding the propagation of electromagnetic waves through materials. The idea behind FDTD technique is to discretize both in time and space, the Maxwell equations with central difference approximations. The study of interaction between the nanostructured semiconductor materials and light is of high relevance in recent years primarily due to the applications of these materials in solar energy conversion process such as solar photovoltaics and solar photocatalysis. Titania nanotube arrays fabricated by anodic oxidation have already attracted considerable attention due to their unique properties and applications. This material has already demonstrated high light scattering and antireflection properties. To obtain a better understanding of nanotube-light interaction we used opti-FDTD software to study the influence of nanotube growth conditions on the optical properties. Simulations were carried out by defining the material properties and using the Lorenz drude model in 380-700nm range. In this presentation we will detail our findings on the correlation between the nanotube array fabrication conditions and its optical properties.

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H1.00266 The magneto-optical properties of non-uniform graphene nanoribbons1, HSIEH-CHING CHUNG, MING-FA LIN, Natl Cheng Kung Univ — When synthesizing few-layer graphene nanoribbons (GNRs), non-uniform GNRs would be made simultaneously. Recently, the non-uniform GNRs, which is a stack of two GNRs with unequal widths, have been fabricated by mechanically exfoliated from bulk graphite. Some theoretical predictions have been reported, such as gap opening and transport properties. Under the influence of magnetic fields, magnetic quantization takes place and drastically changes the electronic properties. By tuning the geometric configuration, four categories of magneto-electronic spectra are exhibited. (1) The spectrum is mostly contributed by quasi-Landau levels (QLLs) of monolayer GNRs. (2) The spectrum displays two groups of QLLs, and the non-uniform GNR behaves like a bilayer one. (3) An intermediate category, the spectrum is composite disordered. (4) The spectrum presents the coexistence of monolayer and bilayer spectra. In this work, the magneto-electronic and optical properties for different geometric configurations are given, such as energy dispersions, density of states, wave functions, and magneto-antimony spectra are presented. Furthermore, the transformation between monolayer and bilayer spectra as well as the coexistence of monolayer and bilayer spectra are discussed in detail.

1One of us (Hsien-Ching Chung) thanks Ming-Hui Chung and Su-Ming Chen for financial support. This work was supported in part by the National Science Council of Taiwan under grant number 98-2112-M-006-013-MY4.

H1.00267 Resonance Raman Spectroscopy of Single-Wall Carbon Nanotubes Separated via Aqueous Two-Phase Extraction. J. R. SIMPSON, Towson University, J. A. FAGAN, A. R. HIGHT WALKER, National Institute of Standards & Technology (NIST) — We report resonance Raman Spectroscopy measurements of single-wall carbon nanotube (SWCNT) samples dispersed in aqueous solutions via surfactant wrapping and separated using aqueous two-phase extraction (ATPE) into chirality-enriched semiconducting and metallic SWCNT species. ATPE provides a rapid, robust, and remarkably tunable separation technique that allows isolation of high-purity, individual SWCNT chiralities via modification of the surfactant environment. We report RRS measurements of individual SWCNT species of various chiral index including, semiconductors, armchair and zigzag metals. Raman provides a powerful technique to quantify the metallic SWCNTs in ATPE fractions separated for metallicity. We measure Raman spectra over a wide range of excitation wavelengths from (457 to 850) nm using a series of discrete and continuously tunable laser sources coupled to a triple-grating spectrometer. The spectra reveal Raman-active vibrational modes, including the low-frequency radial breathing mode (RBM) and higher-order modes. SWCNT chiral vectors are determined from Raman spectra, specifically the RBM frequencies and corresponding energy excitation profiles, together with input from theoretical models.


H1.00268 Roles of Multi-Walled Structures in Thermal Transport Properties of Nanotubes. TOMOYUKI HATA, HIROKI KAWAI, RYOTA JONO, KOICHI YAMASHITA, Department of Chemical System Engineering, Graduate School of Engineering, the University of Tokyo — The molecular structures of carbon nanotubes are thought to be deeply related with various physical properties. Understanding the relationship is one of the challenges in designing potential materials. In the research, we theoretically investigated the thermal transport properties of carbon nanotubes, focusing the multi-walled structures. We investigated the thermal conductance of the double-walled carbon nanotubes (DWCNTs) by using the nonequilibrium Green’s function method. It is found that the inter-layer interaction causes the suppression of thermal conductance at low temperature. The analysis of the transmission coefficients revealed that this suppression was attributed to the energy shifts of the normal modes from the synchronized vibrations. The mechanism of such energy shifts is examined by the coupled vibration model with the parameters extracted from our simulations, and we grasp the multi-wall effects on the thermal transport properties of the nanotube structures.

H1.00269 Couloomb excitations for Gapped Graphene in a perpendicular magnetic field. ANDRII IUROV, University of New Mexico and Hunter College, CUNY, GODFREY GUMBS, Hunter College, CUNY and Donostia International Physics Center (DIPC), DANHONG HUANG, Air Force Research Laboratory, Space Vehicles Directorate — We investigate numerically the Coulomb excitations for gapped graphene and other buckled honeycomb lattices (such as silicene and germanene) in the present of a perpendicular magnetic field. The plasmons are calculated within the random phase approximation. The collective excitations in the presence of a perpendicular magnetic field for such gapped systems are shown to be different from those for both intrinsic gapless graphene as well as a standard two-dimensional electron gas. We present a theoretical description of Bernstein modes that appear due to the coupling between inter-Landau-level excitations and plasmons.

H1.00270 Calculating Observable Quantities for the Hofstadter-Type Spectrum of Graphene. LIUBOV ZHEMCHUZHA, Hunter College, CUNY, DANHONG HUANG, Air Force Research Laboratory, Space Vehicles Directorate, GODFREY GUMBS, Hunter College, CUNY and Donostia International Physics Center (DIPC). ANDRII IUROV, CHTM, University of New Mexico and Hunter College CUNY, SANJAY KRISHNA, CHTM, University of New Mexico — We numerically obtain density of states and the conductivity of the periodically modulated graphene in the presence of a perpendicular magnetic field. The collective excitations in the presence of a perpendicular magnetic field for such gapped systems are shown to be different from those for both intrinsic gapless graphene as well as a standard two-dimensional electron gas. We present a theoretical description of Bernstein modes that appear due to the coupling between inter-Landau-level excitations and plasmons.

H1.00271 Dielectric function for doped graphene layer with barium titanate$^1$, MANUEL MARTINEZ RAMOS, ERIC GARCES GARCIA, FERNANDO MAGANA, GERARDO JORGE VAZQUEZ FONSECA, Univ Nacl Autonoma de Mexico — The aim of our study is to calculate the dielectric function for a system formed with a graphene layer doped with barium titanate. Density functional theory, within the local density approximation, plane-waves and pseudopotentials scheme as implemented in Quantum Espresso suite of programs was used. We considered 128 carbon atoms with a barium titanate cluster of 11 molecules as unit cell with periodic conditions. The geometry optimization is achieved. Optimization of structural configuration is performed by relaxation of all atomic positions to minimize their total energies. Band structure, density of states and linear optical response (the imaginary part of dielectric tensor) were calculated.

We thank Dirección General de Asuntos del Personal Académico de la Universidad Nacional Autónoma de México, partial financial support by Grant IN-106514 and we also thank Mictl\' Super-Computing center the technical assistance.

H1.00272 Direct exfoliation of graphene in ionic liquids with aromatic groups$^1$, ROZANA BARI, GEORGE TAMAS, FAHMIHA IRIN, ADELIA AQUINO, EDWARD QUITEVIS, MICAH GREEN, Texas Tech University — The imidazolium cation of the designed and synthesized novel ionic liquids (ILs) having aromatic groups interact non-covalently with graphene. The graphene stabilized by the IL is neither covalently functionalized nor requires the presence of additive stabilizer and such process results in dispersion of pristine graphene. This graphene dispersion is stable against centrifugation and the concentration of the resulting graphene is high as well. It was observed that the ILs are less effective in dispersing graphene if the cation does not have these aromatic groups. The interaction between the cation and the graphene surface plays an important role in the final yield of graphene. The graphene dispersion was characterized by Raman spectroscopy, X-ray Diffraction, and X-ray photoelectron spectroscopy. The experimental observations were compared with the density functional theory (DFT-D3) calculations and the comparison indicated that the experimental observations and the theoretical calculations were in good agreement. These validated theoretical calculations can further be used in future to design and synthesize the ILs in order to optimize the graphene yield without the need for additional experimentation.

1 National Science Foundation under CRIF-MU instrumentation grant CHE-0840493, National Science Foundation under CAREER award CMMI-1253085, Air Force Office of Scientific Research Young Investigator Program (AFOSR FA9550-11-1-0027).

H1.00273 Physical Adsorption of noble gases on a monolayer graphene sheet using Grand Canonical Monte Carlo Simulation$^1$, SIDI MAIGA, Student, SILVINA GATICA, Howard University — Adsorption is defined as the attachment of atoms, or molecules of a gas, liquid or dissolved solid onto a surface. Using the Method of Grand Canonical Monte Carlo we computed the adsorption of Ar, Kr, and Xe on a monolayer graphene sheet, at various temperatures for each gas. For each temperature, we compute the adsorption isotherm, Energy-gas-surface and Energy-gas-gas, radial distribution function and structure function. We constructed the phase diagrams for 2D Ar and Kr on graphene.

1 Partial funding for this research was provided by the Partnership for Reduced Dimensional Materials (PRDM), an NSF Partnership for Research and Education in Materials (PREM) (Award Number DMR-1205608) and by the CIQM, NSF Grant No. DMR-1231319

H1.00274 Probing weak localization in chemical vapor deposition graphene with wide constriction by scanning gate microscopy$^1$, CHIASHAIN CHUANG, National Taiwan University, M. MATSUNAGA, Chiba University, FAN-HUNG LIU, TAK-PONG WOO, National Taiwan University, NOBUYUKI AOKI, Chiba University, LI-HUNG LIN, National Chiayi University, Y. OCHIAI, Chiba University, CHI-TE LIANG, National Taiwan University, NATIONAL TAIWAN UNIVERSITY COLLABORATION, CHIBA UNIVERSITY COLLABORATION, NATIONAL CHIAYI UNIVERSITY COLLABORATION — We observe weak localization effect in different wide channels on this disordered CVD graphene device. We also perform the low temperature-scanning gate microscopy experiments under weak localization regime on CVD graphene with wide constriction. The movable local gate can sensitively perturb the total conductance in the wide constriction CVD graphene under magnetic field, suggestive the advantages in the design of graphene-based spintronics.

1 The Aim for the Top University Project by National Taiwan University and Chiba University

H1.00275 Micron scale ballistic Josephson junctions in edge-contacted graphene$^1$, SRIJIT GOSWAMI, VICTOR CALADO, GAURAV NANDA, Delft University of Technology, MATHIAS DIEZ, Leiden University, ANTON AKHMEROV, Delft University of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute of Materials Science, LIEN VANDERSYPEN, Delft University of Technology — Despite recent improvements in the electronic quality of graphene, it has remained challenging to make superconducting contacts to it while preserving its high quality. Here, we integrate monolayer graphene encapsulated in hexagonal Boron Nitride with a type-II superconductor (Molybdenum Rhenium – MoRe) via one-dimensional contacts along the edge of the graphene. We observe gate-tunable supercurrents over distances as long as 1.5 $\mu$m. Ballistic, phase coherent transport in these devices causes the switching current to oscillate periodically with the Fermi wave number, thus providing clear evidence of a ballistic Josephson junction. Furthermore, the large critical field of MoRe allows us to resolve several broken symmetry states in the quantum Hall regime, while the MoRe remains superconducting.

H1.00276 Tunable dichroism and optical absorption of graphene by strain engineering$^1$, MAURICE OLIVA-LEYVA, GERARDO G. NAUMIS, Univ Nacl Autonoma de Mexico — Recently, the concept of strain engineering has been experimentally extended to the optical domain. However, strain-induced modifications of optical absorption in graphene have been only quantified in the case of a uniaxial strain. In this sense, our work opens a more rich scenario to explore strained-graphene transparency because it is applicable to an arbitrary uniform strain (e.g., uniaxial, biaxial, and so forth). From the corresponding Dirac-like equation [1], we compute the optical conductivity of graphene under a uniform strain [2,3]. This result allowed us to study the transmittance of linearly polarized light between two media separated by a strained graphene sheet [4]. We analytically characterize the degree of dichroism and the transparency of graphene as a function of an arbitrary uniform strain and the incident polarization. Also, we discuss how measurements of dichroism and transparency for two different polarization directions can be used to determine the magnitude and direction of strain. Ours findings result in very useful tools to tune the graphene absorption by mechanical strain [4]. [1] J. Phys. Rev. B 88, 085430 (2013). [2] J. Phys.: Condens. Matter 26, 125302 (2014). [3] J. Phys.: Condens. Matter 26, 279501 (2014). [4] arXiv: 1411.1376.
H1.00277 Enhanced hot-carrier luminescence in multilayer reduced graphene oxide nanospheres1, QI CHEN, CHUNFENG ZHANG, MIN XIAO, Nanjing Univ — We report a method to promote photoluminescence emission in graphene nanospheres by enhancing carrier scattering instead of directly modifying band structure in multilayer reduced graphene oxide (rGO) nanospheres. We intentionally curl graphene layers to form nanospheres by reducing graphene oxide with spherical polymer templates to manipulate the carrier scattering. These nanospheres produce hot-carrier luminescence with more than ten-fold improvement of emission efficiency as compared to planar nanosheets. With increasing excitation power, hot-carrier luminescence from nanospheres exhibits abnormal spectral redshift with dynamic feature associated to the strengthened electron-phonon coupling. These experimental results can be well understood by considering the screened Coulomb interactions. With increasing carrier density, the reduced screening effect promotes carrier scattering which enhances hot-carrier emission from such multilayer rGO nanospheres. This carrier-scattering scenario is further confirmed by pump-probe measurements.

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H1.00278 Momentum resolved optical pump-probe spectroscopy in monolayer graphene: An analytical model and measurements1, MAXIM TRUSHIN, ALEXANDER GRUPP, GIANCARLO SOAVI, ARNE BUDWEB, University of Konstanz, Germany, DOMENICO DE FAZIO, ANTONIO LOMBARDO, UGO SASSI, ANDREA C. FERRARI, Cambridge Graphene Centre, University of Cambridge, UK, WOLFGANG BELZIG, ALFRED LEITENSTÖRFER, DANIELE BRIDA, University of Konstanz, Germany — Further development in graphene based photonics and optoelectronics requires fundamental information on the evolution of the strongly non-equilibrium charge carrier distribution created by the light-carrier interaction. Here, we report polarization and fluence dependent ultrafast optical pump-probe spectroscopy of high quality CVD-grown monolayer graphene. An analytical model has been developed and employed to describe the experiments. Graphene offers a unique opportunity to probe the photocarrier occupation, not only at different energies but also in different directions in momentum space applying linearly polarized beams. The latter approach is possible due to the pseudospin-momentum coupling which results in an optical pseudospin-selection rule. Our method allows us to quantify and control the relative contributions of both the strongly non-equilibrium anisotropic occupation and the hot Fermi-Dirac photocarrier distribution to the total differential transmission measured. We provide a conclusive and quantitative evidence for an anisotropic photocarrier occupation with a life-time of about 100 fs and claim that its relaxation towards the isotropic distribution occurs mostly due to optical phonon emission.

H1.00279 Probing the Doping level in Graphene Using Surface Plasmon Resonance,1 KAMRUL ALAM, YANG LI, JIMING BAO, University of Houston — The present work describes an investigation of the electrochemically doped large area CVD grown graphene by using surface plasmon resonance (SPR). As graphene was doped electrochemically its conductance changes based on electron and hole concentration, that have an effect on its permittivity which has influence on the refractive index. We have used SPR angle interrogation scheme, generally known as Kretschmann configuration, to detect this change in refractive index of graphene as a shift in the angle of the SPR curve. To verify our results we have use Raman spectroscopy of the graphene-Au hybrid sample that was used for SPR measurement. Shift in the G peak signifies that graphene is doped electrochemically which is also in agreement with the shift in the angle of the SPR curve.

H1.00280 Strain-Engineering of Graphene Based Topological Quantum Devices1, GINETOM S. DINIZ, MARCOS R. GUASSI, FANYAO QU, Institute of Physics, University of Brasilia, Campus Darcy Ribeiro, DF, 70910-900, Brazil — We have investigated the spin-charge transport in quantum devices based on graphene nanoribbons (GNR). Our calculation is based on the surface Green’s function technique, considering the presence of an uniform uniaxial strain, spin-orbit interactions (SOIs), exchange field and a smooth staggered potential. We propose the use of uniaxial strain as an efficient mechanism to tune the conductance profiles of GNR with different edge terminations. Our results show that distinct behaviors can be achieved: for armchair GNR there is a complete suppression of the conductance close to the Fermi level with the formation of a band gap that depends on the direction and strength of the strain deformation, while for zigzag GNR there is only a small conductance suppression. We also discuss the effects of SOIs and the appearance of spin-resolved conductance oscillations, and the local density of states of these GNR devices in the quantum anomalous Hall regime. Furthermore, we demonstrate that the local density of states show that depending on the smoothness of the staggered potential, the edge states of AGNR can either emerge or be suppressed. These emerging states can be probed by scanning tunneling microscope. Our findings can be potentially used in novel GNR based topological quantum devices.

1Supported by FAP-DF, CNPq and CAPES

H1.00281 Physisorption of Fullerenes in Graphene layers and carbon Nanoribbons1, MONICA PACHECO, PEDRO ORELLANA, Universidad Tecnica Federico Santa Maria, JULIAN CORREA, Universidad de Medellin — The study of nanostructures based on carbon allotropes has captured the interest of the scientific community in the last two decades, due to its great versatility. In such structures a simple change of geometry leads to important changes in their physicochemical properties. In this context it has been studied different carbon allotropes complexes in particular for the development of photovoltaic systems. In this paper we show a study of opto-electronic properties of fullerenes physisorbed on graphene nanoribbons. Our calculations are carried out within the framework of density functional theory (DFT) using the SIESTA package. Our results show that effectively the fullerenes bind both to the layer of graphene as well as to the nanoribbons, with binding energies of about 0.5eV. We find that when the complex is formed, the physical properties of fullerenes, graphene and nanoribbons are preserved and when graphene is functionalized with various fullerenes the electronic spectrum is composed of bands of energy which increases the intensity of the optical absorption spectrum of the complex.

1Conicyt ACT 1204, USM 11.14.68

H1.00282 Thermoelectric properties of a trilayer graphene nanoribbon1, PEDRO ORELLANA, NATALIA CORTES, LUIS ROSALES, MONICA PACHECO, Universidad Tecnica Federico Santa Maria, LEONOR CHICO, CSIC — In this work the electronic and thermoelectric properties of a three-layer graphene with AAA stacking type are studied. By using a tight-binding model analytical expressions for the transmission and density of states are obtained. Thermoelectric properties are analyzed by numerical integration and results for thermopower and figure of merit, electronic conductance and thermal conductance are obtained. The results show that the interference effects present in this system, like Fano effect, directly affect the behavior of these thermoelectric properties [1] as well as the Wiedemann-Franz law [2]. There is an enhancement of the thermopower of the system and a violation of the Wiedemann-Franz law in the region of energies close the Fano antiresonances and this has as a consequence an enhancement of the figure of merit of the system.


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H1.00283 Polarized spin and valley transport across ferromagnetic silicene junctions V. VARGIADAMIS, P. VASILOPoulos, Concordia University, V. FEssATIDIS, Fordham University — We study ballistic transport of Dirac fermions through silicene barriers, of width d, with an exchange field M and metallic gates above them that provide tunable potentials of height U. Away from the Dirac point (DP) the spin- and valley-resolved conductances, as functions of U, exhibit resonances and close to it a pronounced dip that becomes a transport gap when an appropriate electric field E_0 is applied. The charge conductance g_e of such a junction changes from oscillatory to a monotonically decreasing function of d beyond a critical E_0. This tuning of g_e can be used to realize electric-field-controlled switching. Further, the field M splits each resonance of g_e in two split-lead peaks. The spin polarization p_y of the current near the DP increases with E_0 or M and becomes nearly perfect above certain of their values. We also show that p_y can be inverted either by varying U or by reversing the direction of M. For two barriers there is no splitting in g_e when the fields M are in opposite directions. Most of these phenomena have no analogs in graphene.

H1.00284 Graphene optical-to-thermal converter1, ALEJANDRO MANJAVacas, Rice University, SUKOSIN THONGRATTANASIRI, Kasetsart University, JEAN-JACQUES GREFFET, Institut d’Optique, Univ. Paris Sud, JAVIER GARCIA DE ABANO, ICF-CThe Institute of Photonic Sciences — Infrared plasmons in doped graphene nanostructures produce large optical absorption that can be used for narrow-band thermal light emission at tunable frequencies that strongly depend on the doping charge. By virtue of Kirchhoff’s law, thermal light emission is proportional to the absorption, thus resulting in narrow emission lines associated with the electrically controlled plasmons of heated graphene. Here [1] we show that realistic designs of graphene plasmonic structures can release over 90% of the emission through individual infrared lines with 1% bandwidth. We examine anisotropic graphene structures in which efficient heating can be produced upon optical pumping tuned to a plasmonic absorption resonance situated in the blue region relative to the thermal emission. An incoherent thermal light converter is thus achieved. Our results open a new approach for designing tunable nanoscale infrared light sources.

H1.00285 Evanescent field coupled graphene plasmon waveguide, WON JONG YOO, JAEHWAN KWEON, EUYHEON HWANG, Sungkyunkwan Univ — Surface plasmon polaritons (SPPs) is propagating electron-light coupled oscillation. There had been various methods to excite graphene plasmon such as fabricating graphene nano-ribbon and NSM micro-tip assisted methods. These methods are used for reducing wavelength of incident light and finally matching desired wavelength to propagating light. Here, we propose that evanescent field coupled graphene plasmon is using different media, evanescent field coupling and excited graphene plasmon properties are still unclear. There are severaladvantages in using this coupling method. We can control the direction of propagating plasmon and effectively find plasmon modes. Interestingly, propagating wavelength is scaled to 50 – 100 times depending on its modes and light is confined into extremely small mode size. Also its optical properties can be easily controlled by biasing voltage on its surface. To analyze graphene plasmon, we use random phase analysis (RPA) so as to figure out optical permittivity of graphene, and then we use the FDTD (finite difference time domain) and FDFD (finite difference frequency domain) computational methods so as to theoretically figure out the propagation of graphene plasmon waveguide. Also we will report various plasmon properties of graphene plasmon propagation such

H1.00286 All-Metallic Vertical Transistors Based on Stacked Dirac Materials, YANGYANG WANG1, ZEYUAN NI, School of Physics, Peking University, QIHANG LIU, University of Colorado, RUGE QUHE, School of Physics, Peking University, JIAxin ZHENG, School of Advanced Materials, Peking University, Shenzen Graduate School, MENG YE, DAPENG YU, JUNJIE SHI, JINBO YANG, School of Physics, Peking University, JU LI, Massachusetts Institute of Technology, JING LU, School of Physics, Peking University, COLLABORATIVE INNOVATION CENTER OF QUANTUM MATTER, BEIJING COLLABORATION — All metallic transistor can be fabricated from pristine semimetallic Dirac materials (such as graphene, silicene, and germanene), but the on/off current ratio is very low. In a vertical heterostructure composed by two Dirac materials, the Dirac cones of the two materials survive the weak interlayer van der Waals interaction based on density functional theory method, and electron transport from the Dirac cone of one material to the one of the other material is therefore forbidden without assistance of phonon because of momentum mismatch. First-principles quantum transport simulations of the all-metallic vertical Dirac mater heterostructure devices confirm the existence of a transport gap of over 0.4 eV, accompanied by a switching ratio of over 1014. Such a striking behavior is robust against the relative rotation between the two Dirac materials and can be extended to twisted bilayer graphene. Therefore, all-metallic junction can be a semiconductor and novel avenue is opened up for Dirac material vertical structures in high-performance model predicts. Our results provide new insight to nanoepitaxy of low dimensional structures especially quantum dots and nanoprecipitates.

H1.00287 Identification of the existence of quantum Hall edge-state in graphene field-effect transistor at high temperatures, JOONG GYU KIM, HAEYONG KANG, JEONGMIN PARK, YOOJOO YUN, THUY KIEU TRUONG, JEONG-GYUN KIM, NAHEE PARK, YOURACK LEE, CINAP, IBS, Department of Energy Science, Sungkyunkwan University, HOYEOL YUN, SANG WOOK LEE, School of Physics, Konkuk University, YOUNG HEE LEE, DONGSEOK SUH, CINAP, IBS, Department of Energy Science, Sungkyunkwan University — Quantum Hall effect (QHE) is one of the unique properties of two-dimensional electronic systems providing the universal standard of electrical resistance. Due to edge-state transport features in quantum Hall regime, the two-terminal graphene field-effect transistor (FET) is frequently examined for the study of the integer as well as the fractional QHEs of graphene. In this work, we present a simple method to identify the existence of quantum Hall state in the graphene FET especially at high temperatures. Using the monolayer graphene FET sample with fully broken degeneracy, we modified the equipotential line inside graphene and identified the existence of quantum Hall state in the graphene FET by the addition of extra electrode for the clear identification of the quantum Hall state formation at given temperature and magnetic field. We suggest a simple model to explain the difference and similarity between two-terminal and multi-terminal configurations, including the discussion about the QHE devices connected in series.

H1.00288 SUPERLATTICES, NANOSTRUCTURES AND OTHER ARTIFICIALLY STRUCTURED MATERIALS

H1.00289 Three-Dimensional Lattice Matching for Epitaxially Embedded Nanoparticles BRELON MAY, Peter ANDERSON, RObERTO MYERS, Ohio State Univ — Columbus — Since Mathews-Blakeslee developed a theory of atomic lattice matched thin films, epitaxy has been modeled using only 2D lattice matching conditions between arbitrary films. For a given degree of in-plane lattice mismatch, the theory predicts a critical film thickness above which interface defects form to relax the film strain. Here we present a three-dimensional model to predict the conditions for epitaxially encased nanoparticles, which includes not only the in-plane lattice matching, but also the out-of-plane mismatch. We find that the consideration of the out-of-plane strain, due to the Poisson effect and particle shape change, can greatly alter the critical volume compared to what the Mathews-Blakeslee model predicts. Our results provide new insight to nanoparticle/nanostructures of low dimensional structures especially quantum dots and nanoprecipitates.
H1.00290 A DFT analysis of structure and energetics of Mg/Nb multilayers, ANIL KUMAR, IRENE BEYERLEIN, JIAN WANG, Los Alamos National Laboratory — Magnesium and its alloys, the lightest structural materials, have attracted the attention of the automotive industry for reducing the vehicle’s weight to increase its fuel efficiency. The magnesium phase characterized within Mg/Nb multilayers can adopt either body-centered cubic (bcc-Mg) or hexagonal close packed (hcp-Mg) structure depending on the Mg layer thickness. The bcc-Mg has a similar weight density as the hcp-Mg, but low Young’s modulus, high shear modulus and conventional slip systems of bcc structure. In this work, using first-principles density functional theory, we studied both structural and mechanical properties of bcc-Mg and hcp-Mg in Mg/Nb multilayers as a function of Mg layer thickness and developed a simple theoretical model to predict the structural stability of the bcc-Mg/Nb and hcp-Mg/Nb multilayers. We show that the bcc-Mg/Nb multilayer is energetically favorable when the bcc-Mg layer is less than 4.2 nm. We also studied the mechanism such as inter-mixing of Mg and Nb atoms, creation of vacancies and doping of solute atoms at Mg/Nb interface to minimize the Mg/Nb interface energy. We found that solute atoms such as Zr, Cd and Zn, whose metallic radius are smaller than Mg, can easily segregate at Mg/Nb interface and lower the interface energy.

H1.00291 Layer by Layer Fabrication of 3D Photonic Crystals by Substrate Conformal Imprint Lithography (SCIL) from Titania Nanoparticle Solutions, IRENE HOWELL, University of Massachusetts-Amherst, MARC VERSCHUUREN, Philips Research, ROHIT KOTHARI, JAMES WATKINS, University of Massachusetts-Amherst — We demonstrate a method for fabricating well-aligned, large-area, log-pile 3D photonic crystals. Using 15 nm titania (anatase) nanoparticles dispersed in a mixture of propanediol and methanol, we show that these nanoparticles can be patterned to produce robust, reproducible, 1 µm pitch, 500 nm line-width gratings. By planarizing the grating with an organic UV-curable resin (Norland Optical Adhesive 60), subsequent titania layers can be patterned in the proper orientation, ending with a calcination step to remove the organic resin and create a 3D photonic crystal. This method allows for a photonic stop band in the infrared region, but the limitations in feature size and alignment capability prevent fabrications of a photonic crystal with a band gap at shorter wavelengths. By applying Substrate Conformal Imprint Lithography (SCIL) technology to this method, we can produce 3D photonic crystals with features suitable for a band gap in the visible region. SCIL utilizes a higher modulus PDMS (X-PDMS) to easily achieve sub-500 nm features. Additionally, the alignment method, involving box-in-box and Moire patterns, enables reproducible, precise alignment of sequential layers within 5 nm.

H1.00292 Phonon Scattering at Nanoparticles in LuAs:InGaAs Nanocomposites, FENG HE, RODOLFO SALAS, SETH ROBERT BANK, YAGUO WANG, University of Texas System — Nanocomposites of III-V semiconductors embedded with semi-metallic rare earth nanoparticles grown with molecular beam epitaxy (MBE) have been widely using in optoelectrics and thermoelectrics. Manipulating the growth parameters, e.g. growth rate, particle concentration and surfactant, will allow precise control of electronic and thermal transport properties for specific applications. Fundamental understanding of phonon scattering at nanoparticles in these nanocomposites under various growth conditions is not only scientifically important, but also will facilitate the material growth and device design. We have investigated the ultrafast dynamics of coherent acoustic phonons (CAP) in LuAs:InGaAs nanocomposites with standard two-color femtosecond pump-probe technique. Phonon frequency and life time have been measured in samples grown under different conditions. Our results show that CAP lifetime increases with increasing LuAs deposition, as well as pump fluences. We have also studied the influences of growth rate and surfactant on phonon lifetime.

H1.00293 Study of plasmon-polariton in 1-D photonic crystals of dielectric and magneto optical layers under the effects of external magnetic field in the polar configuration, JAIME ANDRES GIRON SEDAS, EDWIN MONCADA VILLA, Solid State Group, NELSON PORRAS MONTENEGRO, Solid State Group, Universidad del valle, Cali, Colombia — Photonic crystals (PCs) are artificial microstructures with a periodic spatial distribution of the dielectric constant, which enables us to manipulate and control the photons. In particular, the existence of photonic bands in the energy spectrum as well as photonic band gaps, forbidden frequency regions for light propagation have permitted quite a number of analogies with physical properties of semiconductor, this provides a perfect base for the construction of great varieties of photonic devices. In this case the superlattice is composed of alternating slabs of two materials, one is a dielectric, and the other is magneto-optical material. The interaction between plasma excitations and the electromagnetic radiation in the frequency region around null electric and magnetic responses in these arrangements, it gives a requisite for the existence of longitudinal waves, results in the excitation of modes that couple plasmons and optical fields. Those are known as Plasmon- Polaritons. We analyze the magneto-optic response of this PCs and the Plasmon-Polaritons behavior when an external magnetic field is placed in the growth direction of the structure using the scattering matrix approach for anisotropic layer stacks.

H1.00294 Electronic structure of palladium and gold-palladium nano clusters, both free and supported on MgO(100), CARLOS QUINTANAR, REYNA CABALLERO, RAUL ESPEJEL, ELIZABETH CHAVIRA, Universidad Autónoma de México, MAGALI UGALDE, FRANCISCO ESPINOZA, Centro de Investigación en Materiales Avanzados, SAMUEL TRICKEY, University of Florida — Ideal (or model) metal nano-clusters, both free and supported on MgO(100), have been the subject of numerous experimental studies. This work probes the characteristics of non-ideal systems. For that, palladium nano clusters first were synthesized using a sol-gel-microwave method. A mono-phase of metallic Pd was obtained as corroborated by thermo gravimetric analysis, x-ray powder diffraction, scanning electron microscopy, and high resolution transmission electron microscopy studies (HRTEM). Among the HRTEM micro-graphs we found an almost planar nano-surface (facet) with only forty six atoms (Pd_{46}). From that micro-graph we obtained the coordinates of the atoms in the Pd_{46} nano-surface. With those coordinates, we did a DFT study of the Pd_{46} nano-surface electronic structure. From the Pd_{46} nano-surface, nine and eighteen Pd atoms were chosen to build A and Pd_{18} clusters respectively. Starting from a near-planar Au8 cluster, the Au_{8} geometry was optimized over the fixed Pd_{9} and Pd_{18} nano-surfaces, charge transfer was determined with charge density difference analysis (CDDA) and Fukui analysis was done and. The Au_{8}Pd_{9} cluster was positioned on an MgO(100) surface with an O vacancy and charge transfer was determined with CDDA

H1.00295 Formation of finite layer MoS2 using ultrasonic agitation, TIM KIDD, RUI HE, ERIC CLAUSEN, University of Northern Iowa — We have developed a process in which finite layer MoS2 can be produced using ultrasonic agitation. The material shows optical properties consistent with an average layer thickness of less than five layers. The process uses ultrasonic agitation of MoS2 in an suspension using isopropanol. Interestingly, side products involving carbon nanoparticles are also produced. These side products are quite small, and become the dominant material when using a centrifuge to separate out the smallest particles. These carbon nanoparticle side products appear to include nanometer scale particles as well as materials with sizes consistent with fullerenes and graphene with nanoscale lateral dimensions. This process appears to represent a novel method for producing finite layer MoS2 and some forms of carbon nanoparticles using a relatively simple method.
**H1.00297 Bimodal Distribution of Cadmium Selenide Quantum Dots Prepared by UV-Photolithography**
AJITH DESILVA, University of West Georgia, M. KAVEH, University of Cincinnati, RAGHVEER R. GADIPALLI, SARAH G. MARTINO, University of West Georgia, H.P. WAGNER, University of Cincinnati — We employed wet chemical and UV photolithography methods to synthesize CdSe quantum dots (QDs). The dynamics of excitons in the QDs were studied using temperature-dependent photoluminescence (PL) ranging from 17 to 300 K. The inhomogeneous shape and size of the QDs led to an asymmetric PL spectrum at 17 K, which was approximately decomposed into two Gaussian emission bands, with peak energies at 2.182 and 2.299 eV and widths of 40 and 30 meV, respectively. These bands are attributed to the existence of two CdSe QDs ensembles with differently sized QDs. With increasing temperature the PL intensities of both bands weakly change, the PL yield of the larger QDs being higher at low temperatures while the smaller QDs show the stronger emission at higher temperatures. The stronger PL quenching of the larger QDs with increasing temperature is tentatively assigned to a higher density of defects at the grain boundary compared with small QDs. TEM images of the sample revealed a distribution of nanoparticles with average sizes around 10 and 15 nm supporting the existence of a bimodal QD distribution.

**H1.00298 AlN nanowire growth using InN crystalline powders by physical vapor deposition**
NAOTO KENMOCHI, HIRAKU OTA, MIKKA NISHITANI-GAMO, NOBORU WADA, Toyo University, Japan — AlN nanowires were grown by heating an evacuated quartz ampule which contained InN crystalline powders and an Al substrate at 1300 °C. Both EDX and Raman spectroscopy yielded that the nanowires should be crystalline InN. Almost all the nanowires exhibited a spherical head at the end, implying that the growth mechanism might be the vapor-liquid-solid (VLS) growth. The diameter typically varied from 30 nm to 500 nm, while the length could be several microns meters long. The nanowire growth was quite significant on the Al substrate close to the InN powder source. When the samples were kept at high temperatures for a longer time, both the spherical heads and nanowires were found to be thicker. The detailed mechanism for the growth and the growth conditions will be discussed.

**H1.00300 Metallic Nanoparticles Confined in Silica Matrices**
SHIN-HYUN KANG, MIN-JAE LEE, JEEUN LEE, JUN-KI LEE, SUNG-MIN CHOI, KAIST — Metallic nanoparticles are widely studied due to their noble properties based on the high surface area. In order to increase the practical applications, the nanoparticles should be protected from thermal damage which can cause agglomeration. A facile way of protecting metallic nanoparticles with a silica matrix is presented. Metal nanoparticles are synthesized and functionalized in aqueous solution, and are collectively confined in a silica matrix which is thermally stable enough to protect the embedded nanoparticles. The structure and morphology are investigated by small angle scattering measurements, transmission electron microscopy and scanning electron microscopy. Physical and chemical properties of the heterogeneous system would be presented, too.

**H1.00301 Synthesis, Electrical and Structural Properties of $Mg_x Pb_{(1-x)}TiO_3$ produced by mecanosynthesis**
JALDAIR NOBREGA, ARIANO DE GIOVANNI RODRIGUES, MICHELVENET ZAMBRANO, PAULO SERGIO SILVA JUNIOR, JULIO CESAR CAMILO ALBORNIZDIAZ, PAULO SERGIO PIZANI, Univ Fed de Sao Carlos, ESPETROSCOPIA RAMAN EM MATERIAIS NANOESTRUTURADOS COLLABORATION, METALURGIA FISICA E DE ESPECTROSCOPIA MECANICA COLLABORATION — Over last decades scientific studies about ceramic materials based in metallic oxides have pointed to an increasing wide range of applications. Among them, $PbTiO_3$ has been significantly applied to electronic components and optoelectronics devices. Another example can be found in the microwave dielectric $MgTiO_3$, which has been used on the production of devices. The development of a compound that combines the physical properties of these well-known materials aims the achievement of a new type of ceramics presenting distinctive applications. We report the production of $Mg_x Pb_{(1-x)}TiO_3$ by means of mecanosynthesis techniques. Electric measurements were carried out in order to verify the dielectric behavior of the system. By analyzing the signatures of characteristic phases of $PbTiO_3$ and $MgTiO_3$ in X-Ray diffractograms, we could confirm that the stoichiometry of our solid solutions could be controlled by properly adjusting the amounts of the oxides used as precursors. The Raman spectroscopy analysis showed us the behavior of the soft mode, typical of ferroelectric, which is present in all composition. By determining the dependence of its energy with temperature variation, we could estimate the temperatures of phase transition for each composition.

**H1.00302 Synthesis and Characterization of Magnetic Nanoparticle Assemblies**
MIN-JAE LEE, HO-HYUN KIM, SHIN-HYUN KANG, SUNG-MIN CHOI, KAIST — The superstructure of magnetic nanoparticles, which may provide new properties, are of great interest for various potential applications as well as its own scientific merits. Despite recent advances in the fabrication and characterization of magnetic nanoparticle structures, it remains challenges to exploit for controllable organization of magnetic nanoparticles at the nanoscale. Here, we will report the synthesis and functionalization of monodisperse magnetic nanoparticles and their self-assembled structure.
H1.00303 Microwave metal-dielectric metamaterials with magnetic inclusions, BRITTANY BATES, BRANDON ALLISON, Norfolk State Univ, NICOLE GREENE, Cornell Univ, NATALIA NOGINHOVA, Norfolk State Univ — Use of natural magnetic materials as a constituent part of metamaterials is attractive as they provide a possibility to tune material parameters at microwave range and THz frequency with external magnetic fields. Metal-dielectric multilayers and wire arrays structures were fabricated using both ferromagnetic and nonmagnetic metals. These structures were studied in free space microwave propagation experiment. We show that a cube of such a metamaterial operates as a focusing lens and a polarizer with a possibility of tuning with external magnetic field.

H1.00304 Magnetic, structural and adsorption properties for methylene blue of PAA/MnFe$_2$O$_4$ nanocomposite, WEI WANG, ZUI DING, School of Science, Beijing University of Chemical Technology, Beijing 100029, China. J. PING LIU, Department of Physics, University of Texas at Arlington, Arlington, TX 76019, USA — PAA/MnFe$_2$O$_4$ nanocomposite was fabricated by a hydrothermal procedure and ultrasonic wave-assisted method. The morphology of the synthesized MnFe$_2$O$_4$ ferronanocrystals reached 74.6 nm. FTIR spectrum confirms the coating of PAA on the surface of MnFe$_2$O$_4$ ferronanocrystals. Here, the PAA coating does not lead to a deterioration in magnetic performance. Moreover, the PAA/MnFe$_2$O$_4$ nanocomposites were applied to remove Methylene Blue (MB) from wastewater. Compared with the nanoparticles without coating, the PAA coating significantly enhanced the adsorption capacity of MB onto MnFe$_2$O$_4$ magnetic nanoparticles, where a rapid and efficient removal of MB was observed. The research suggests that as-synthesized PAA/ MnFe$_2$O$_4$ nanocomposites have promising and potential applications in water treatment for removal of dyes.

H1.00305 Synthesis and Characterization of Au@Pd@Au core-shell nanostructures, ALEJANDRA LONDONO-CALDERON, J. JESUS VELAZQUEZ-SALAZAR, MIGUEL JOSE YACAMAN, Univ of Texas, San Antonio — In this work we present a systematic study on the synthesis of (Au@Pd)@Au nanostructures by a seed mediated method in aqueous solution. In the first step, single crystal Au octahedra nanoparticles are used as seeds to promote a metallic Au core-shell nanocube of 40 nm in size. The growth mechanism of successive Au layers on the Au@Pd nanocube and the crystallinity on the Au/Pd and Pd/Au interfaces are studied by the use of Scanning Electron Microscopy (SEM), High Resolution Transmission Electron Microscopy (HTEM) and Scanning Transmission Electron Microscopy (STEM). A transformation from cubes to truncated polyhedrons is observed by Electron Tomography in the reconstruction of the surface.

H1.00306 Real-space and nanoscopic observation of phase transition behaviors of VO$_2$ thin films using Kelvin probe force microscopy, DONG-WOOK KIM, AHRUM SOHN, Department of Physics, Ewha Womans University, TERUO KANKI, KOUTARO SAKAI, HIDEKAZU TANAKA, The Institute of Scientific and Industrial Research, Osaka University — VO$_2$ undergoes a metal-insulator transition (MIT) and a tetragonal-monoclinic structural phase transition (SPT) near room temperature. We carry out transport and KPFM (Kelvin probe force microscopy) measurements on epitaxial VO$_2$/TiO$_2$ thin films simultaneously in the temperature range of 285-330 K. The samples have large grains due to very small lattice mismatch, which allows us to study inherent nature of the phase transition in quasi-2D VO$_2$ system. The sample’s work function decreases from 5.1 eV to 4.9 eV, while spanning the transition temperature. The work function maps can clearly reveal coexistence of the two distinct states at the intermediate temperature range, well explained by the 2D percolation theory.

H1.00307 Plasmon Excitations for a Coulomb-coupled Graphene Layer and a Thick Conductor, GODFREY GUMBS, Hunter College, CUNY and Donostia International Physics Center (DIPC), ANDRII IUROV, University of New Mexico and Hunter college, CUNY, NORMAN HORNING, Stevens Institute of Technology — Self-consistent field theory is used to obtain the plasmon dispersion relation of monolayer graphene which is Coulomb coupled to a thick conductor. We calculate numerically the undamped plasmon excitation spectrum for arbitrary wave number. For gapped graphene, both the low-frequency (acoustic) and high frequency (surface) plasmons may lie within the opening within the particle-hole region. Additionally, we obtain plasmon excitations in a region of the frequency-wave vector space which does not exist for free standing gapped graphene.

H1.00308 One and two dimensional shock waves of light, RICARDO FERRO, HASANUZZAMAN RAHMAN, GERMAN KOLMAKOV, MANAS KULKARNI, New York City College of Technology, City University of New York — By using numerical simulations for the dynamics of an exciton polaron condensate in an optical microcavity, we demonstrate that strongly nonlinear, spatially localized waves can be formed during the propagation of the condensate perturbations. We show that at the terminal stage of their evolution, the condensate density waves acquire the universal shape of a shock wave, which is similar to that known from a classical rarefied interacting gas dynamics. Since the exciton-polaritons in the condensate include photons as their constituents, this allows new possibilities for multiphoton quantum imaging and measuring the phase coherence of a two-dimensional condensate. We also discuss the effects of the scattering of the photon on the shock structure of the defects in the cavity, and the effects of the phase coherence during mutual scattering of two and more shock waves.

H1.00309 A quantum interferometer for studies of the exciton and polaron drag effects, ANDY HE, ROMAN YA. KEZERASHVILI, GERMAN V. KOLMAKOV, New York City College of Technology CUNY — Recently, the drag effects of excitons and cavity polaron condensates by an electric current running in a quantum well embedded in a cavity were theoretically predicted. These effects provide one with a useful tool to control the exciton and photons propagation in optical integrated circuits by external electric signals. Applications of such the drag effects in the design of semiconductor- and graphene-based devices for optical computing have recently been discussed in the literature. In our report, we propose a setup suitable for the studies of the exciton and polaronate condensate drag effects based on self-interference of a split condensate in the presence of the driving current. By numerically simulating an output signal of a ring-shaped interferometer, we determine the range of parameters, at which the exciton and polaron drag effects in a microcavity can be observed and utilized in optical nanodevices.

H1.00310 Dynamics of self-trapped excitons in layered Pb$_1$−$X$Cd$_X$I$_2$ semiconductors, YURIY GNATENKO, ANATOLII BUKIVSKII, YURIY PIYATINSKI, Institute of Physics of National Academy of Science of Ukraine — The dynamics of self-trapped excitons, localized on stretched Pb-I chemical bonds which are formed on PbI$_2$ nanocluster surface was investigated. It should be noted that these nanoclusters are naturally formed in Pb$_2$I$_4$ nanocrystals. To study the excited state properties and the excited state lifetime of Pb$_2$I$_4$ nanocrystals, the measurements of photoluminescence (PL) spectra and kinetics of PL intensity decay for those materials were performed at T=300 K. The kinetic dependences were obtained for the maximum of PL band (600 nm) and for its short-wave shoulder (550 nm). It was shown that PL decay kinetics is well approximated by stretched exponential function $I(t) = I_0 \exp(-t/\tau_d)$. Obtained values of $\tau_d$ and $\beta$ for $X = 0.5$ are equal about 800 ns and 0.76 at 600 nm. At 550 nm these values are 700 ns and 0.74, respectively. Similarly for $X = 0.7$ these values correspond about 800 ns and 0.80 at 600 nm. At 550 nm they are 800 ns and 0.82. Application of the Inverse Laplace Transformation (ILT) to our experimental data gave us an opportunity to estimate the probability density function of self-trapped exciton state lifetimes for Pb$_2$I$_4$ nanocrystals ($X = 0.3, 0.5$ and $0.7$). The position of the maximum of $F(\tau)$ gives us the average decay time $<\tau>$ which is about 1250 ns which significantly differs from $\tau_d$ which is about 800 ns (for $X = 0.5$ nm). This complex dynamics of excitons is associated with strong heterogeneity of the investigated system.
Half-metallicity in a BiFeO$_3$/La$_2$Sr$_{1/3}$MnO$_3$ heterostructure: A first-principles study

JILILI JIUWER, KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia, ULRICH ECKERN, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany, UDO SCHWINGENSCHLOGL, KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia — We present first principles results for the electronic, magnetic, and optical properties of the BiFeO$_3$/La$_2$Sr$_{1/3}$MnO$_3$ heterostructure as obtained by spin polarized calculations using density functional theory. The electronic states of the heterostructure are compared to those of the bulk compounds. Structural relaxation turns out to have only a minor impact on the chemical bonding, even though the oxygen octahedra in La$_2$Sr$_{1/3}$MnO$_3$ develop some distortions due to the interface strain. While a small charge transfer affects the heterointerfaces, our results demonstrate that the half-metallic character of La$_2$Sr$_{1/3}$MnO$_3$ is fully maintained. (Reference: EPL, 102, 67009, 2013)

Magnetoresistance Anomalies in LaAlO$_3$/SrTiO$_3$(110): Fingerprints of Flat $d_{yz}/d_{xz}$ Band along [1-10] zigzag chain

HAIJJIAO MA, NUSNNI-NanoCore and Physics Department, NUS, QINFANG ZHANG, Yancheng Institute of Technology, YANG LIU, Laboratoire SPMS, Ecole Centrale Paris, ANIL ANNADI, NUSNNI-NanoCore, NUS, WENXIONG ZHOU, NUSNNI-NanoCore and Physics Department, NUS, THIRUMALAI VENKY VENKATESAN, ARIANDO ARIANDO, NUSNNI-NanoCore and Physics Department, NUS, ARIANDO RESEARCH GROUP COLLABORATION$^1$. Q. F. ZHANG TEAM, Y. LIU TEAM — We report novel features in the in-plane magnetoresistance (MR) of anisotropic two-dimensional electron gas (2DEG) at LaAlO$_3$/SrTiO$_3$(110) heterostructures, which unveil the existence of a flat band in this system. One of the striking features is an anisotropy of the MR with a "$d_{yz}/d_{xz}$"-wave"-like symmetry upon rotating the magnetic field $H$ within [110] plane at low temperature, which is caused by the existence of flat $d_{yz}/d_{xz}$ band. Combining with theoretical and experimental results, we confirm that a flat $d_{yz}/d_{xz}$ band formed along [1-10] Ti-O-Ti zigzag chain direction which might be very interesting for searching for topological state such as in superconducting regime.

Double perovskites nanoparticles: synthesis and magnetic properties (La$_2$NiMnO$_6$ vs La$_3$CoMnO$_6$)

YUANBING MAO, University of Texas-Pan American — Nanoparticles of double perovskite La$_2$BMnO$_6$ (B = Ni and Co) with average particle size of about 50 nm were successfully prepared using a facile, environmentally friendly, scalable molten-salt synthesis method at 700 °C in air. Their structural and morphological properties were characterized by X-ray diffraction and transmission electron microscopy. Their magnetic properties were evaluated using dc magnetic M–T and M–H, and ac magnetic susceptibility versus frequency, temperature, and field for the first time. The magnetic properties of these double perovskite nanoparticles indicate that they possess very different magnetic behaviors. The following results will be discussed: (i) field-cooled and zero-field-cooled magnetization curves become divergent at their Curie temperature, i.e. 275 K and 210 K for La$_2$NiMnO$_6$(LNMO) and La$_2$CoMnO$_6$(LCMO) nanoparticles, respectively, which are almost unchanged from their bulk and thin film counterparts. (ii) ac susceptibility indicates that the LNMO particles are much more complex structurally and may have anti-site defects or a second-phase with a different transition temperature. For a better understanding of the nature of the magnetic state and dynamic characteristics observed here for these LNMO and LCMO nanoparticles, further detailed studies are needed.

Possible Mechanisms in Atomic Force Microscope-Induced Nano-Oxidation Lithography (negative AFM tip case) in La$_{0.67}$Ba$_{0.33}$MnO$_{3-\delta}$ Thin Films on SrTiO$_3$(001)

GRACE YONG, Towson University, WILLIAM VANDERLINDE, Laboratory for Physical Sciences, E. KEVIN TANYI, Norfolk University, DAVID SCHAEPFER, CHRISTOPHER STUMPF, RAJESWARI M. KOLAGANI, Towson University — In this paper, we present possible microscopic mechanisms for La$_{0.67}$Ba$_{0.33}$MnO$_{3-\delta}$ films that have been nano-oxidized by an AFM tip that is negatively biased with respect the sample. Further analysis of comparative EDS elemental profile for unmodified film versus AFM negative tip-modified films yield fresh insights. We can qualitatively explain many of the observations with electrochemical half reactions, electrochemical migration and electromigration.

Heat flow and $\delta$-layers in Si nanowires

MEHMET B. BEBEK, T. MICHAEL GIBBONS, STEFAN K. ESTREICHER, Texas Tech — Modern semiconductor growth techniques allow the use of heterostructures in semiconductor devices such as $\delta$-layers or superlattices, and their behavior regarding heat flow is generating considerable interest. However, there is no fully 'first-principles' theoretical description of the interactions between heat flow and the interface between two dissimilar materials. In this contribution, we present the result of ongoing ab-initio, microcanonical, non-equilibrium MD simulations on Si/Ge or Si/C interfaces in a Si nanowire. We show that the 'spatially-localized vibrational modes' (SLMs) associated with the interface trap incoming bulk phonons for lengths of time ranging from dozens of hundreds of periods of oscillation. Then, the trapped phonons decay into lower frequency bulk phonons. This decay depends on the availability of receiving modes on either side of the interface rather than on the origin of the incoming flow of heat.

Local electrical imaging of tetragonal domains and field-induced ferroelectric domains in conducting SrTiO$_3$

HAIJJIAO MA, Nanocore and Physics D. NUS, S. SCHARINGER, U. Tuebingen, S.W. ZENG, Nanocore, M. LANGE, A. STHR, U. Tuebingen, Z. HUANG, T. VENKATESAN, Nanocore, R. KLEINER, U. Tuebingen, M. COEY, Nanocore, D. KOELLE, U. Tuebingen, A. ARIANDO, Nanocore and Physics D., NUS, NANO CORE TEAM, DIETER TEAM — We report intrinsic electric mapping of local conductivity due to tetragonal domains and twin boundaries in conducting STO. Multidomains and stripe monodomains were observed in different samples at low temperatures. The distribution of these domains changes on thermal cycling above the STO cubic-to-tetragonal structural transition temperature and on electric field gating. The domains split into narrower domains when we applied side gating and we attributed this to field-induced ferroelectric domain. Twin boundaries with different orientations were observed. Angles of these domain boundaries in (110) plane are 0, 55, 125 and 145 degrees. These angles were calculated from the intersection of twin planes and substrate cutting orientation. The domains split into narrower domain segments when T decreases below 30 K.

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$^1$Ariando Research Group is part of Department of Physics and of NUSNNI-NanoCore, the inter-faculty and multidisciplinary Nano-Institute at the National University of Singapore.

$^2$We acknowledge support from the NSF grant ECCS 1128586 at Towson University.
H1.00317 Probing the mechanical properties and microstructure of WS$_2$/Si$_x$Ge$_{1-x}$ multiphase thermoelectric material by nanoindentation, electron and focused ion beam microscopy methods

, FRANCISCO SOLA, FREDERICK DYNYS, NASA Glenn Res Ctr — Silicon germanium (SiGe) thermoelectric (TE) alloys have been traditionally used in radioisotope thermoelectric generators (RTG) NASA applications. While RTG applications is the main driver of our current research, we are exploring other applications in the energy harvesting arena. There is still a need to improve the TE figure of merit (ZT) of SiGe based TE alloys and we have been working on ways to improve it by incorporating tungsten di-silicide (WS$_2$) phases in to the matrix by directional solidification process. Considerable efforts have been focused until now in microstructural engineering methods that can lead to ZT improvement by microstructure optimization. Although critical for the previous mentioned applications, work pertinent to the mechanical integrity of WS$_2$/SiGe based TE materials is lacking. In this presentation, we report local mechanical properties (hardness, modulus and fracture toughness) and microstructure of WS$_2$/SiGe multiphase thermoelectric material by nanoindentation, scanning electron microscopy, focused ion beam and transmission electron microscopy methods.

H1.00318 Nanophononic metamaterial: Thermal conductivity reduction by dispersion-resonance hybridization

, MAHMOUD I. HUSSEIN, HOSSEIN HONARVAR, LINA YANG, University of Colorado Boulder — Engineered manipulation of phonons can yield beneficial thermal properties in semiconducting materials. One pivotal application relates to thermoelectric materials, or the concept of converting energy in the form of heat into electricity and vice-versa. The ability to use nanostructuring to reduce the thermal conductivity without negatively impacting the power factor provides a promising avenue for achieving high values of the thermoelectric energy conversion figure-of-merit, ZT. In this work, we propose a novel nanostructured material configuration that seeks to achieve this goal. Termed “nanophononic metamaterial,” the configuration is based on a silicon thin-film with a periodic array of pillars erected on one or two of the free surfaces. The pillars qualitatively alter the base thin-film phonon spectrum due to a hybridization mechanism between their local resonances and the underlying atomic lattice dispersion. Using lattice dynamics calculations and molecular dynamics simulations, we predict a drop in the thermal conductivity to as low as 50% of the corresponding uniform thin-film value despite the fact that the pillars add more phonon modes to the spectrum.

H1.00319 Magneto-thermoelectric effects in the two-dimensional electron gas of a HgTe quantum well due to THz laser heating by cyclotron resonance absorption

, MEHDI PAKMEHR, University at Buffalo, the State University of New York, CHRISTOPH BRUJÈNE, HARTMUT BUHMANN, LAURENS MOLENKAMP, University of Wuerzburg, BRUCE MCCOMBE, University at Buffalo, the State University of New York — HgTe quantum wells (QWs) have shown a number of interesting phenomena over the past 20 years, most recently the first two-dimensional topological insulating state. We have studied thermoelectric photovoltages of 2D electrons in a 6.1 nm wide HgTe quantum well induced by cyclotron resonance absorption (B = 2 - 5 T) of a focused THz laser beam. We have estimated thermo-power coefficients by detailed analysis of the beam profile at the sample surface and the photovoltage signals developed across various contacts of a large Hall bar structure at a bath temperature of 1.6 K. We obtain reasonable values of the magneto-thermopower coefficients.

1Work at UB was supported by NSF DMR 1008138 and the Office of the Provost, and at the University of Wuerzburg by DARPA MESO contract N6001-11-1-4105, by DFG grant HA5893/4-1 within SPP 1666 and the Leibnitz Program, and the EU ERC-AG Program (Project 3-TOP.

H1.00320 The concept of position-dependent mass and its consideration in the study of a particle subjected to different types of potential

, MARTIN MOLINAR-TABARES, Organismo de Cuenca Noroeste, Comisión Nacional del Agua, LAMBERTO CASTRO-ARCE, CARLOS FIGUEROA-NAVARRO, Departamento de Física e Ingeniería, Unidad Regional Sur, Universidad de Sonora, JULIO CAMPOS-GARCÍA, Departamento de Ciencias de la Salud, Departamento Cajeme, Universidad de Sonora — We present a study where is used the concept of position-dependent mass for a particle subjected to three kind of potential: infinite quantum potential well, harmonic oscillator potential and step potential. We solve the time-independent Schrödinger equation for each potential, considering different forms for the functional dependence of the mass respect the position. We obtain the ground state energy, the energies of some excited states and the corresponding probability densities. We make a comparison of the results with those that we would obtain if we consider an average mass for the particle.

H1.00321 Investigation of insulator-sandwich MCBJ device for single molecule detection

, AKIHIDE ARIMA, MAKUSU TSUTSUI, MASATERU TANIGUCHI, The Institute of Scientific and Industrial Research, Osaka University — Mechanically controllable break junction (MCBJ) is one of the most excellent methods for accurate measurements of electron transport through single molecules because of its stability and repeatability of nanometer-scale gap distance. This method has been recently used to investigate electric conductivity of individual nucleotides in an aqueous solution. However, traditional bare electrodes of MCBJ substrate generates unexpected ionic current, which deteriorates S/N ratio and distorts accurate control of the gap distance. To solve this problem, we report the novel MCBJ device architecture. Briefly, we covered whole junctions with insulating material. This insulator-sandwich architecture enables us to suppress such ionic current and flesh electrode surface can be used in measurement because the gap distance is controlled with a high accuracy. To solve this problem, we report the novel MCBJ device architecture. Briefly, we covered whole junctions with insulating material. This insulator-sandwich architecture enables us to suppress such ionic current and flesh electrode surface can be used in measurement because the gap distance is controlled with a high accuracy.

H1.00322 Sheared graphene: Electronic properties shaped by a mechanical instability

, ANDRES CONCHA, School of Engineering and Sciences, Adolfo Ibáñez University, Santiago, Chile., SHENGFENG CHENG, Department of Physics, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061, USA, LUCIAN COVACI, Department Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium, L. MAHADEVAN, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138,USA. — We explore the effects of shearing graphene ribbons on its geometry, and electronic properties. Inspired by macroscopic experiments, we show that spontaneous patterns appear when their local resonances and the underlying atomic lattice dispersion. Using lattice dynamics calculations and molecular dynamics simulations, we predict a drop in the thermal conductivity to as low as 50% of the corresponding uniform thin-film value despite the fact that the pillars add more phonon modes to the spectrum.

2H1.00317 Probing the mechanical properties and microstructure of WS$_2$/Si$_x$Ge$_{1-x}$ multiphase thermoelectric material by nanoindentation, electron and focused ion beam microscopy methods

AC was partially supported by Conicyt grant 79112004, and Fondecyt under grant 11130075. LC acknowledges individual support from FWO-Vlaanderen.
H1.00323 Ultrafast optical measurements of surface waves on a patterned layered nanostructure

BRIAN DALY, MATTEO BJORNSSON, AINE CONNOLLY, SUSHANT MAHAT, BRYAN RACHMILOWITZ, Vassar College, GEORGE ANTONELLI, Antonelli Research & Technology LLC, ALAN MYERS, HUI-JAE YOO, KANWAL SINGH, SEAN KING, Illinois Corporate — We report ultrafast optical pump-probe measurements of 12 – 54 GHz surface acoustic waves (SAWs) on patterned layered nanostructures. These very high frequency SAWs were generated and detected on the following patterned film stack: 25 nm physically vapor deposited TiN / 180 nm porous PECVD-grown a-SiO\(_2\)C:H dielectric / 12 nm non-porous PECVD-grown a-SiO\(_2\)C:H etch-stop / 100 nm CVD-grown a-SiO\(_2\) / Si (100) substrate. The TiN layer was dry plasma etched to form lines of rectangular cross section with pitches of 420 nm, 250 nm, 180 nm, and 168 nm and the lines were oriented parallel to the [110] direction on the wafer surface. The absorption of ultrafast pulses from a Ti:sapphire oscillator operating at 800 nm generated SAWs that were detected by time-delayed probe pulses from the same oscillator via a reflectivity change (ΔR). In each of the four cases the SAW frequency increased with decreasing pitch, but not in a linear way as had been seen in previous experiments of this sort. By comparing the results with mechanical simulations, we present evidence for the detection of different types of SAWs in each case, including Rayleigh-like waves, Sezawa waves, and leaky or radiative waves.

H1.00324 Molecular Dynamics Simulations of Surface Acoustic Waves on Patterned Layered Nanostructures

MATTEO BJORNSSON, AINE CONNOLLY, SUSHANT MAHAT, BRYAN RACHMILOWITZ, BRIAN DALY, Vassar College, GEORGE ANTONELLI, Antonelli Research & Technology LLC, ALAN MYERS, KANWAL SINGH, MIU-JAE YOO, SEAN KING, Illinois Corporation — We report coarse-grained molecular dynamics (MD) simulations of surface acoustic waves on patterned layered nanostructures. The simulations were designed for comparison with samples consisting of the following patterned film stack: 25 nm physically vapor deposited TiN / 180 nm porous PECVD-grown a-SiO\(_2\)C:H / 12 nm non-porous PECVD-grown a-SiO\(_2\)C:H etch-stop / 100 nm CVD-grown a-SiO\(_2\) / Si (100) substrate. Ultrafast optical experiments on these samples have detected high frequency surface waves in the range of 10s of GHz. The MD simulation demonstrates the presence of strongly excited modes at frequencies that closely match those found in the experiments. Moreover, the simulation predicts that the type of surface wave mode detected should change depending on the pitch. For larger pitch, Rayleigh-like waves are predicted, but for smaller pitch, Sezawa waves (surface waves with properties similar to free plate modes of the thin films) are predicted. The MD simulation also demonstrates the cutoff wavelength for the Sezawa modes, as is reflected in the experimental results and as is also predicted by isotropic elastic calculations of the surface modes of a thin film on an infinite substrate.

H1.00325 Evolution of interface and surface structures of ZnO/Al2O3 multilayers upon rapid thermal annealing

H.H. LIU, Q.Y. CHEN, C.F. CHANG, W.C. HSIEH, National Sun Yat-Sen University, Taiwan, P.V. WADEKAR, University of Liverpool, UK, H.C. HUANG, National Sun Yat-Sen University, Taiwan, H.H. LIAO, Enli Technology Inc., Taiwan, H.W. SEO, University of Arkansas, USA, W.K. CHU, University of Houston, USA — ZnO/Al2O3 multilayers were deposited on sapphires by atomic layer deposition at 85°C. This low substrate temperature ensures good interface smoothness useful for study of interfacial reaction or interdiffusion. Our study aimed at the effects of rapid thermal annealing at different annealing temperatures and times and P\(_{O_2}\)/P\(_{N_2}\). RHEED patterns during and post deposition of Ag thin films on MgO, Al2O3, STO and Si. HR-TEM and electron diffraction were carried out to correlate the microstructures and interfacial alignments as a result of the reactions.

H1.00326 Pulsed Laser Deposition and Reflection High-Energy Electron Diffraction studies of epitaxial long range order, nano- and microstructured Ag thin films grown on MgO, Al2O3, STO and Si

DANIEL VELAZQUEZ, RACHEL SEIBERT, HAMDI MAN, LINDA SPENTZOURIS, JEFF TERRY, Illinois Institute of Technology — Pulsed Laser Deposition is a state-of-the-art technique that allows for the fine tunability of the deposition rate, highly uniform and epitaxial sample growth, the ability to introduce partial pressures of gases into the experimental chamber for growth of complex materials without interfering with the energy source (laser). Pulsed Laser Deposition is a state-of-the-art technique that allows for the fine tunability of the deposition rate, highly uniform and epitaxial sample growth, the ability to introduce partial pressures of gases into the experimental chamber for growth of complex materials without interfering with the energy source (laser). An auxiliary in situ technique for growth monitoring, Reflection High-Energy Electron Diffraction, is a powerful characterization tool for predictability of the surface physical structure both, qualitatively and quantitatively. RHEED patterns during and post deposition of Ag thin films on MgO, Al2O3, Si and STO substrates are presented and their interpretations are compared with surface imaging techniques (SEM, STM) to evidence the usefulness of the technique.

H1.00327 Indeterminate form 0/0 and tunneling in double quantum wells

IGOR FILIKHIN, BRANISLAV VL AHOC, North Carolina Central University — We study single electron tunneling between localized and delocalized states in double InAs/GaAs quantum wells (DQWs). Spectral distribution of localized (or delocalized) states demonstrates high sensitivity on inter-dot distance. The tunneling goes consecutively from the higher energy levels to the ground state when the inter-dot distance decreases. The spectrum is presented by set of quasi-doublets and may be described by three parts: localized states, delocalized states, and states with different probability for localization in each QW of DQW. For the last states, the ratio W/ ΔE of the wave functions overlapping integral W and the electron energy difference ΔE of isolated left and right QWs is a weight coefficient in the expansion of wave function on the basis of the wave functions of isolated QWs. In case of weakly coupled QWs in DQW the indeterminate form 0/0 takes a place for the electron wave function. It is found that a small violation of the DQW shape symmetry drastically affects tunneling. This effect also appears as a numerical instability calculations for small variations of input parameters of numerical procedure.

H1.00328 Emission energy control of semiconductor quantum dots using phase change material

SHOHEI KANAZAWA, YU SATO, ARIYOSHI YAMAMURA, TOSHIHARU SAIIK, Keio Univ — Semiconductor quantum dots have paid much attention as it is a promising candidate for quantum, optical devices, such as quantum computer and quantum dot laser. We propose a local emission energy control method of semiconductor quantum dots using applying strain by volume expansion of phase change material. Phase change material can change its phase crystalline to amorphous, and the volume expand by its phase change. This method can control energy shift direction and amount by amorphous religion and depth. Using this method, we matched emission energy of two InAs/InP quantum dots. This achievement can connect to observing superradiance phenomenon and quantum dot coupling effect.
H1.00320 Magnetic field effects and nodal ground states in InP nanowire. TIAGO DE CAMPOS, PAULO EDUARDO DE FARIÁ JÚNIOR, Universidade de São Paulo, State University of New York at Buffalo, IGOR ZUTIC, State University of New York at Buffalo, GUILHERME SIPAHNI, Universidade de São Paulo, State University of New York at Buffalo — Semiconductor nanowires (NWs) have attracted great interest in the last decade because of their unique optical, electronic, and spin-dependent properties. They are among the leading candidates to observe exotic states, such as Majorana Fermions [1]. In asynnealing situation of a single particle confined in a quantum dot, it was predicted that the valence band ground state with a node is possible and was attributed to the formation of orbital textures [2]. This peculiar behavior may also be present in wurtzite InP NWs with a diameter less than 10 nm [3]. The presence of nodal state modifies its basic optical properties, such as the degree of off-linear polarization. Here we study the change in these states when an external magnetic field is applied along nanowire axis. We studied wurtzite InP [0001] and zincblende InP NWs calculated within a k.p method formulation that describes both crystal phases in a single-particle Hamiltonian [4] and account for the applied magnetic field.


H1.00330 Polarization dependent Optical Reflectance and Electroreflectance measurements of GaAs/AlGaAs multiple quantum well Bragg structure. MIM NAKARMI, Department of Physics, Brooklyn College-CUNY, NARESH SHAKYA, Department of Applied Physics, NYU-Polytechnic School of Engineering, VLADIMIR CHALDYSHEV, Ioffe Physico-Technical Institute, Russia. — Electoreflectance spectroscopy provides sharp and derivative-like spectral features in the energy region of excitonic transitions, while suppressing uninteresting background effects due to electro-modulation. We employed both electroreflectance and optical reflectance spectroscopy to probe excitonic transitions in a GaAs/AlGaAs multiple quantum well (MQW) Bragg structure. The sample used in this experiment consists of 60 periods of quantum well structures with GaAs well layer (13 nm) and AlGaAs barrier layer (94 nm), grown by molecular beam epitaxy on a semi-insulating GaAs substrate. We observed a significant enhancement of excitonic features at the x(e2-hh2) exciton transitions due to double resonance along with sharp features of heavy-hole and light-hole ground state x(e1-hh1) and x(e1-lh1) exciton transitions around incident angle of 23 degree. We will present results on polarization dependent optical reflectance and electroreflectance measurements of this structure and discuss the effect of polarization in the first and second energy states.

1This work was partially supported by PSC-CUNY research grant.

H1.00331 Effective masses of Quasi-2D electrons in InGaAs/GaAsSb modulation-doped heterostructures. IMTIAZ TANVEER, BRUCE MCCOMBE, University at Buffalo, The State University of New York, HERMANN DETZ, GOTTFRIED STRASSER, Vienna University of Technology, Vienna, Austria — The electronic properties of In0.53Ga0.47As/GaAsSb.0.5Sb.0.52 2D electron gas (2DEG) systems, in spite of their use in high power electronics, have not been extensively investigated. Recently, they have been suggested as potential materials for IR quantum devices such as quantum cascade lasers (QCL), and they also show a strong Rashba effect. Here accurate values of the effective masses are important. Two remotely donor (Si)-doped samples grown by MBE with a 2DEG at the single heterostructure interface were studied by FIR magneto-transmission spectroscopy with a BOMEM FTIR spectrometer. The maximum mobilities (near 70 K) are 43,000 cm2/Vs and 36,000 cm2/Vs with corresponding carrier densities of 1.07 × 10^{12} cm^{-2} and 2.13 × 10^{12} cm^{-2}, respectively. Cyclotron resonance measurements between 4T and 9T yielded m* = 0.0495 m0 for the more heavily doped sample. Individual transmission profiles in this case showed broadening toward high-energy, which may be due to contributions to the overall absorption profile from higher occupied subbands. The lower density sample shows an energy vs B dependence that does not extrapolate to zero at B = 0. The origin of this behavior will be discussed.

H1.00332 Carrier thermalization dynamics in single Zincblende and Wurtzite InP nanowires. YUDA WANG, HOWARD JACKSON, LEIGH SMITH, Dept. of Physics, Univ. of Cincinnati, TIM BURGESS, SURIATI PAINAM, PHILIPPE CAROFF, HOE TAN, CHENNUPATI JAGADISH, Dept. of Electronic and Materials Engineering — Using transient Rayleigh scattering (TRS) measurements, we obtain photoexcited carrier thermalization dynamics for both zincblende (ZB) and wurtzite (WZ) InP single nanowires (NW) with picosecond resolution. A phenomenological fitting model based on direct band to band transition theory is developed to extract the electron-hole plasma density and temperature as a function of time from TRS measurements of single nanowires which have complex valence band structures. We find that the thermalization dynamics of hot carriers depends strongly on material (GaAs NW vs. InP NW) and less strongly on crystal structure (ZB vs. WZ). The thermalization dynamics of ZB and WZ InP NWs are similar. But a comparison of the thermalization dynamics in ZB and WZ InP NWs with ZB GaAs NW reveals more than an order of magnitude slower relaxation for the InP NWs. We interpret these results as reflecting their distinctive phonon band structures which lead to different hot phonon effects. Knowledge of hot carrier thermalization dynamics is an essential component for effective incorporation of nanowire materials into electronic devices. We acknowledge the NSF through DMR-1105362, 1105121 and ECCS-1100489, and the Australian Research Council.

H1.00333 Fluorescent DNA-templated silver nanoclusters. DAMYTO NYKYPANCHUK, Brookhaven National Laboratory, RUOQIAN LIN, YOLANDA SMALL, CUNY — Silver nanoclusters synthesized in the presence of templating DNA molecules show tunable optical properties that depend on cluster size and structure as well as on templating DNA sequence. In this paper we study the effect of DNA sequence and temperature on the cluster photoluminescence and discuss the results in the context of thermodynamics of DNA bases binding to the silver atoms in the clusters.

H1.00334 Plasmon Enhanced Ultrathin Film Broad-Band Nanoporous Absorber. JIN-YOU LU, Masdar Institute of Science and Technology, LONG LIU, Tsinghua University, KYLIE WILKE, MIT, SUMAYA NOORULLA, Masdar Institute of Science and Technology. — Ultra-thin absorbing films have attracted much attention due to their strong interference persisted inside the lossy dielectric film, which has much smaller thickness compared with conventional resonators. The absorber was realized by coating a lossy dielectric film with tens of nanometers in thickness on a metallic substrate. The ultrathin absorber was further developed to achieve broad-band absorption. This concept is realized by coating ultrathin absorbing Ge/Au films on nanoporous substrate, where the LSP mode is supported by pore-shape cavities. The near-field optical properties of ultrathin film on nanoporous substrate are analyzed by using the finite difference time domain method to study the spectroscopy and energy flow patterns. Simulation shows the absorption increases with the pore radius until the pore is too large to sustain LSP. Light is trapped in nanopores and penetrated into the lossy dielectric film around the pore entrance.

1Supported by cooperative agreement between Masdar Inst and MIT.
H1.00335 Optical Properties of CdSe Nanocrystalline Photoanodes AMANDA LESAR, ROHANA GARUTHARA, Hofstra University — Cadmium selenide (CdSe) nanocrystalline photoanodes were prepared by chemical solution deposition, with deposition time varied from 24 hours to 120 hours. Photoluminescence (PL) spectroscopy, reflectance and transmittance spectra, and photoelectric current were measured to optically characterize each sample. Photoelectric current was measured in a liquid junction configuration, with sodium sulfide as the electrolyte and platinum foil as the electrode. The PL, reflectance, and transmittance spectra were measured for each sample from 79 K to room temperature. Chemical solution deposition should lead to quantum size effects, as longer deposition times form larger size nanocrystals. Quantum size effects were observed, as longer depositions times led to a shift towards lower energy in the peak of the PL spectra. The temperature dependence of the PL peak energy position was also analyzed; as the temperature increased, the peak shifted towards higher energy. Using the reflectance and transmittance spectra, the absorption coefficient $\alpha$ was calculated, and the Tauc’s plot of $(\alpha h\nu)^2$ versus $(h\nu)$ was graphed. A correlation between the observed absorption edge and the PL spectra was seen, as the absorption edge energy was approximately equal to the PL energy peak.

H1.00336 Plasmon excitations of multi-layer graphene interacting with a conducting substrate , PAULA FEKETE, US Military Academy at West Point, NY, GODFREY GUMBS, Hunter College, City University of New York — We generalize the procedure for calculating the plasmon excitations of a 2D layer that is Coulo-coupled to a thick conducting substrate to the case when there is an arbitrary number of layers. In this work, we will present results for the plasmon excitations for up to five layers with arbitrary separation, energy gap between the valence and conduction bands for graphene and doping concentrations. Our procedure involves determining the inverse dielectric function for the composite hybrid system in the random-phase approximation (RPA). Effects due to nonlocality will be investigated.

H1.00337 Invisibility’s Flicker: Detecting Thermal Cloaks via Transient Effects1, SOPHIA SKLAN, Massachusetts Inst of Tech-MIT, XUE BAI, BAOWEN LI, National University of Singapore, XIANG ZHANG, University of California, Berkeley — Recent research on the development of a thermal cloak has concentrated on engineering an inhomogeneous thermal conductivity and homogeneous volumetric heat capacity. While the perfect cloak of inhomogeneous $\kappa$ and $\rho_c$ is known to be exact (no signals scattering or penetrating to the cloak’s interior), no such analysis has been considered for this case. Using analytic, computational, and experimental techniques, we demonstrate that these approximate cloaks are detectable. Although they work as perfect cloaks in the steady-state, their transient (time-dependent) response is imperfect and a detectable amount of heat is scattered. This is sufficient to determine the presence of a cloak and any heat source it contains, but the material composition hidden within the cloak is not detectable in practice.

H1.00338 Generating Steep Phase Anisotropy With Zero-Backscattering By Arrays of Coupled High Permittivity Dielectric Nanoresonators , FENG WANG, CINT, Los Alamos National Lab, QI-HUO WEI, Liquid Crystal Institute, Kent State University, HAN HTOON, CINT, Los Alamos National Lab — Simultaneous excitation of electric and magnetic dipolar modes in high-permittivity dielectric nano-resonators can lead to zero-backscattering, i.e. full transmission. Here, we numerically demonstrate that stable or unstable zero-backscattering by 2-dimensional (2D) arrays of Si nano-resonators can be realized. We also show that this Si nano-resonator array with anisotropic periodicity can generate approximate 2π optical phase anisotropy for the transmitted light at the wavelength of zero-backscattering. By introducing strong Fano-type coupling into unit cells of the array, ultra-steep phase anisotropy can be achieved. These special optical properties promise applications in various transmissive photonic devices, and we show their potential applications in transmissive polarization conversion and sensing.

H1.00339 Calculus of bands and profiles of study the system mirror - resonance of the Fibonacci Pt/Zn, LAMBERTO CASTRO-ARCE, Departamento de Fisica e Ingenieria, Unidad Regional Sur, Universidad de Sonora, CARLOS FIGUEROA-NAVARRO, Departamento de Ingenieria Industrial, Universidad Regional Centro, Universidad de Sonora, JULIO CAMPOS-GARCIA, Departamento de Ciencias de la Salud, Unidad Cajeme, Universidad de Sonora, MARTIN MOLINAR-TABARES, Organismo de Cuenca Noroeste, Comision Nacional del Agua, FELIPE RAMOS-MENDIETA, Departamento de Investigacion en Fisica, Universidad Regional Centro, Universidad de Sonora, BETZABE MANZANARES-MARTINEZ, Departamento de Fisica, Universidad Regional Centro, Universidad de Sonora — In order to analyze the behavior of a mirror — located resonance of 2pi, in a given system and with a given filling factor equal to 0.4 a study has been realized in an arrangement fibonacci, also in periodic slabs jobs. It is observed how in a study of profile that some waves are annulled giving birth to the mirror placed in 2pi. With regard to the resonance in a profile study the maxima are in certain structure Pt Pt Zn Pt Pt. Even if we increase the number of repetitions these are preserved, that means that they are related to effects of segments isolated inside the multilayer.

H1.00340 Atomic structure prediction of metal clusters using the evolutionary algorithm , NABIL AL-AQTASH, University of Nebraska- Omaha, KHALDOUN TARAWNEH, Princess Sumaya University for Technology, RENAT SABIRIANOV, University of Nebraska- Omaha — The evolutionary algorithm coupled with density functional (DFT) method is used to identify the global energy minimum atomic structure of metal clusters. Using evolutionary crystal structure optimization algorithm, as implemented in USPEX, we studied the atomic structure, binding energies, and magnetic properties of 13-atom Cu, Co and Cr clusters. A set of metastable and global minimum atomic structures are identified. Several new lower energy configurations were identified for 13-atom Cu, Co and Cr clusters and previous known atomic structures were confirmed by our calculations. We found that the Cu13 cluster has a distorted hexagonal bilayer (HBL) –like structure, which is composed by two layers as in the ideal HBL structure. The distorted HBL Cu13 is 1.17 eV lower in total energy compared to close-packed icosahedral (ICO) configuration, which reported as the lowest-energy structure for Cu13 in previous studies. Our calculations show that Cu13 has an ideal HBL structure and Cr13 cluster has distorted ICO structure, which are consistent with the previous studies. Moreover, our calculations show that Cr13 has another lower energy atomic configuration with 0.003 eV difference form ICO. Cr13 has ferrimagnetic (FIM) interaction which plays an important role in finding the lowest energy structure. We discuss the predictive capabilities of evolutionary algorithms for nanoclusters.

H1.00341 Electron with position-dependent mass confined in a two-dimensional infinite square well , MARTIN MOLINAR-TABARES, Organismo de Cuenca Noroeste, Comision Nacional del Agua, CARLOS RUVALCABA-CORNEJO, Departamento de Matematicas, Unidad Regional Centro, Universidad de Sonora — In order to have a case of study for introduce the concept of position-dependent mass, we propose to analyze the following case. Creating a rectangular crystal structure from the two-dimensional deposit of GaAs and Al0.35Ga0.65As on a substrate, we study the confinement of an electron with position-dependent effective mass. Knowing how the electron mass of the electron and its potential energy varies with the concentration of the semiconductor, we solve the time-independent Schrödinger equation using a linear combination of wave functions of a particle enclosed inside a two-dimensional square well with infinite potential walls. The ground state energy and the energies of some excited states with the probability density of these states are found. Making a two-dimensional growth of the structure we analyze if appears sub-bands energy and if the Bloch theorem manifests. We compare our results with those that we would obtain if we consider and constant effective mass inside the crystal.
Conformational electroresistance and hysteresis in nanoclusters

H1.00344

Conformational electroresistance and hysteresis in nanoclusters

ZHANG, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida — Abstract: Existence of multiple thermodynamically stable isomer states is one of the most fundamental properties of small clusters. We show that the conformational dependence of the Coulomb charging energy of a nanocluster leads to a giant electroresistance, where charging induced conformational distortion changes the blockade voltage. The intricate interplay between charging and conformation change is demonstrated in a nanocluster Zn$_3$O$_4$ by combining a first-principles calculation with a temperature-dependent transport model. The predicted hysteretic Coulomb blockade staircase in the current-voltage curve adds another dimension to the rich phenomena of tunneling electroresistance. The new mechanism provides a better controlled and repeatable platform to study conformational electroresistance.

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H1.00343

Finite-size scaling study of the one-dimensional Bose-Hubbard model via matrix product state representations

SUNG-BEEN PARK, MIN-CHUL CHA, Hanyang University — The Bose-Hubbard model is a prototypical simple model showing quantum phase transition with a continuous symmetry. In one dimension, the quantum critical properties of the model has been studied via various methods, but still some basic properties remain unknown, such as the exact location of the critical point. It is a computational challenge to study this model with more elaborated numerical methods. The matrix product state (MPS) representations are new variational solutions to one-dimensional quantum systems. By using this method to find the ground state, we study the critical properties of the one-dimensional Bose-Hubbard model with a periodic boundary condition. Finite-size scaling analysis provides the phase diagram and the critical exponents.

H1.00345

Solution of the homogeneous electromagnetic wave equation with velocity time depending on the discrete space-time

JULIO CAMPOS-GARCIA, Departamento de Ciencias de la Salud, Universidad Caxem, Universidad de Sonora, MARTIN MOLINAR-TABARES, Organismo de Cuenca Noroeste, Comision Nacional del Agua, LAMBERTO CASTRO-ARCE, Departamento de Fisica e Ingenieria, Universidad Regional Sur, Universidad de Sonora, CARLOS FIGUEROA-NAVARRO, Departamento de Ingenieria Industrial, Universidad Regional Centro, Universidad de Sonora, RODRIGO ROSAS-BURGOS, Departamento de Fisica, Universidad Regional Centro, Universidad de Sonora — We present in this meeting the solution of the homogeneous electromagnetic wave equation with a speed of light time depending on the discrete space-time. The solutions are compared with those that are obtained for a standard case, where the speed of light is constant. In addition, the limiting cases of the discrete and continuum space-time are analyzed.

H1.00346

Fabrication and In-situ TEM Characterization of Freestanding Graphene Nanoribbons Devices

QING WANG, RYO KITAURA, SHOJI SUZUKI, HISANORI SHINOHARA, Department of Chemistry, Nagoya University, SHINOHARA TEAM — Edge-dependent electronic properties of graphene nanoribbons (GNRs) have attracted intensive interests. To fully understand the electronic properties of GNRs, the combination of precise structural characterization and electronic property measurement is essential. For this purpose, a new experimental technique using freestanding GNR devices has been developed, leading to the simultaneous characterization of electronic properties and edge structure of GNRs. To prepare freestanding GNR devices, graphene was first transferred on a Si substrate with an open slit covered by a silicon dioxide layer, and then silicon dioxide membrane underneath the graphene was etched away by buffered hydrogen fluoride acid. The so-prepared freestanding graphene device was assembled to a home-made TEM holder for in-situ characterization. The freestanding graphene was sculpted by a focused electron beam in TEM, purified and narrowed by Joule heating down to several nanometers width. Structure-dependent electronic properties were performed in TEM. We have observed significant increase in resistance and semiconductive behavior became more dominant with decreasing width of GNR.

H1.00347

Surface Premelting Coupled with Bulk Phase Transitions in Colloidal Crystals

BO LI, FENG WANG, DI ZHOU, XIN CAO, YI PENG, The Hong Kong University of Science and Technology, RAN NI, Universiteit van Amsterdam, MALJIA LIAO, YILONG HAN, The Hong Kong University of Science and Technology — Colloids have been used as outstanding model systems for the studies of various phase transitions in bulk, but not at interface yet. Here we obtained equilibrium crystal-vapor interfaces using tunable attractive colloidal spheres and studied the surface premelting at the single-particle level by video microscopy. We found that monolayer crystals exhibit a bulk isostructural solid-solid transition which triggers the surface premelting. The premelting is incomplete due to the interruption of a mechanical-instability-induced bulk melting. By contrast, two- or multilayer crystals do not have the solid-solid transition and the mechanical instability, hence they exhibit complete premelting with divergent surface-liquid thickness. These novel interplays between bulk and surface phase transitions cast new lights for both types of transitions.

H1.00348

Entrance Pressure Fluctuation of LLDPE in Capillary Flow

HAIQING HU, SHUAI LI, LUYAO YAN, TONGJIE SUN, LINLIN LIU, Ministry of Education/Shandong Provincial Key Laboratory of Rubber-plastics; Qingdao University of Science and Technology, HE CHENG, Dongguan Institute of Neutron Physics, China; China Spallation Neutron Source, Institute of High Energy Physics CAS, Dongguan — Oscillating flow, which usually refers to the whole capillary pressure oscillation under constant piston speed, has been widely studied as an important instability phenomenon in capillary flow. The coil-stretch transition of entangled polymer molecules can be considered as a critical factor resulting in oscillating flow, which is only observed under controlled piston speed. It has been theorized by Weill since 1980 that the appearance of surface distortions may originate from a high-frequency oscillatory flow created at the die entry, but no experimental evidence has been found to prove it over 30 years. Wall slippage plays an important role in capillary extrusion flow instability for LLDPE melt. Local stick-slip transition leads to perturbations on the exit stress and sharkskin distortion, while global stick-slip transition perturbations on the exit pressure flow. This article has revealed the correspondence relationship between entrance pressure fluctuation and exit stress perturbation experimentally and illuminated it by Uhland model. We have further confirmed the idea that local wall-slip transition can induce the entrance pressure fluctuation. In brief, the molecular disentanglement in die exit determines the critical shear stress of entrance pressure fluctuation.

3 This work was supported by NSFC (51373884)

H1.00349

Superconductivity and Magnetism from First Principles

ANDREAS LINSCHEID, ANTONIO SANNA, FRANK ESSENBERGER, E.K.U. GROSS, Max Planck Institute of Microstructure Physics — Magnetism has intriguing effects in superconductors. On the one hand static magnetic fields are known to suppress the superconducting state while dynamic spin-fluctuations are the probable candidate to explain the pairing in the Fe-based Superconductors. Achieving an ab-initio description is important. First, because this allows to compute the critical field and whether a local coexistence of magnetic and superconducting phases exist. Second, the critical temperature of a material is among the predicted properties which allows to search yet unknown superconductors on a computer. The Density Functional Theory for Superconductors (SCDFT) has been very successful in predicting Tc of phonon mediated superconductors. We include the magnetic density into SCDFT so that the electronic Kohn-Sham system now reproduces the electronic density ρ(r), the order parameter of superconductivity Δ(r, y) and the magnetic density n(r). We derive the xc-potential and discuss some first results. Furthermore, we discuss an effective electron interaction mediated by spin-flip processes based on the exact spin susceptibility. We drive a xc-functional for SCDFT that includes this effective interaction and present some results.
H1.00350 Iterative backflow renormalization procedure for many-body ground state wave functions of strongly interacting normal Fermi liquids. MICHELE RUGGERI, DEMOCRITOS National Simulation Center, Istituto Officina dei Materiali del CNR and SISSA, Via Bonomea 265, I-34136 Trieste, Italy, MICHELE TADDEI, Dipartimento di Fisica, Sapienza Universita' di Roma Piazzale A. Moro 2, I-00185, Roma, Italy, SAVERIO MORONI, DEMOCRITOS National Simulation Center, Istituto Officina dei Materiali del CNR and SISSA, Via Bonomea 265, I-34136 Trieste, Italy, MARKUS HOLZMANN, LPMC, UMR 5493 of CNRS, Universite’ Grenoble Alpes, F-38100 Grenoble, France — We propose a novel trial wavefunction for the ground state of a normal Fermi liquid. We apply iterative backflow transformations to obtain a sequence of renormalized coordinates. At each iteration two and three body correlations between quasiparticles are taken into account. We use these wavefunctions to compute the ground state energy of liquid 3He at freezing density in two dimensions with Variational and Diffusion - Fixed Node Monte Carlo simulations. Comparing with exact transient estimate results for systems with small number of particles, we find that variance extrapolations provide accurate results for the true ground state together with stringent lower bounds. For larger systems these bounds can in turn be used to quantify the systematic bias of fixed-node calculations. These wave functions are size consistent and the scaling of their computational complexity with the number of particles is the same as for standard backflow wave functions.

H1.00351 Comparative Study Between GGA and LDA Approximation Using First-Principles Calculations of Structural, Electronic, Optical and Vibrational Properties of CaTiO3 Crystal , SUBENIA MEDEIROS, MAEVA ARAUJO, Universidade Federal Rural do Semi-Árido — The structural, electronic, vibrational, and optical properties of perovskite CaTiO3 in the cubic, orthorhombic, and tetragonal phase are calculated in the framework of density functional theory (DFT) with different exchange-correlation potentials by CASTEP package. The calculated band structure shows an indirect band gap of 1.88 eV at the Γ - H points in the Brillouin zone to the cubic structure, a direct band gap of 2.41 eV at the Γ - I points to the orthorhombic structure, and an indirect band gap of 2.31 eV at the M – I’ points to the tetragonal phase. It is still known that the CaTiO3 has a static dielectric constant that extrapolates to a value greater than 300 at zero temperature, and the dielectric response is dominated by low frequency (ν ≈ 90cm⁻¹) polar optical modes in which cation motion opposes oxygen motion. Our calculated lattice parameters, elastic constants, optical properties, and vibrational frequencies are found to be in good agreement with the available theoretical and experimental values. The results for the effective mass in the electron and hole carriers are also presented in this work.

H1.00352 Electron relaxation of DNP free radicals BDPA and DPPH at W-band , ARMIN KHAMOSHI, UT Dallas, PAVANEET KAUR, LKAI SONG, NHMF, LLOYD LUMATA, UT Dallas — The stable, spin-1/2 organic free radicals BDPA and DPPH are efficient polarizing agents for dissolution dynamic nuclear polarization (DNP). Despite the hydrophobic nature of these two free radicals, BDPA and DPPH can be dissolved in specialized solvents such as sulfurane or dimethyl sulfoxide. In this work, we have investigated the temperature dependence of the spin-lattice relaxation rate 1/T1 of these two DNP free radicals at W-band from 250 K down to 4 K. We have found that at high temperature above 40 K the relaxation rates of these free radicals (at optimum DNP concentration) behave closely according to the Raman process prediction. At lower temperature below 40 K, the relaxation rate slows down according to the direct process behavior. The results obtained here may elucidate the correlation between the relaxation of electrons and the efficiency of these free radicals in DNP.

H1.00353 Power laws and extreme values in antibody repertoires , SEBATIEN BOYER, DIPANWITA BISWAS, NATALA SCARAMOZZINO, ANANDA SOSHEE KUMAR, Laboratoire Interdisciplinaire de Physique - CNRS & Universite Grenoble Alpes, CLEMENT NIZAK, ESPCI ParisTech/CNRS, OLIVIER RIVOIRE, Laboratoire Interdisciplinaire de Physique - CNRS & Universite Grenoble Alpes — Evolution by natural selection involves the succession of three steps: mutations, selection, and proliferation. We are interested in describing and characterizing the result of selection over a population of many variants. After selection, this population will be dominated by the few best variants, with highest propensity to be selected, or highest “selectivity.” We ask the following question: how is the selectivity of the best variants distributed in the population? Extreme value theory, which characterizes the extreme tail of probability distributions in terms of a few universality class, has been proposed to describe it. To test this proposition and identify the relevant universality class, we performed quantitative in vitro experimental selections of libraries of > 10⁶ antibodies using the technique of phage display. Data obtained by high-throughput sequencing allows us to fit the selectivity distribution over more than two decades. In most experiments, the results show a striking power law for the selectivity distribution of the top antibodies, consistent with extreme value theory.

H1.00354 Single Crystal Diffuse X-ray Scattering Using Continuous Rotation1, MATTHEW KROGSTAD, OMAR CHMAISSEM, KEITß TÁDEDEI, Northern Illinois University, Argonne National Laboratory, JARED ALLRED, RAYMOND OSBORN, STEPHAN ROSENKRANZ, JUSTIN WOZNIAK, Argonne National Laboratory — Single crystal diffuse scattering provides a measure of the 3D pair distribution function and is thus useful for investigating short-range order in materials. Using very bright synchrotron X-ray sources and fast area detectors, large volumes of reciprocal space can be mapped quickly with a dynamic range large enough to measure both Bragg peaks and the much weaker diffuse scattering. With the appropriate tools for processing and analyzing large data sets (10 to 30GB), this technique can be used to track changes in the defect structures of a material as a function of different parameters, providing a sensitive and efficient method for investigating phenomena associated with disorder. We have been developing methods of measuring diffuse scattering using continuous sample rotations (shutterless mode) at the Advanced Photon Source, and will show data from several systems, including iron nitrides, for a range of temperatures and doping levels.

1Supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

H1.00355 Chemical Bonding Forces and Metalization of Hydrogen , IVAN NAUMOV, RUSSELL HEMLEY, Carnegie Inst of Washington, CARNEGIE INST OF WASHINGTON COLLABORATION — Recent theoretical and experimental studies reveal that compressed molecular hydrogen at 200-350 GPa transforms to layered structures consisting of distorted graphene sheets. The new phases of dense solid hydrogen contrast with the long-held view that symmetric close-packed, ambient alkali-metal-like structures form at these high pressures — this raises the question about the nature and fate of molecular bonding in hydrogen on compression. The realization of such unexpected structures can be explained by consideration of simple low-dimensional model systems— H6 rings and graphene-like monolayers. Both molecular quantum chemistry and well-tested solid state approaches show that these model systems like aromatic hydrocarbons exhibit a special stability, associated with the completely filled set of bonding orbitals or valence bands. This close-shell effect persists in progressing to the real layered structures where it prevents the dielectric energy gap from closing, thus delaying the pressure-induced metalization. The latter nevertheless can occur upon further compression via destroying the closed shell electronic structure which is mainly determined by the 1S electrons. The most likely scenario is the lowering of the bonding bands (their bottoms) stemming from the unoccupied atomic 2s and 2p orbitals [1]. This research was supported by EFRee, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DESC0001057. [1] I. Naumov and R. J. Hemley, Acc. Chem. Res. 47, 3551-3559 (2014).
H1.00356 Generation of internal gravity waves by tidal flow over random oceanic topography

JIAJUN ZHAO, Natl Univ of Singapore, LIKUN ZHANG, HARRY SWINNEY, University of Texas at Austin — Internal waves (IW) are gravity waves that propagate within density-stratified fluids such as the ocean, atmosphere, and protoplanetary disks. IWs generated by tidal flow over oceanic topography provide much of the energy needed to sustain vertical mixing, which plays a critical role in ocean circulation and global climate. Therefore, it is important to determine the amount of energy that is extracted from tidal flow over topography and radiated into IWs. We conduct 2D numerical simulations to determine the IW power generated by tidal flow over random topographies that have the seafloor spectrum. The power is found to saturate with increasing topographic roughness, and to scale linearly with the characteristic height of the topography. The linear dependence on the topographic height is, surprisingly, nearly independent of the value of the exponent characterizing the topographic spectrum. Our results should lead to improved predictions of the IW power generated by tidal flow over global ocean topography.

Research supported by the Office of Naval Research and the Texas Advanced Computing Center. JZ is supported also by the Presidents Graduate Fellowship from the National University of Singapore.

H1.00357 Photoresponse of Single Mn doped ZnO nanowires in UV application

MON-SHU HO, Department of Physics, National Chung Hsing University — This paper reports the fabrication of Mn doped ZnO nanowires (NWs) using a low temperature hydrothermal method. The resulting nanowires were characterized using field emission scanning electron microscopy, energy dispersive spectroscopy, X-ray diffraction analysis, transmission electron microscopy and photoluminescence spectroscopy. A single Mn doped ZnO NW UV sensor with high performance sensing capabilities was then assembled using a focused ion beam technique. The photoresponse of the ZnO NW sensors was investigated under irradiation from 365 nm and 400 nm ultra-violet lamps. The proposed sensor exhibited rapid photoresponse speeds and short recovery times with a photocurrent ratio (ΔI = I_{light} / I_{dark}) superior to that of pure ZnO NW sensor. A possible mechanism to account for adsorption-desorption of oxygen and water molecules on Mn/ZnO NW surfaces was finally proposed to give the expression.

Photoresponse of Single Mn doped ZnO nanowires in UV application

H1.00358 Power-law-like correlation between condensation energy and superconducting transition temperatures in iron pnictide/chalcogenide superconductors: Beyond the BCS understanding

JIE XING, SHENG LI, Center for Superconducting Physics and Materials, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, BING MU, BING SHEN, National Laboratory for Superconductivity, Institute of Physics and National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, J. SCHNEELOCH, R.D. ZHONG, T.S. LIU, G.D. GU, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, HAI-HU WEN, Center for Superconducting Physics and Materials, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University — Superconducting condensation energy \( U_{0}^{\alpha} \) has been determined by integrating the electronic entropy in various iron pnictide/chalcogenide superconducting systems. It is found that \( U_{0}^{\alpha} \propto T_{c}^{n} \) with \( n = 3 \) to 4, which is in sharp contrast to the simple BCS prediction \( U_{0}^{\alpha,BCS} = 1/2N_{P} \Delta_{P}^{2} \), with \( N_{P} \) the quasiparticle density of states at the Fermi energy and \( \Delta_{P} \), the superconducting gap. A similar correlation holds if we compute the condensation energy through \( U_{0}^{\alpha,eff} = 3\gamma_{n} \Delta_{P}^{2}/4n_{eff}^{2}k_{B}^{2} \), with \( \gamma_{n} \) the effective normal state electronic specific heat coefficient. This indicates a general relationship \( \gamma_{n} \propto T_{c}^{m} \) with \( m = 1 \) to 2, which is not predicted by the BCS scheme. A picture based on quantum criticality is proposed to explain this phenomenon.
is high enough to generate a distinct NEXAFS resonance at 286.2 eV (1s → π\(^+\)) the electronic states of chlorinated graphene on different substrates, including surface binding energy, dopant concentration and work function shift by use of X-ray spectroscopy provides us a sensitive probe to investigate the surface states of functionalizing dopants in graphene. Here, we systematically studied KONG, MILDRED DRESSELHAUS, TOMAS PALACIOS, Massachusetts Institute of Technology, THEANNE SCHIROS, Columbia University, DENNIS NORDLUND, SLAC National Accelerator Laboratory, YONG CHEOL SHIN, JING XU ZHANG, Massachusetts Institute of Technology, MIT/COLUMBIA UNIVERSITY/SLAC COLLABORATION.

Institute of Technology, THEANNE SCHIROS, Columbia University, DENNIS NORDLUND, SLAC National Accelerator Laboratory, YONG CHEOL SHIN, JING XU ZHANG, Massachusetts Institute of Technology, MIT/COLUMBIA UNIVERSITY/SLAC COLLABORATION — Plasma-based chlorination is a promising technique to realize controllable doping in graphene, while maintaining its high mobility. Meanwhile, synchrotron-based X-ray spectroscopy provides us a sensitive probe to investigate the surface states of functionalizing dopants in graphene. Here, we systematically studied the electronic states of chlorinated graphene on different substrates, including surface binding energy, dopant concentration and work function shift by use of Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy, XPS and photoemission threshold measurements. The concentration of absorbed chlorine is high enough to generate a distinct NEXAFS resonance at 286.2 eV (1s → π\(^+\) transition for C-Cl bonds). It is remarkable that the sp2 core carbon-hole exciton (291.85eV) retained its sharpness even after treatment, indicating the long-range periodicity in graphene is largely preserved. This distinguishes our approach as a noninvasive and effective doping method. The interaction between Cl and graphene also exhibits strong substrate effects: for Cu, graphene’s Fermi level is shifted downwards by 0.35eV, while for graphene on SiO2, the much (4-5 times) higher chlorine concentration causes EF to shift by 0.9eV.

3:18PM J1.00003 Near-edge X-ray Absorption Fine Structure (NEXAFS) Spectroscopy study on Chlorinated Graphene through Plasma-based Surface Functionalization. XU ZHANG, Massachusetts Institute of Technology, THEANNE SCHIROS, Columbia University, DENNIS NORDLUND, SLAC National Accelerator Laboratory, YONG CHEOL SHIN, JING XU ZHANG, Massachusetts Institute of Technology, MIT/COLUMBIA UNIVERSITY/SLAC COLLABORATION — Plasma-based chlorination is a promising technique to realize controllable doping in graphene, while maintaining its high mobility. Meanwhile, synchrotron-based X-ray spectroscopy provides us a sensitive probe to investigate the surface states of functionalizing dopants in graphene. Here, we systematically studied the electronic states of chlorinated graphene on different substrates, including surface binding energy, dopant concentration and work function shift by use of Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy, XPS and photoemission threshold measurements. The concentration of absorbed chlorine is high enough to generate a distinct NEXAFS resonance at 286.2 eV (1s → π\(^+\) transition for C-Cl bonds). It is remarkable that the sp2 core carbon-hole exciton (291.85eV) retained its sharpness even after treatment, indicating the long-range periodicity in graphene is largely preserved. This distinguishes our approach as a noninvasive and effective doping method. The interaction between Cl and graphene also exhibits strong substrate effects: for Cu, graphene’s Fermi level is shifted downwards by 0.35eV, while for graphene on SiO2, the much (4-5 times) higher chlorine concentration causes EF to shift by 0.9eV.

3:30PM J1.00004 First Principles Study of Chemically Functionalized Graphene1, SANJIV JHA, IGOR VASILIEV, New Mexico State University — The electronic, structural and vibrational properties of carbon nanomaterials can be affected by chemical functionalization. We applied ab initio computational methods based on density functional theory to study the covalent functionalization of graphene with benzene, carboxyl groups and tetracyanoethylene oxide (TCNEO). Our calculations were carried out using the SIESTA and Quantum-ESPRESSO electronic structure codes combined with the local density and generalized gradient approximations for the exchange correlation functional and norm-conserving Troullier-Martins pseudopotentials. The simulated Raman and infrared spectra of graphene functionalized with carboxyl groups and TCNEO were consistent with the available experimental results. The computed vibrational spectra of graphene with carboxyl groups showed that the presence of point defects near the functionalization site affects the Raman and infrared spectroscopic signatures of functionalized graphene.

1Supported by NSF CHE-1112388

3:42PM J1.00005 The influence of selective chemical doping on clean, low-carrier density SiC epitaxial graphene1. CHIASHAIN CHUANG, YANFEI YANG, National Institute of Standard and Technology, LUNG-I HUANG, CHI-TE LIANG, National Taiwan University, RANDOLPH E. ELQUIST, National Institute of Technology, NATIONAL INSTITUTE OF OF STANDARDS AND TECHNOLOGY COLLABORATION, NATIONAL TAIWAN UNIVERSITY, DEPARTMENT OF PHYSICS COLLABORATION — The charge-transfer effect of ambient air on magneto-transport in polymer-free SiC graphene was investigated. Interestingly, adsorption of atmospheric gas molecules on clean epitaxial graphene can reduce the carrier density to near charge neutrality, allowing observation of highly precise v = 2 quantum Hall plateaus. The atmospheric adsorbates were reproducibly removed and pure gases (N\(_2\), O\(_2\), CO\(_2\), H\(_2\)O) were used to form new individual adsorbates on SiC graphene. Our experimental results (v = 2) support the theoretical prediction that the ratio of transport relaxation time \(\tau_r\) to quantum lifetime \(\tau_q\) in clean graphene. The analysis of the Shubnikov-de Haas oscillations at intermediate doping levels indicates that the carrier scattering is reduced by water and oxygen so as to increase both the classical and quantum mobility. This study points to the key dopant gases in ambient air and also paves the way towards extremely precise quantized Hall resistance standards in epitaxial graphene systems with carrier density tuned by exposure to highly pure gases and vacuum annealing treatment.

1National Institute of Standard and Technology

3:54PM J1.00006 ABSTRACT WITHDRAWN —

4:06PM J1.00007 Electroless deposition of metal nanoparticles on graphene with substrate-assisted techniques1. ANNA M. ZANIEWSKI, CHRISTIE J. TRIMBLE, VERONICA MEEKS, ROBERT J. NEMANICH, Arizona State University — We present the electroless reduction of solution-based metal ions for nanoparticle deposition on a variety of substrates. The substrates include graphene-coated metals, insulators, doped semiconductors, and patterned ferroelectrics. We find that the metal ions are spontaneously reduced on a wide variety of graphene substrates, and the substrates play a large role in the nanoparticle coverage. For example, the reduction of gold chloride to gold nanoparticles on graphene/lithium niobate results in 3% nanoparticle coverage compared to 20% coverage on graphene/silicon and 60% on graphene/copper. Given that the work function of graphene is approximately 4.4eV, the Fermi level is ~0.1 V vs the normal hydrogen electrode (NHE). Since the reduction potential of gold chloride is +1.02 V, the spontaneous transfer of electrons from the graphene to the metal ion is energetically favorable. However, we find substrates with similar work functions nevertheless result in varied deposition rates, which we attribute to electron availability. We also find that patterned ferroelectrics can be used as a template for patterned nanoparticle deposition, with and without graphene.

1This work is supported by the National Science Foundation under Grant # DMR-1206935.

4:18PM J1.00008 Quantum Transport in Few-Layer Graphene and Phosphorene Devices. CHUN NING (JEANIE) LAU, University of California, Riverside — I will present our results on transport measurements in bilayer and trilayer graphene devices with mobility as high as 400,000 cm\(^2\)/Vs. We demonstrate the presence of an intrinsic gapped state in bilayer and trilayer graphene at the charge neutrality point, a “new” spectroscopy technique for measuring the Landau level gaps, the distinct competing states at filling factor 2 and crossing between symmetry-broken Landau levels. Our results underscore the fascinating many-body physics in these 2D membranes. Finally, I will present our recent results on fabrication of air-stable few-layer phosphorene heterostructures and observation of quantum oscillations in these devices.
5:4PM J1.00009 Multi-mode Fabry-Pérot Interferences in SiO₂-supported Single Layer Graphene, in Large Aspect Ratio 2-terminal Devices¹. JOSEPH LAMBERT, Drexel University; STEVEN CARABELLO, Penn State Harrisburg and Drexel University; ROBERTO RAMOS, Indiana Wesleyan University — The Fabry-Pérot (F-P) interference of charge carriers in graphene occurs in 2-dimensional cavities defined by p-n interfaces. Typically, p-n interfaces form by local doping of metallic contacts, and serve as partially reflecting mirrors for ballistic charge carriers. Here, we report on observed F-P resonances in very large aspect ratio devices. For all devices studied, the inter-lead distance is L ≈ 0.2 μm, and the graphene channel widths range from W ≈ 5 to 17 μm, resulting in aspect ratios up to W/L ≈ 74. In maps of conductance versus source-drain and gate voltages, we observe long-range tapestry patterns, extending over the gate voltage range from Vgs = –60 V to 20 V. These features are observed at a temperature of T = 20 K. Upon lowering the temperature, an additional mode appears around T ≈ 3 K, and remains fairly unchanged down to T ≈ 30 mK. From the lowest energy features, we estimate the phase coherence length to be on the order of 1 to 2 μm. Using FFT, we have identified two modes: the fundamental longitudinal, and one of the transverse modes, which we propose is a result of smaller cavities formed by the disorder-induced charge puddles.

¹We gratefully acknowledge Prof. Fred Wellstood, University of Maryland, for access to fabrication facilities.

5:06PM J1.00010 Graphene Transport Under the Influence of Polar Molecules¹. BARRETT WORLEY, SEOHEE KIM, SAUNGEUN PARK, Univ of Texas, Austin; PETER ROSSKY, Rice University; DEJI AKINWANDE, ANANTH DODABALAPUR, Univ of Texas, Austin — Charged defects and impurities play a very important role in charge transport in graphene field-effect transistors (FETs). They influence the mobility, residual doping, and the Dirac voltage. Long-range scattering by charged impurities in fabricated graphene FETs lowers the mobility of charge carriers, while short range scattering affects the value of residual carrier concentration. Our group has shown that the electrical properties of graphene FETs are significantly improved upon exposure to fluoropolymers or polar organic vapors. We have demonstrated favorable Dirac voltage shifts, increases in mobility, and reduction in residual carrier concentration as a result of polar molecules altering the dielectric environment surrounding the graphene/substrate interface of a graphene FET. Screening of charged impurity scattering is hypothesized to be the principal effect by which the polar molecules of the altered dielectric layer bring about improvements. We employ computational chemistry to model polar organic molecule-graphene systems. Such modeling will help explain experimental results.

¹We acknowledge support from NASCENT NSF EEC-1160494 and NSF CHE-1362381.

5:18PM J1.00011 Theory of anharmonic phonons in graphene. SEBASTIAN COSTAMAGNA, Instituto de Fisica de Rosario (IFIR-CONICET); FRANCOIS M. FEETERS, KARL H. MICHEL, University of Antwerp — Anharmonic effects in an atomic monolayer thin crystal with honeycomb lattice structure are studied by analytical and numerical lattice dynamical methods. Starting from a semi-empirical model for anharmonic couplings of third and fourth order, we study the in-plane and out-of-plane (flexural) mode components of the generalized wave vector dependent Gruneisen parameters, the thermal tension and the thermal expansion coefficients as function of temperature and crystal size. From the resonances of the displacement-displacement correlation functions we study the renormalization and decay rate of in-plane and flexural phonons as function of temperature, wave vector and crystal size. Numerical evaluations are made with graphene as a specific model. The work is complementary to crystalline membrane theory and computational studies of anharmonic effects in two-dimensional crystals.

Tuesday, March 3, 2015 2:30PM — 5:30PM
Session J2 DMP: Focus Session: Beyond Graphene - Strongly Correlated Phenomena 001B - Kin Fai Mak, Pennsylvania State University

2:30PM J2.00001 Control of Metastable Charge Density Wave Phases in Ultrathin 1T-TaS₂. ADAM TSEN, Columbia University; ROBERT ROVDEN, Cornell University; DEENNIS WANG, YOUNG DUCK KIM, Columbia University; YU LIU, WENJIAN LU, YUPING SUN, Chinese Academy of Sciences, JAMES HONE, Columbia University; LENAFITTINGKOURKOUTIS, Cornell University; PHILIP KIM, Harvard University; ABHAY PASUPATHY, Columbia University — Among the most intriguing aspects of reduced dimensionality in condensed matter systems is the enhancement of various correlation effects (electron-electron, electron-phonon, etc.). In quasi-2D metallic chalcogenides, they lead to electronic instabilities that give rise to a wealth of exotic ground states such as charge density waves (CDWs), spin density waves, and superconductivity. 1T-TaS₂ is a unique layered material which exhibits a number of different CDW states as well as a Mott phase at low temperatures. Although its electronic structure is largely two dimensional, the CDWs are stabilized by an out-of-plane stacking. By combining low temperature transmission electron microscopy with electrical transport measurements, we investigate how the various CDW phases in 1T-TaS₂ change as it approaches the physical 2D limit. We find that in well-controlled samples, the lock-in transition from a nearly commensurate CDW to a fully commensurate CDW gradually disappears with reduced thickness as both phases become increasingly metastable. I will discuss the physical reasons underlying this behavior as well as demonstrate how to manipulate this phase transition in few-layer samples by application of an in-plane electric field.

2:42PM J2.00002 Tantalum Disulfide Ionic Field-Effect Transistors. YUAN YU, FANGYUAN YANG, Fudan University, XIU FANG LU, YA JUN YAN, University of Science and Technology of China; Y. H. CHO, Rutgers University; LIGUO MA, XIAOHAI NIU, Fudan University, SEJOONG KIM, YONG-WOO SON, Korea Institute for Advanced Study, DONGLAI FENG, SHIYAN LI, Fudan University, SANG-WOOK CHEONG, Rutgers University, XIAN HUI CHEN, University of Science and Technology of China; YUANBO ZHANG, Fudan University — The ability to tune material properties using gate electric field is at the heart of the modern electronic technology. Electrolyte gating has recently emerged as an important technique to reach extremely high surface charge carrier concentration in a variety of materials through the formation of electric double layer (EDL) at the sample surface. Here we demonstrate a new mechanism of electrolyte gating that modulates the volumetric carrier density by gate-controlled intercalation in layered materials. We fabricate field-effect transistors (referred to as ionic field-effect transistor, iFET) based on transition metal dichalcogenides 1T-TaS₂ and 2H-TaS₂. The unprecedented large doping induces dramatic changes in the transport properties of the sample, including CDW phase transitions, superconductivity and metal-to-insulator transitions. The controllable and reversible intercalation of different ion species into layered materials opens up new possibilities in searching for novel states of matter in the extreme charge-carrier-concentration limit.

2:54PM J2.00003 Scanning Tunneling Microscopy and Spectroscopy of the commensurate charge density wave phase of 1T-TaS₂. ADINA LUCIAN-MAYER, ANDREW DILULLO, YANG LI, SAW WAH-HLA, Argonne National Laboratory — The 1T polymorph of TaS₂, 1T-TaS₂, has one of the richest phase diagrams among the transition metal dichalcogenides: It is metallic at higher temperatures; it has four temperature-dependent charge density wave (CDW) phases with different structures; at low temperatures it shows Mott insulator behavior and under pressure and doping it becomes superconducting. In this talk, we focus on the low temperature commensurate charge density wave phase. Using scanning tunneling microscopy and spectroscopy, we explore the spatial variation of the electronic properties of the commensurate CDW phase at the atomic level. The role that defects play in the formation of this phase will also be discussed.
3:42PM J2.0005 New STM Tip-induced Phases in 1T-TaS_2
LIGUO MA, YIJUN YU, State Key Laboratory of Surface Physics, Department of Physics, Fudan University, XIU FANG LU, YA JUN YAN, Heifei National Laboratory for Physical Science at Microscale and Department of Physics, University of the Science and Technology of China, YUANBO ZHANG, State Key Laboratory of Surface Physics and Department of Physics, Fudan University — Transition metal dichalcogenide 1T-TaS_2 is a layered material featuring a unique set of charge density wave (CDW) phases. The close proximity of the CDW phases in energy makes the material prone to external perturbation, and the intricate electron-phonon and electron-electron interactions often lead to electronic/structural phase transitions in 1T-TaS_2. Here we report a new phase transition from the insulating commensurate CDW (also known as a Mott state) to a new metallic CDW state that is induced in 1T-TaS_2 by voltage pulses from an STM tip at low temperatures. We study the topographic and spectroscopic properties of the metallic CDW phase in detail with STM and Scanning Tunneling Spectroscopy (STS).

3:54PM J2.0006 Controlling non-equilibrium CDW states in 1T-TaS_2 nano-thick crystals
MASARO YOSHIDA, YIJIN ZHANG, RYUJI SUZUKI. Quantum-Phase Electronics Center (QPEC) and Department of Applied Physics, The University of Tokyo, Japan, JIANTING YE, Zernike Institute for Advanced Materials, University of Groningen, The Netherlands, YOSHIIRO IWASA, Quantum-Phase Electronics Center (QPEC) and Department of Applied Physics, The University of Tokyo, Japan — Two-dimensional (2D) crystals provide an ideal platform for exotic electronic band structures in mono- or multi-layer form. The thinning to nano-scale may also affect collective phenomena in interacting electron systems and can lead to unconventional states that are dramatically different from those in bulk. In this presentation, we report the systematic control of charge-density-wave (CDW) transitions by changing thickness and cooling rate in nano-thick crystals of 1T-type tantalum disulfide (1T-TaS_2). First, we discovered a new super-cooled nearly-commensurate CDW state, which shows metallic behavior at low temperatures. Furthermore, we achieved current-induced switching between various CDW states. The glassy behavior and non-linear response, possibly due to the reduced dimensionality, manifest the emergent complex nature of correlated electrons in 2D crystals with nanometer thickness.

4:06PM J2.0007 Effects of Dimensionality on the Charge-Density Wave Phases of Transition-Metal Dichalcogenides
DANilo ROMERO, ECE Department, University of Maryland, College Park, MD 20740 and NIST Gaithersburg, MD 20899, JEFFREY SIMPSON, Towson University and NIST Gaithersburg, MD 20899, HELMUTH BERGER, EPSL, Lausanne, Switzerland, ANGELA HIGHT-WALKER, NIST Gaithersburg, MD 20899 — We investigate the effects of dimensionality on the electronic properties of the transition-metal dichalcogenides (TMDCs). We observe phase transitions between commensurate and incommensurate CDW phases in thin films of 1T-TaS_2 and 1T-TaSe_2. These effects are attributed to the reduced electron-phonon coupling and the reduced electron-electron interactions.

4:18PM J2.0008 Ultrafast Two-Pulse Photocurrent Correlation Measurements of Single Atomic Layer MoS_2 Photodetectors
HAINING WANG, CHANGJIAN ZHANG, WEI-MIN CHAN, OKAN KOKSAL, SANDIP TIVITY, FARHAN RANA, Cornell Univ — We present, for the first time, results from ultrafast measurements of carrier transport and carrier dynamics in monolayer MoS_2 photodetectors by time resolved two-pulse photocurrent correlation technique [1]. The photocurrent transient contains information on the recombination dynamics and transport physics of the photoexcited carriers and excitons. The measured photocurrent correlation data shows two distinct decay time constants: one fast around 5 ps and one much slower around 100 ps. The observed dynamics are largely independent of temperature (10K to 300K) and pump fluence (1 to 16 μJ/cm²). The fast decay is attributed to the fast recombination of the photoexcited carriers rather than to the transport and extraction of the photoexcited carriers from the device. The decay time scales, the temperature and the pump fluence dependence of the observed dynamics are in good agreement with defect-assisted carrier recombination model via Auger scattering. The observed time scales also agree well with our all-optical pump-probe studies. The strong Coulomb interactions and resulting strong electron-hole correlations in monolayer MoS_2, make carrier and exciton capture by defects the dominant carrier recombination mechanism.

4:30PM J2.0009 Proximity-induced superconductivity in transition metal dichalcogenides
DRISS M. BADIANE, William & Mary Coll, CHRISTOPHER TRIOLA, E. ROSSI, Department of Physics, College of William and Mary, Williamsburg, Virginia 23187, USA — In this work we study the proximity-induced superconductivity in a monolayer of the transition metal MoS_2 placed on top of a superconducting substrate. We investigate the symmetries of the proximity-induced superconducting pairing amplitude and we find that superconducting substrates with spin-orbit coupling can induce odd-frequency pairing in the MoS_2 monolayer. We discuss the relevant experimental signatures of the proximity-induced superconducting phase in the MoS_2 monolayer.

4:42PM J2.0010 In search of single layer superconductivity in semiconducting transition metal dichalcogenides
EFREn NAVARRO-MORATALLA, YAFANG YANG, HUGH CHURCHILL, PABLO JARILLO-HERRERO, Department of Physics, Massachusetts Institute of Technology — Charge carrier density control is a keystone in the study of 2D semiconductors. The use of ionic liquids as gate electrodes gives rise to the formation of high capacitance electrical double layers (EDLs) that permit exploring very high carrier density regimes (n ≈ 10^{15} cm^{-2}), opening the door for the study of field-induced correlated states, such as ferromagnetism or superconductivity. Though pioneering works on transition metal dichalcogenides have provided proof of the use of EDLs for the induction of superconductivity in bulk crystals or in the surface of thick flakes, no reports of single layer superconductivity have been put forward. We take advantage of crystal growth techniques, the EDL approach, the wide range of metal dichalcogenides and the van der Waals stacking to fabricate ultraflat samples that will permit exploring the high carrier density regime in search for switchable single layer superconductivity. The use of a liquid gate opens the possibility of studying the effect that strain or even the presence of molecular species may have in the superconducting state.
4:54PM J2.00011 Electronic and magnetic properties of NbSe$_2$ monolayer doped vacancy and transition metal atoms$^{1}$. PRIYANKA MANCHANDA, DAVID SELLMYER, RALPH SKOMSKI, Univ of Nebraska - Lincoln — Two-dimensional transition-metal dichalcogenides (2D TMDs) have attracted much attention recently due to potential applications including optoelectronic devices. Atomically thin layers of materials such as MoS$_2$, WS$_2$, NbS$_2$, NbSe$_2$, TaTe$_2$ can easily be synthesized by exfoliation techniques and exhibit variety electronic phases such as metal, semiconductor, superconductor depending on the choice of metal. Most of the TMDs are nonmagnetic and various techniques have been proposed to induce or modulate magnetic properties that are essential for nanoelectronic device applications. We use DFT calculations to analyze the effect of strain, hydrogen adsorption, and doping. Emphasis is on the magnetic properties of NbSe$_2$ monolayers containing vacancies and 3d transition metal atoms. We find that magnetism can be induced by vacancy creation and transition metal-substitution in NbSe$_2$, with effects similar to strain and hydrogen adsorption. The moment mainly arises from the localized nonbonding 3d electrons of the transition-metal atoms. Our findings contribute to the ongoing search for “better-than-graphene” thin-film materials for novel electronic devices.

$^1$This research is partially supported by DOE BES (DE-FG02-04ER46152).

5:06PM J2.00012 Superconductivity Series of Ion-gated Transition Metal Dichalcogenides. WU SHI, JIANTING YE$^1$, YIJING ZHANG, RYUJI SUZUKI, MASARO YOSHIDA, NAOKO INOUE, YU SAITO, YOSHIHIRO IWASA, Univ of Tokyo — Semiconducting transition metal dichalcogenides (TMDs) have attracted considerable interest as typical two-dimensional (2D) materials. By mechanical cleavage, atomically flat and chemically stable thin flakes of TMDs can be readily obtained from bulk crystals. Recently, coupling with high efficient ionic media, TMD thin flakes have exhibited extraordinary electronic and opto-vascular properties in the form of electrical double layer transistors (EDLTs). The introduction of high-density carriers have also induced metal-insulator transition and superconductivity in MoS$_2$, revealing an enhanced Tc and a dome-like phase diagram that is inaccessible through conventional chemically doping. In this work, we report the discovery of a superconductivity series based on a further exploration of high-density carriers and both magnetic and transport measurements of this materials physical properties.

Tuesday, March 3, 2015 2:30PM - 4:54PM — Session J3 COM FIAP: Invited Session: Research and Opportunities in Nanoscience: An Industrial Perspective 002AB - Alfredo Alexander-Katz, Massachusetts Institute of Technology

2:30PM J3.00001 Nanofabrication in the Magnetic Recording Industry: Past, Present and Future. RICARDO RUIZ, HGST, a Western Digital Company — The magnetic recording industry stands out as an example of multidisciplinary nanotechnology that keeps pushing the envelope in terms of controlling matter and events at the nanometer length scale. From magnetic media composed of sub-10 nm grains, to overcoat protecting layers that are only 2-3 nm thick, to read sensors that are ~ 30 nm wide, to recording heads that fly at ~ 5 nm heights with speeds up to 100 mi/hr, nanotechnology and nanofabrication have been inseparable to the success and extendibility of hard disk drives. Looking into the future, as the demand for data storage continues to increase in a data-centric, cloud-connected environment, future magnetic recording will need to scale accordingly to accommodate ever increasing demands for areal density gains. Future storage technologies such as heat assisted magnetic recording that employs plasmonic antennas or magnetic bit patterned media that requires self-assembly of block copolymers, also stake their success in the advances of nanoscience. I will review research opportunities in this industry with a personal perspective of a decade’s worth in self-assembly for lithographic applications.

3:06PM J3.00002 From silicon nanowire sensors to making living safer. MONIKA WEBER, Yale University

3:42PM J3.00003 Control of crystal morphology and orientation in nano-confined semi-crystalline polymer films to obtain superior barrier performance. BERNARD OBI, The Dow Chemical Company — Several global megatrends are driving the need for packaging films that offer much more superior barrier to oxygen and water vapor transmission than have been traditionally achieved, whilst maintaining high levels of transparency. For food packaging applications targeting aluminum foil barrier performance, OTR and WVTR of approximately 10$^{-4}$ cc/m$^2$/day-atm are typically required. The U.S. flexible packaging market was predicted to exceed $26.5$ billion by 2010 with an annual growth rate of over 67 wt %. We have worked at understanding the parameters that control the transmission of small penetrating molecules through these thin transparent polymeric flexible barrier films, and how to design for high barrier performance. The dispersion of large aspect ratio impervious inclusions in an In-plane oriented morphology into these films lead to very high tortuosity and correspondingly very high barrier performance. A physical model that describes mechanistically the spatial control of crystallization kinetics in a nano-confined geometry using micro-layer technology to obtain predominantly “In-plane” lamellae orientation in semi-crystalline barrier polymer films was validated for providing up to 200X improvement in barrier performance.

4:18PM J3.00004 Integrated Ge laser for silicon photonics platform. RODOLFO CAMACHO, Intel Corporation — The exponential increase of data transfers and requirements have produced difficult constraints that silicon photonics is posed to solved. The integrated platform of silicon photonics. In this ecosystem one of the main barriers is the fabrication of integrated transceivers, which translates into lasers on Si. A material proposed is germanium. Growth techniques, laser design and theory are demonstrated concluding in the creation of a 0.2% biaxial strain and highly n-type doped Ge laser exhibiting gain > 1000 cm$^{-1}$.

Tuesday, March 3, 2015 2:30PM - 5:30PM — Session J4 FOEP: Invited Session: Forum on Outreach and Engaging the Public Mayor Cockrell Room 004 - R. Micahael Barnett, Lawrence Berkeley National Laboratory
Room 005 - Anderson Janotti, University of California, Santa Barbara

and disseminate the results of efforts that are enhancing the quality and visibility of broader impacts activities in whatever form they take. As access to a community of colleagues working at the nexus of scientific research and informal education for further exploration. Through heightened awareness, (STEM) education professionals provide researchers, graduate students and staff resources to tap into as they consider their broader impacts directions. Web conditions in fostering science learning and literacy in informal settings, as well as an expanding network of informal science, technology, engineering and math (STEM) education opportunities. By creating exhibits, media or programming that will convey the scientific concepts and processes involved in research and engage students and learning goals or other intended impacts. One approach to developing such plans is to partner with an informal science education institution, program, project or individual to create exhibits, media or programming that will convey the scientific concepts and processes involved in research and engage students and public audiences in appreciation for, and understanding of. A growing body of evidence-based knowledge about what works for whom and under what conditions in fostering science learning and literacy in informal settings, as well as an expanding network of informal science, technology, engineering and math (STEM) education professionals provide researchers, graduate students and staff resources to tap into as they consider their broader impacts directions. Web infrastructure like the informalscience.org website and others offer aggregated, vetted, and searchable examples of successful partnerships and strategies, as well as access to a community of colleagues working at the nexus of scientific research and informal education for further exploration. Through heightened awareness, stronger connectivity and a growing repository of knowledge, projects like the Center for Advancement of Informal Science Education (CAISE) hope to support and disseminate the results of efforts that are enhancing the quality and visibility of broader impacts activities in whatever form they take.

3:06PM J4.00002 Quantum physics reimagined for the general public, JULIEN BOBROFF, LPS, Université Paris Sud — Quantum Physics has always been a challenging issue for outreach. It is invisible, non-intuitive and written in sophisticated mathematics. In our “Physics Reimagined” research group, we explore new ways to present that field to the general public. Our approach is to develop close collaborations between physicists and designers or graphic artists. By developing this new kind of dialogue, we seek to find new ways to present complex phenomena and recent research topics to the public at large. For example, we created with web-illustrators a series of 3D animations about basic quantum laws and research topics (graphene, Bose-Einstein condensation, decoherence, pump-probe techniques, ARPES...). We collaborated with designers to develop original setups, from quantum wave animated models or foldings to a superconducting circus with levitating animals. With illustrators, we produced exhibits, comic strips or postcards displaying the physicists in their labs, either famous ones or even our own colleagues in their daily life as researchers. With artists, we recently made a stop-motion picture to explain in an esthetic way the process of discovery and scientific publication. We will discuss how these new types of outreach projects allowed us to engage the public with modern physics both on a scientific and cultural level and how the concepts and process can easily be replicated and expanded by other physicists. We are at the precise time when creative tools, interfaces, and ways of sharing and learning are rapidly evolving (wikipedia, MOOCs, smartphones...). If scientists don’t step forward to employ these tools and develop new resources, other people will, and the integrity of the science and underlying character of research risks being compromised. All our productions are free to use and can be downloaded at www.PhysicsReimagined.com (for 3D quantum videos, specific link: www.QuantumMadeSimple.com)

3:42PM J4.00003 Developing a Global Science and Math Education System Based on Real Astronomy Data, CARLTON PENNYPACKER, Lawrence Berkeley National Lab and UC Berkeley — Global Hands-On Universe (GHOU) is an educational system where students use real astronomy data from (largely optical) telescopes to learn fundamental physics, math, astronomy, and technology. GHOU is a good example of a collaborative global education project, where data, software, teacher training methods, curriculum, activities, telescopes, and human resources are developed by many members of GHOU and then shared internationally. Assessments show that in this program students learn more science and math than in conventional classroom teaching, and students change their attitudes towards choosing careers in science and technology. GHOU is an exemplar of appropriate use of computers in the classroom for real data analysis. The International Asteroid Search program of GHOU has helped students discover over 700 asteroids. Half a dozen high schools have named the asteroids they have found after their high school (some from here in Texas)!

4:18PM J4.00004 The Role of Outreach in NSF Proposals, RANDAL C. RUCHTI, University of Notre Dame — The NSF has two merit criteria that must be addressed in proposals, intellectual merit and broader impacts. While the former is generally well understood, that latter less so. This presentation will review the issues of broader impacts, of which outreach is but one possible approach, and give a view from the perspective of a research scientist who recently served as a program director in the NSF Division of Physics.

4:54PM J4.00005 Developing Broader Impacts Activities through Informal STEM Education Collaborations and Strategies, JAMES BELL, Center for Advancement of Informal Science Education — With the National Science Foundation and other funding agencies’ renewed emphasis on broader impacts merit criterion in proposals, investigators and directors of education, outreach and engagement are challenged to identify, plan and implement innovative and transformative activities that engage a variety of audiences in the broader impacts of scientific research. These activities are also often required to have an evaluation plan for assessing the effectiveness of the strategies employed to achieve learning goals or other intended impacts. One approach to developing such plans is to partner with an informal science education institution, program, project or individual to create exhibits, media or programming that will convey the scientific concepts and processes involved in research and engage students and public audiences in appreciation for, and understanding of. A growing body of evidence-based knowledge about what works for whom and under what conditions in fostering science learning and literacy in informal settings, as well as an expanding network of informal science, technology, engineering and math (STEM) education professionals provide researchers, graduate students and staff resources to tap into as they consider their broader impacts directions. Web infrastructure like the informalscience.org website and others offer aggregated, vetted, and searchable examples of successful partnerships and strategies, as well as access to a community of colleagues working at the nexus of scientific research and informal education for further exploration. Through heightened awareness, stronger connectivity and a growing repository of knowledge, projects like the Center for Advancement of Informal Science Education (CAISE) hope to support and disseminate the results of efforts that are enhancing the quality and visibility of broader impacts activities in whatever form they take.

Tuesday, March 3, 2015 2:30PM - 5:30PM
Session J5 FIAP GERA DMP: Electricity to Light Conversion: Solid State Lighting, Juan Gorman
Room 005 - Anderson Janotti, University of California, Santa Barbara
2:30PM J5.00001 Accurate treatment of spontaneous polarization in III-nitrides1, CURTIS E. DREYER, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — The III-nitride compounds assume the wurtzite crystal structure in the ground state and therefore exhibit spontaneous and piezoelectric dipole moments in the c direction. Discontinuities in these moments at heterostructure interfaces result in electric fields in the layers, which can be detrimental because they separate electrons and holes in quantum wells. Accurate values for polarization differences are critical for understanding and engineering III-nitride heterostructures. Direct experimental measurement of spontaneous polarization has not been possible to date, and calculations are complicated by the necessity to choose a reference structure. The universal choice of reference structure for wurtzite has been zincblende; we demonstrate that this choice does not allow consistent determination of the differences of spontaneous polarizations between materials, which determine their physical manifestation. Using first-principles techniques based on hybrid density functional theory, we have determined polarization discontinuities using a consistent reference based on the hexagonal layered structure of these materials. We will discuss the results in light of available experimental data, and outline consequences for device simulations.

1Work supported by DOE.

2:42PM J5.00002 Electronic and optical properties of AlN/GaN superlattices from first-principles calculations, DYLAN BAYERL, EMMANOUIL KIOUPAKIS, University of Michigan — Group-III-nitrides are important materials for efficient light emitters in the ultraviolet and visible range. Superlattices of AlN/GaN quantum wells are especially promising for ultraviolet light emission. We use first-principles calculations to investigate the electronic and optical properties of AlN/GaN quantum well superlattices. Density functional theory with quasiparticle corrections from the GW method provides accurate electronic band structures. We then solve the Bethe-Salpeter equation to predict exciton binding energies and fundamental optical emission energies from first principles, yielding good agreement with available experimental measurements. Ultimately, we elucidate the relationship between optical emission energy and well/barrier thickness, as well as demonstrate mitigation of the quantum confined Stark effect in ultra-narrow wells for enhanced radiative recombination efficiency. This research was supported by the J. Robert Byaster Computational Innovation Graduate Fellowship and in part by C3S, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science. Computational resources were provided by the DOE NERSC facility.

2:54PM J5.00003 Correlation between optical properties and strain relaxation in thick InGaN epitaxial films,2, WEN-CHE TSAI2, Chung Yuan Christian University in Taiwan, CHIA-HE HSU, SHAO-FU FU, FANG-WEI LEE, CHIN-YU CHEN, WU-CHING CHOU, WEI-KUO CHEN, WEN-HAO CHANG1, Department of Electrophysics, National Chiao Tung University — The alloy compositions, strain distributions and emission properties of thick In$_x$Ga$_{1-x}$N layers with x ranging from 0.13 to 0.38 are investigated. High resolution x-ray diffractions (XRD) and reciprocal space mapping (RSM) along an asymmetric axis reveal that the In composition inhomogeneity is accompanied by strain relaxations during the growth of thick InGaN layers. Photoluminescence (PL) results together with RSMs indicate that the observed double PL peaks are associated with the strained and relaxed phase in the InGaN films. It is further indicated that the relaxed phase in InGaN films exhibits better emission efficiency than the strained phase from the temperature-dependent PL measurements. Recombination dynamics from time-resolved PL measurements reveal that the carrier localization effect is more pronounced in the relaxed phase. According to the optical properties, the emission efficiency is strongly correlated with the localization effect in thick InGaN films.

2This work was supported in part by the program of MOEATU and the National Science Council of Taiwan under Grant No. NSC-101-2628-M-009-002-MY3.

2:56PM J5.00004 Characterization of M-plane InGaN/GaN Quantum Wells Grown on Mis-oriented γ-LiAlO$_2$ by Plasma-Assisted Molecular Beam Epitaxy, YU-CHIAO LIN, IKAI LO, CHENG-HUNG SHIH, ZHANG WEI XIANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan, MING-CHI CHOU, Department of Materials and Optoelectronic Science, National Sun Yat-Sen University, Kaohsiung, Taiwan — We have grown a series of InGaN/GaN quantum wells on misoriented LiAlO$_2$ (LAO) substrate with different growth parameters by plasma-assisted molecular beam epitaxy (PAMBE). The sample structure consists of M-plane InGaN/GaN quantum wells with 25nm GaN barrier/5nm InGaN well) with a ~225nm GaN buffer layer between the quantum wells and LAO substrate. The mis-cut angle of LAO substrate was tilted 11° off [011] direction to match the atoms of GaN lattice. From the X-ray diffraction (XRD) measurement, we found two peaks of 34.6° and 32.2°, indicating the LAO(100) substrate and [110] oriented (M-plane) for the InGaN thin films, respectively. The surface morphology, optical property and microstructure of the samples were investigated by scanning electron microscope (SEM), photoluminescence (PL) and transmission electron microscope (TEM) measurements, as well.

3:18PM J5.00005 Growth of high-quality InN thin films on InGaN buffer layer by plasma-assisted molecular beam epitaxy, CHE-NCHI CHAO, IKAI LO, CHENG-HUNG SHIH, CHIA-HSUAN HY, YING-CHIEH WANG, YU-CHIAO LIN, CHENG-DA TASI, SHOU-TING YOU, Department of Physics, Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan, R. O. C. — Four samples were grown on 2 inch c-plane (0001) sapphire substrates with 4μm-thick GaN template. The InN thin films were grown on InGaN buffer layer by low-temperature plasma-assisted molecular beam epitaxy (PAMBE) system. These samples were grown under a varied temperature of InGaN buffer layers: 500°C, 540°C, 570°C, and 600°C. The structure properties of these samples were analyzed by X-ray diffraction (XRD). The interference fringes of InN grown on the sample 1 (the growth temperature of InGaN buffer layer at 500°C) exhibit prominent oscillations, which indicates that the sample has a high quality and layer by layer epitaxial structure. The surface morphology and microstructure of samples were investigated by scanning electron microscopy (SEM), atomic force microscopy (AFM), and transmission electron microscopy (TEM). We confirmed the smooth surface and high quality crystalline for the sample.

3:30PM J5.00006 Microstructure of Er optical centers in the large-bandgap semiconductor GaN, DEEPU GEORGE, ALI CHARKHESHT, Virginia Tech, STEPHEN MCGILL, National High Magnetic Field Laboratory, HONGXING JIANG, Texas Tech University, JOHN ZAVADA, NYU Polytechnic, NGUYEN VINH, Virginia Tech — Photoluminescence properties of Er optical centers in GaN epi-layers grown by metal-organic chemical vapor deposition are investigated in magnetic fields up to 17 T and high-resolution time-resolved PL spectroscopy. The magnetic field induced splitting is observed for all the main lines of the Er-related photoluminescence spectrum. For the most intense emission line, angular dependence of the splitting is measured in the (1120) crystallographic plane of the sample. The effective g-tensor, corresponding to the difference between individual g-tensors of the lowest multiplets of the ground and the first excited states, is experimentally determined. The neto-mageto-optical measurements, the time-resolved photoluminescence and the temperature dependence of the photoluminescence spectroscopy show that the samples have two main optical centers and they can be excited selectively under band-to-band and resonance excitations.
3:42PM J5.00007 Effect of Dopant Activation on Device Characteristics of InGaN-based Light Emitting Diodes — NICHOLAS LACROCE, GUANYU LIU, CHEE-KEONG TAN, Center for Photonics and Nanoelectronics, Department of Electrical and Computer Engineering, Lehigh University; RONALD A. ARIF, SOO MIN LEE, Veeco Instruments, Inc.; NELSON TANSU, Center for Photonics and Nanoelectronics, Department of Electrical and Computer Engineering, Lehigh University — Achieving high uniformity in growths and device characteristics of InGaN-based light-emitting diodes (LEDs) is important for large scale manufacturing. Dopant activation and maintaining control of variables affecting dopant activation are critical steps in the InGaN-based light-emitting diodes (LEDs) fabrication process. In the epitaxy of large scale production LEDs, in-situ post-growth annealing is used for activating the Mg acceptor dopant in the p-AlGaN and p-GaN of the LEDs. However, the annealing temperature varies with respect to position in the reactor chamber, leading to severe uniform dopant activation issue across the devices. Thus, it is important to understand how the temperature gradient and the resulting variance in Mg acceptor activation will alter the device properties. In this work, we examine the effect of varying p-type doping levels in the p-GaN layers and AlGaN electron blocking layer of the GaN LEDs on the optoelectronic properties including the band profile, carrier concentration, current density, output power and quantum efficiency. By understanding the variations and its effect, the identification of the most critical p-type doping layer strategies to address this variation will be clarified.

3:54PM J5.00008 Electrical contact of wurtzite GaN microdisks on p-type GaN template — CHENG-DA TSAI, IKAI LO, YING-CHIEH WANG, YU-CHI HSU, CHIA-HSUAN HU, MITCH M.C. CHOU, CHEN-CHI YANG, YU-CHIAO LIN, Department of Physics, Department of Materials and Optoelectronic Science, Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University — We developed a back processing to fabricate a secure electrical contact of wurtzite GaN microdisk on a p-type GaN template with the orientation, [10-10]_disk // [10-10]_template. GaN microdisks were grown on LiAlO_2 substrate by using plasma-assisted molecular beam epitaxy [1]. In the further study, we analyzed the TEM specimen of a sample with annealed GaN microdisk/p-typed GaN template by selection area diffraction (SAD) to confirm the alignment of the microdisks with the template at the interface. From the I-V measurements performed on the samples, we obtained a threshold voltage of ∼ 5.9 V for the current passing through the GaN microdisks with a resistance of ∼ 45 KΩ. The electrical contact can be applied to the nanometer-scaled GaN light-emitting diode.


4:06PM J5.00009 Spatially resolved visible broad band multi-photon luminescence in GaN micro-pyramids — SWEEN BUTLER, Univ of North Texas, MOHAMED FIKRY, KLAUS THONKE, Ulm University, ARUP NEOGI, Univ of North Texas, ULM UNIVERSITY COLLABORATION — Multi-photon induced visible broad band luminescence was observed in position controlled m-polar GaN hexagonal micro-pyramids using a tunable near-infrared femtosecond laser source at room temperature. The GaN micro-pyramids were grown by molecular beam epitaxy on the high quality GaN template by using the epitaxial lateral overgrowth method. Excitation wavelengths corresponding to near band gap and below band gap energies were used. Spatially resolved optical characterization from a single micro-structure was achieved using multi-photon microscopy and spectroscopy. We observed broad band luminescence in the range of 400 nm to 600 nm for both near band gap and below band gap excitations. Power dependent excitation dependence confirms the origin of broad band visible emission as multi-photon induced luminescence (MPL). Band width of broadband light emission due to MPL can be controlled by selective spatial excitation of the GaN micro-pyramid.

4:18PM J5.00010 High Efficiency Alternating Current Driven Organic Light Emitting Devices Employing Active Semiconductor Gate Layers — GREGORY SMITH, JUNWEI XU, DAVID CARROLL, Wake Forest University — In this work, we describe the role of semiconductor-polymer interfaces in alternating current (AC) driven organic electroluminescent (EL) devices. We implement inorganic semiconductor materials between the external contact and the active layers in organic light EL devices. Precise control of capacitance and charge injection is required to realize bright and efficient large area AC driven devices. We show how this architecture results in active gating to the polymer layers, resulting in the novel ability to control the capacitance and charge injection characteristics. We propose a model based on band bending at the semiconductor-polymer interface. Furthermore, we elucidate the influence of the semiconductor-polymer interface on the internally coupled magnetic field generated in an alternating current driven organic light emitting device configuration. Magnetic fields can alter the ratios of singlet and triplet populations, and we show that internal generation of a magnetic field can dramatically alter the efficiency of light emission in organic EL devices.

4:30PM J5.00011 Elasto-optic effect in semiconductors: a first principle approach using Maximally Localized Wannier Functions — XIN LIANG, SOHRAB ISMAIL-BEIJI, Applied Physics, Yale University — Strain-induced changes of optical properties are of use in the design and functioning of devices that couple photons and phonons. The elasto-optic (or photo-elastic) effect describes a general materials property where strain induces a change in the dielectric tensor. Despite a number of experimental and computational works on this area, it is fair to say that a basic understanding of the effect and its materials dependence is lacking: for example, we know of no materials design rules for enhancing (or suppressing) elasto-optic response. Here, we begin by computing the elasto-optic tensor of silicon using Density Functional Theory (DFT). By analyzing the longitudinal dielectric response to uniaxial strain, we find that a promising avenue to physical understanding of the basis of the effect is to work in a real space representation and to employ Maximally Localized Wannier Functions (MLWFs). We describe our results based on this approach. This work is supported by the National Science Foundation through grant NSF DMR-0808665.

4:42PM J5.0012 Directional Control of Plasmon-Exciton interaction with Plexcitonic Crystals — SINAN BALCI, Department of Astronautical Engineering, University of Turkish Aeronautical Association, 06790 Ankara, Turkey, ERTU-GRUL KARADEMIR, COSKUN KOCABAS, ATILLA AYDINLI, Department of Physics, Bilkent University, 06800 Ankara, Turkey — Plexcitons [1] are strongly coupled plasmon excitons. In this work, we developed a platform, consisting of one and two dimensional corrugated surface patterns coated with a thin metal film and a dye solution. This system shows a controlled coupling action based on the excitation direction of SPP modes [2]. Our scheme is based on the control of wavelengths of the forbidden SPP modes. Three kinds of patterns have been tested: a one dimensional uniform, a triangular, and a square lattice type crystals. For all three cases, lowest wavelength of the band gap is observed in $\Gamma$ to M direction. For triangular and square lattice cases, band gap center oscillates between two finite values for every $60^\circ$ and $90^\circ$, respectively. We utilized this behavior to control SPP and J-aggregate coupling. We observe directional dependence of Rabi splitting energy varying between 0 meV and 60 meV. Square lattice gives the ability to tune a larger band gap, whereas triangular lattice gives higher number of symmetry points. Simulations show that, an 80 nm deep triangular lattice with 280 nm periodicity can result in omnidirectional decoupling of plexcitons.

4:54PM J5.00013  Thermochemical and electronic properties of amorphous oxides, nitrides and sulfides, PAWEŁ ZAWADZKI, STEPHAN LANY, National Renewable Energy Laboratory — Amorphous thin films materials become increasingly important components of many functional devices such as thin film displays, photovoltaic cells or thin film transistors. Due to lack of grain boundaries, they have superior uniformity and smoothest, flexibility and corrosion resistance. Amorphous thin films are typically prepared using physical vapor deposition (PVD) techniques at temperatures well below the melting point of deposited material (\(<0.2Tm\)). Computational models of amorphous structures, however, are almost elusively constructed from a high temperature equilibrated crystal melt using simulated annealing (SA) protocol. To account for low temperature growth conditions of amorphous thin films we recently developed a new simulation technique [1]. The method, kinetically limited minimization (KLM), starts from a randomly initialized structure and minimizes the total energy in a number of local structural perturbation-relaxation events. We apply KLM to model amorphous structures of 20 binary oxides, nitrides and sulfides and compare their thermochemical, structural and electronic properties.


5:06PM J5.00014 Colossal photoconductivity in transparent perovskite semiconductor BaSnO$_3$, JISUNG PARK, USEONG KIM, KOOKRIN CHAR, Seoul Natl Univ — We compare photoconductivities of BaSnO$_3$ (BSO) and SrTiO$_3$ (STO). Photoconductivity of STO has been intensively studied for its high potential for UV detector and optical devices. On the other hand, BSO has recently started to draw a large attention for its high electron mobility and thermal stability. BSO and STO have the same perovskite structure and similar band gap. Epitaxial thin films of BSO and STO were grown by pulsed laser ablation. The spectral responses measured by the monochromatic light showed peaks around the band gap of each film, an evidence that the electron-hole pair generation is the main mechanism for the photoconductivity in both materials. We have found the photoconductivity of BSO to be several orders of magnitude higher than that of STO. In addition, there exists a larger “persistent” photoconductivity in BSO. The high mobility of BSO, which is two orders of magnitude larger than that of STO at room temperature, should be partially responsible for the higher photoconductivity. The small difference between the direct gap and indirect gap of BSO may make band to band transition easier. We are also investigating the effect of dislocations on the “persistent” photoconductivity.

5:18PM J5.00015 $m$-Plane GaN Growth on “Double Miscut” Bulk Substrates for Blue Diode Applications, LEAH KURITZKY, DANIEL MYERS, KATHRYN KELCHNER, SHUJI NAKAMURA, STEVE DENBAARS, CLAUDE WEISBUCH, JAMES SPECK, Univ of California — Santa Barbara — Although nearly 100% of today’s commercial GaN devices are grown on the c-plane, the nonpolar $m$-plane is an alternative orientation that is free from polarization-induced electric fields, which separate carrier wavefunctions in c-plane InGaN quantum wells (QWs) and reduce carrier combination rates compared to m-plane. Performance of m-plane blue laser diodes is currently limited by low In uptake and broad linewidth in the blue spectrum compared to c-plane. This work examines the impact of m-plane surface miscut on these performance aspects. The morphology was examined by atomic force microscopy for homoepitaxy on co-loaded substrates: on-axis, $1^\circ$ c−miscut, $1^\circ$ a−miscut. All three films showed regions of diagonal a−c step direction where pure a− or c−direction steps were expected. These a+c regions also emitted longer wavelength in fluorescence and cathodoluminescence than other step directions. “Double miscut” substrates in the combined a− and c−directions take advantage of the observed stable a+c step direction and redshift. Multi-QWs on double miscut substrates exhibited <30 nm linewidth in the blue spectrum and higher In uptake than ever achieved for standard miscut m−plane.

Tuesday, March 3, 2015 2:30PM - 5:18PM - Session J6 DMP, DCOMP: Focus Session: Phonons, Spins, Charge and Orbital ordering in Complex Oxides 006A - Roman Engel-Herbert, Pennsylvania State University

2:30PM J6.00001 Nonlinear phononics and ultrafast control at complex interfaces, ANDREA CAVALLERI, Max-Planck Research Group for Structural Dynamics, Univ. Hamburg — No abstract available.

3:06PM J6.00002 Capturing photoinduced structural distortion within a unit cell of BiFeO$_3$, HAIDAN WEN, Argonne Natl Lab, MICHEL SASSI, Pacific Northwest National Laboratory, ZHENLIN LUO, University of Science and Technology of China, CAROLINA ADAMO, Stanford University, DARRELL SCHLOM, Cornell University, ROSSO KEVIN, Pacific Northwest National Laboratory, XIAOYI ZHANG, Argonne Natl Lab — The interaction of light with correlated materials has been an intensively studied research forefront in which the coupling of radiation energy to selective degrees of freedom offers a novel contact-free control knob to tune functionalities on ultrafast time scales. We studied a photoexcited multiferroic BiFeO$_3$ thin film using time-resolved x-ray absorption spectroscopy aided by density functional theory calculations. The study revealed a uniaxial deformation of the unit cell at a constant volume with a minimal oxygen octahedron rotation, consistent with the influence of photoinduced carriers to the ferroelectric polarization. These important findings illustrate a microscopic picture of local structural reconfiguration around iron atoms at atomistic length scales during a photocarrier-mediated nonequilibrium process in polar materials.

3:18PM J6.00003 Neutron Scattering Study of Low Energy Phonons and Spin Waves in Multiferroic BiFeO$_3$, ZHIJUN XU, UC Berkeley, GUANGYONG XU, JOHN SHNEELOCK, Brookhaven National Lab, JINSHEANG WEN, Nanjing University, PETER GEHRING, NIST, CHRIS STOCK, The University of Edinburgh, BARRY WINN, MASAAKI MATSUUDA, MA JIE, Oak Ridge National Lab, GENDA GU, Brookhaven National Lab, TOSHIMITSU ITO, AIST, STEPHEN SHAPIRO, Brookhaven National Lab, ROBERT BIRGENEAU, UC Berkeley — We have performed inelastic neutron scattering studies of the low-energy phonon and spin-wave modes in the multiferroic BiFeO$_3$. The low-energy phonon and spin wave dispersion relations along different directions have been mapped out over a broad temperature range from 100K to 750K. The temperature dependence of the intensities, dispersion relations, and lifetimes (inverse energy width) of these phonon and spin wave modes will be presented. Possible interactions between the lattice and spin dynamics will also be discussed. This work is supported by the Office of Basic Energy Sciences, DOE.

3:30PM J6.00004 Engineering orbital polarization in three-component nickelate heterostructures, CHARLES AHN, Yale University — The interplay between the structural and physical properties of transition metal complex oxides allows for the engineering of their functional properties by tuning atomic-scale structure using interfacial coupling. We show how this principle can be used to achieve orbital polarization and two-dimensional electronic conductivity in nickelate heterostructures [1, 2]. Using a combination of first principles theory and synchrotron-based experiments, we identify key structural features in LaNiO$_3$ thin films grown using molecular beam epitaxy, allowing one to correlate differences in physical structure with electronic transport properties and x-ray absorption spectroscopy measurements. By using general design principles, such as charge transfer and inversion symmetry breaking, which lead to degeneracy breaking of the Ni 3d orbitals, one can design and fabricate tri-component superlattices to engineer the electronic and orbital properties of rare-earth nickelate compounds, achieving a two-dimensional single band electronic surface at the Fermi energy.

4:06PM J6.00005 Time-resolved hard X-ray nano-diffraction study on the long-lived strain in BiFeO₃, induced by optical transient grating

YI ZHU, Argonne National Lab, QINGTENG ZHANG, PICE CHEN, University of Wisconsin, Madison, CAROLINA ADAMO, Cornell University, ZHONGSHOU CAI, DONALD WALKO, ERIC DUFRESNE, Argonne National Lab, DARRELL SCHLOM, Cornell University, PAUL EVANS, University of Wisconsin, Madison, HAIDAN WEN, Argonne National Lab, ARGONNE NATIONAL LAB TEAM, UNIVERSITY OF WISCONSIN, MADISON TEAM, CORNELL UNIVERSITY TEAM — Optical transient grating excitation was applied to induce spatially modulated strain in a BiFeO₃ thin film. The spatial profile and the dynamics of the photo-induced strain were measured by time-resolved hard X-ray nano-diffraction at beamline 7-ID of the Advanced Photon Source. By interfering two ultrafast laser beams at 400nm wavelength and ~ 100fs pulse duration, an optical transient grating with ~ 5 micron period sinusoidal profile was created and used to excite the BiFeO₃ sample. By using the nano-focused ultrafast X-ray pulses, both the strain profile and the dynamics induced by the photo-generated carriers were mapped out. We found the out-of-plane strain profile remained sinusoidal while the strain amplitude modulation lasted tens of microseconds, indicating the non-thermal nature of this photo-induced strain in BiFeO₃.

1Supported by U.S. DOE Contract No. DE-AC02-06CH11357 and Argonne LDRD Grant 2013-36.

4:18PM J6.00006 Phonon dispersion relation in cubic BaTiO₃

IZUMI TOMENO, Akitu University, JAIME FERNANDEZ-BACA, RIKI KOBAYASHI, SONGKUE CHI, Oak Ridge National Laboratory, KUNIHIKO OKA, National Institute of Advanced Industrial Science and Technology, YORIHIKO TSUNODA, Waseda University — The lattice dynamics of cubic BaTiO₃ (Tc = 405 K) has been investigated along the [100], [110], and [111] directions at T = 453, 700 and 890 K using inelastic neutron scattering. The transverse acoustic (TA) phonon dispersion is relatively isotropic. This indicates that all the measured TA branches are mainly governed by the Ba atom motion against the O atoms. The zone-boundary TA phonon energies for BaTiO₃ are approximately twice as large as those for cubic PbTiO₃. These differences cannot be explained by the A-site atomic mass alone. The large Ba-O force-constant reflects the ionic nature of Ba atom in BaTiO₃. The softening of the transverse optical (TO) ΔΣ and Σ branches in a wide q range at T = 453 K is in contrast to the steep softening of the TO Σ1 branch toward the zone center. The TO Σ1 mode is heavily damped in the range q ≤ 0.25 at 453 K, whereas the well-defined TO Σ1 peak for q = 0.25 is observed at 890 K. The low-lying TO ΔΣ1 and Σ1 branches are primary due to the low-frequency Ti-O-Ti chain-like motion along [001]. The soft mode behavior in BaTiO₃ is discussed in comparison with the previous study on PbTiO₃.

4:30PM J6.0007 [001] electric field effect on phonons in PMN-32PT

JOHN SCHNEELOCH, Brookhaven National Laboratory, ZHUJUN XU, University of California, Berkeley, BARRY WINN, Oak Ridge National Laboratory, CHRIS STOCK, University of Edinburgh, PETER GEHRING, National Institute of Standards and Technology, GUANGYONG XU, Brookhaven National Laboratory — We report inelastic neutron scattering measurements on a single crystal of the relaxor ferroelectric 68%Pb(Mg₁₋ₓTiₓ)O₃-32%PbTiO₃ (PMN-32PT) under an external [001] electric field (0.5 kV/cm). In addition to the partial suppression of diffuse scattering intensities, as previously reported, we also see a field-induced change in acoustic phonon intensities and energies. The change is anisotropic, with clear differences between the [100] and [011] directions. We will discuss these results and their relation to possible changes in the domain structure under field and coupling between diffuse scattering and phonon modes.

1DOE under Contract No. DE-AC02-98CH10886 and the DOE Center for Emergent Superconductivity.

4:42PM J6.0008 Magnetic field induced directed dichroism of spin waves in multiferroic BiFeO₃ at THz frequencies

URMAS NAGEL, T. RÖÖM, Nat.-I. Inst. of Chem. Phys. & Biophys., Tallinn, Estonia, S. BORDÁCS, I. KÉSZMÁRKI, Budapest University of Technology and Economics, Hungary, H.T. YI, S.-W. CHEONG, Rutgers Univ., New Jersey, JUN HEE LEE, RANDY S. FISHMAN, Oak Ridge National Laboratory, Tennessee — Using far infrared spectroscopy in high magnetic fields we show that spin excitations in BiFeO₃ simultaneously interact with the electric and magnetic field components of light resulting in directional dichroism (DD) of absorption. DD in BiFeO₃ arises because an applied static magnetic field induces a toroidal moment in the cycloidal spin structure. Strong DD is observed even in the room-temperature state of the material. The results are explained on the microscopic level as an interplay of five different interactions: isotropic exchange couplings between nearest and next nearest neighbors, an easy-axis anisotropy along the ferroelectric polarization, Dzyaloshinskii-Moriya (DM) interaction that creates the cycloid and DM interaction that causes spin canting.

1Research sponsored by the Estonian Ministry of Education and Research (IUT23-3), Estonian Science Foundation (ETF8703), and U.S. Department of Energy (EJL), Office of Science, Materials Sciences and Engineering Division (RF and JL) and Office of Basic Enn

4:54PM J6.0019 Charge Density Behavior of Ionic Liquid Gated Strontium Titanate Nanowires

TERENCE BRETZ-SULLIVAN, ALLEN GOLDMAN, University of Minnesota — Measurements of the current-voltage characteristics of ionic liquid gated nanometer scale channels of strontium titanate have been carried out. These characteristics exhibit a high voltage threshold for conduction and a nonlinear power law behavior at all temperatures measured. The source-drain current of these nanowires scales as a power law of the difference between the source-drain voltage and the threshold voltage. The temperature dependence of the threshold voltage appears to be related to the inverse of the temperature dependent dielectric constant of strontium titanate in qualitative agreement with a simple model of charge density wave depinning. These observations, when taken together, are evidence that a gate induced charge density wave has been induced, and is depinned by strong electric fields. * This work was supported by DOE Basic Energy Sciences Grant DE-FG02-02ER44004. Samples were fabricated at the Minnesota Nanofabrication Center. Parts of this work were carried out in the University of Minnesota Characterization Facility, a member of the Materials Research Facilities Network (www.mrfn.org) funded via the NSF MRSEC program.

5:06PM J6.0010 Neutron and X-ray studies in suppressing orbital order in FeV2O4 with Cr doping

DALMAU REIG-I-PLESSIS, ZHANGSU WEN, ALEXANDER THALER, U. of Illinois, VIASEL O. GARLEA, Oak Ridge National Lab, HAIDONG ZHOU, U. of Tennessee, JACOB RUFF, Cornell U., GREGORY MACDOUGALL, U. of Illinois — Fe₂V₂O₇ is a spinel compound with an orbitally active V⁵⁺ cation on a frustrated pyroclore sublattice and Jahn-Teller active Fe³⁺ on a diamond sublattice. Previous studies show that this material has three structural and two magnetic transitions, and that orbital order leads to coupling between the spin and lattice degrees-of-freedom. The opposite end of the doping series is the multiferroic, FeCr₂O₇, which has spin, but no orbital degree of freedom on the Cr⁴⁺ and only two structural transitions. Although both materials show a higher temperature collinear ferrimagnetic state and a non-collinear phase at lower temperature, the physics must be different since the canting transition in Fe₂V₂O₇ is associated with the orbital order at the lowest temperature. In this talk, I will present the results of synchrotron X-ray and neutron powder diffraction studies of the structural and magnetic transitions in the doping series Fe₂₋ₓCrₓO₇. Specifically, I will comment on the doping-temperature phase diagram we extract from these measurements, and the region of co-existence between distinct non-collinear spin orders which exist at finite doping.

1This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under award number DE-FG02-07ER46453.

2:30PM J7.00001 Spin-Polarized Tunneling Study on Spin-Momentum Locking in Topological Insulators Bismuth Selenide, CHING-TZU CHEN, LUQIAO LIU, IBM TJ Watson Research Center, ANTHONY RICHARDELLA, Department of Physics, Penn State University, ION GARATE, Department of Physics, University of Sherbrooke, YU ZHU, IBM TJ Watson Research Center, NITIN SAMARTH, Department of Physics, Penn State University — In this talk, we will demonstrate that the helical spin texture on topological insulator (TI) surfaces can be electrically detected using four-terminal tunnel junction devices with ferromagnetic top electrodes. Consistent results are obtained in both the Edelstein and spin-galvanic effect configurations, allowing a quantitative determination of the charge-spin conversion efficiency in bismuth selenide. By applying finite DC biases at the junction, we further extract the energy dependence of the effective spin polarization in bismuth selenide. The observed temperature stability up to 200K suggests that TIs can be highly promising for room-temperature spintronics applications.

2:42PM J7.00002 Tunable Intrinsic Spin Hall Conductivities in Bi$_2$(Se,Te)$_3$ Topological Insulators$^1$, CUÑEYT ŞAHIN, MICHAEL E. FLATTÉ, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa, Iowa City, Iowa 52242, USA — It has been recently shown by spin-transfer torque measurements that Bi$_2$Se$_3$ exhibits a very large spin Hall conductivity (SHC)$^1$. It is expected that Bi$_2$Te$_3$, a topological insulator with similar crystal and band structures as well as large spin-orbit coupling, would also exhibit a giant SHC. In this study we have calculated intrinsic spin Hall conductivities of Bi$_2$Se$_3$ and Bi$_2$Te$_3$ topological insulators from a tight-binding Hamiltonian including two nearest-neighbor interactions. We have calculated the Berry curvature, used the Kubo formula in the static, clean limit and shown that both materials exhibit giant spin Hall conductivities, consistent with the results of Ref. 1 and larger than previously reported Bi$_{1-x}$Sb$_x$ alloys$^2$. The density of Berry curvature has also been computed from the full Brillouin zone in order to compute the dependence of the SHC in these materials on the Fermi energy. Finally we report the intrinsic SHC for Bi$_2$(Se,Te)$_3$ topological insulators, which changes dramatically with doping or gate voltage. [1] A.R. Mellnik et al., Nature 511, 449 - 451 (2014) [2] C.Şahin and M.E.Flatté, arXiv:1410.7319

$^1$This work was supported in part by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA.

2:54PM J7.00003 Inverse spin galvanic effect in topological-insulator based heterostructures$^1$, MARTIN RODRIGUEZ-VEGA, Department of Physics, College of William and Mary, Williamsburg, VA 23187, USA, GEORG SCHWIETE, JAIRO SINOA, Institut für Physik, Johannes Gutenberg Universität Mainz, Mainz, Germany, ENRICO ROSSI, Department of Physics, College of William and Mary, Williamsburg, VA 23187, USA — We study the inverse spin galvanic effect in heterostructures formed by a layer of a three dimensional strong topological insulator (TI) and a magnetic material. We consider different configurations for the heterostructure and for the contacts. We carefully treat the effect on the TI bands of the proximity of a magnetic material and take into account both intra-band and inter-band contributions to the current-induced spin polarization of the TI surface states. Finally, we discuss the relevance of our results for recent experiments.

$^1$Work supported by ONR-N00014-13-1-0321, ACS-PRF # 53581-DNI5, and the Jeffress Memorial Trust.

3:06PM J7.00004 Low energy electrodynamics of topological insulator thin films, N. PETER ARMITAGE, Johns Hopkins University — Topological insulators are recently discovered states of matter with robust metallic surface states protected by the topological properties of their bulk wavefunctions. A quantum phase transition from a topological insulator to a conventional insulator and a change in topological class can occur only when the bulk bandgap closes. In this work, we have used time-domain terahertz spectroscopy to investigate the low-frequency conductance in (Bi$_{1-x}$In$_x$)$_2$Se$_3$ as we tune through this transition by In substitution. Above certain substitution levels we observe a collapse in the transport lifetime that indicates the destruction of the topological phase. We associate this effect with the threshold where states from opposite surfaces hybridize. The substitution level of the threshold is thickness dependent and only asymptotically approaches the bulk limit $x \sim 0.06$ where a maximum in the mid-infrared absorption is exhibited. This absorption can be identified with the bulk bandgap closing and change in topological class. The correlation ength associated with the quantum phase transition appears as the evanescent length of the surface states. The observation of the thickness-dependent collapse of the transport lifetime shows the unusual role that finite-size effects play in this topological quantum phase transition. In even more recent work on bulk insulating films, we have identified a cyclotron resonance feature. At high magnetic fields we identify an anomalous increase of the scattering rate. I will discuss the reasons for this increase and put it in the context of existing theories for charge transport in topological insulators.

3:42PM J7.00005 Evidence for surface-generated photocurrent in (Bi,Sb)$_2$Se$_3$ and (Bi,Sb)$_2$Te$_3$ thin films$^1$, YU PAN, ANTHONY RICHARDELLA, BING YAO, JOON SUE LEE, THOMAS FLANAGAN, ABHINAV KANDALA, NITIN SAMARTH, the Pennsylvania State University, ANDREW YEATS, PETER MINTUN, DAVID AWSCHALOM, University of Chicago — Illumination with circularly polarized light can produce a helicity-dependent photocurrent in topological insulators such as Bi$_2$Se$_3$. However, the exact origin of this effect is still unclear since it is observed with photons well above the bulk band gap. We report measurements of the polarization-dependent photocurrent in a series of (Bi,Sb)$_2$Se$_3$ thin films with different carrier densities and find that the photocurrent is enhanced as we increase the population of the surface states. This finding is supported by a study of helicity-dependent photocurrents in back-gated (Bi,Sb)$_2$Te$_3$ thin films, where the chemical potential is varied electrostatically. By illuminating our samples at different wavelengths, we show that the helicity-dependent photocurrent is enhanced when the photon energy approaches the energy difference between the lowest and first excited (unoccupied) topological surface states. This leads us to attribute the helicity-dependent photocurrent in topological insulators to optical excitations between these two spin-textured surface states. We will also discuss experiments imaging the spatial variation of these helicity-dependent photocurrents.

$^1$This work is supported by ONR.
while the chemical potential of a topological insulator (Bi,Sb) 

polarization throughout the surface state. We report the electrical probing of the spin-polarized surface state using a magnetic tunnel junction as a spin detector 
in topological insulators has been demonstrated very recently, there have not been any electrical measurements to demonstrate the entire mapping of the spin 
reversal symmetry protected three-dimensional topological insulator is the helically spin-textured surface state. Although electrical detection of spin polarization 
from Bi$_2$Te$_2$Se$_1$. Such an observation is consistent with the spin-momentum locking of the surface states. The largest Kerr rotation we measured is 4x10$^{-6}$ radians/(A/cm$^2$)) 
superspin function film thickness. 
of Kerr rotation in ultrathin films, allowing us to explore the predicted [Lu et al., PRB, 2010] transitions between topologically trivial and non-trivial states as a 
variation and the nonideal band dispersions of TSS in actual materials by modeling. The surface g factor in Sb$_2$Te$_2$Se and Bi$_2$Se$_3$ is estimated as -10 and 16, 
been successfully observed, the expected features in TSS still lack experimental proof. With scanning tunneling microscopy and spectroscopy, we observed the 
Zeeman shifting of zeroth LL in the TSS of Bi$_2$Se$_3$ and Sb$_2$Te$_2$Se unambiguously. Moreover, we exclude the intrinsic influence on LL shifting from potential 
variations and the nonideal band dispersions of TSS in actual materials by modeling. The surface g factor in Sb$_2$Te$_2$Se and Bi$_2$Se$_3$ is estimated as -10 and 16, 
respectively. This observation indicates that the g factor of TSS is significantly material dependent, which may be related to the atomic orbital character of the 
compound. 

Institute of Technology — Dirac fermions in the topological surface state (TSS) have helical spin textures. This is different from those in graphene, which are 
both valley and spin degenerated. The spin degeneracy can be lifted by Zeeman effect, which is manifested as a spin-splitting of Landau levels (LLs). In the case of TSS, LLs instead should exhibit monotonic shift with magnetic field since the spin degeneracy is lacking. While the Zeeman splitting of LLs in graphene has been successfully observed, the expected features in TSS still lack experimental proof. While scanning tunneling microscopy and spectroscopy, we observed the 
Zeeman shifting of zeroth LL in the TSS of Bi$_2$Se$_3$ and Sb$_2$Te$_2$Se unambiguously. Moreover, we exclude the intrinsic influence on LL shifting from potential 
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Tuesday, March 3, 2015 2:30PM - 5:18PM
Session J8 GSOFT: Colloids: Crystals and Other Phases 006C - Cynthia Olson-Reichhardt, Los Alamos National Laboratory

2:30PM J8.00001 Transitions from hard-sphere colloidal crystals to colloidal crystals with strong attractive interactions1, MATTHEW GRATALE, YE XU, ARJUN YODH, Department of Physics and Astronomy, University of Pennsylvania — Recently, colloid experiments have probed and found interesting differences in the properties of disordered glassy media as a function of the sign of the interparticle interaction [1-3]. Here, we report a similar kind of experiment, this time involving colloidal crystals wherein the interparticle interaction between constituent particles evolves from hard-sphere repulsive to attractive. This change in sign of the interparticle interaction is achieved through use of temperature-tunable depletion agents assembled from surfactants. The depletion-driven entropic attraction between particles in suspension grows with increasing temperature. Increasing temperature changes particle interactions in a dense crystal from repulsive to attractive, and accompanying variations in structure and dynamics of the crystal can be tracked. The increase in attractive interaction can also be turned on slowly and rapidly. Preliminary experiments on polycrystalline hard-sphere samples show accompanying decreases the lattice constant and a fluid-crystal coexistance phase consisting of small, dense “attractive” crystalline domains separated by “voids” filled with dilute colloidal fluid. These voids appear to originate at grain boundaries and near lattice defects in the original hard-sphere polycrystal. Further work explores the dense parts of the colloidal phase diagram with depletion interactions. [1] Eckert et al., PRL 89, 125701 (2002). [2] Pham et al., Science 296, 5565 (2002). [3] Kaufman et al., J. Chem. Phys. 125, 074716 (2006).

2:42PM J8.00002 Melting of colloidal crystals in small cavities1, YAFEI YANG, Hong Kong University of Science & Tech — We studied the melting behaviors of small colloidal crystals in different sized and shaped small cavities by video microscopy. The crystals were composed of temperature-sensitive N-isopropyl acrylamide (NIPA) microgel spheres. The cavity shape and defects can dramatically alter the melting kinetics and the vibration modes. The melting point can increase or decrease with size of colloid crystal, depending on the shape of the cavity. Single defect-free crystals melt from edges via nucleation mechanism in large hexagonal cavities, but melt catastrophically without nucleation when the cavity is smaller than a threshold. The smaller-angled cavity better promotes the melting.

5:06PM J7.00012 Quantum Spin Hall Effect in Ultrasonic Metamaterials, S. HOSSEIN MOUSAVI, University of Texas at Austin, ALEXANDER B. KHANIKAEV, City University of New York, ZHENG WANG, University of Texas at Austin — The discovery of topological order without breaking time-reversal symmetry, such as that in Quantum Spin Hall (QSH) effect and Topological Insulators, is one of the most groundbreaking advancements of recent years in condensed matters physics. The approach to topological order without breaking time-reversal symmetry is particularly important in elastics because no natural elastic materials show linear nonreciprocal response. Here we illustrate the first elastic-wave system emulating QSH effect and demonstrate existence of topologically protected elastic edge states. The system represents an elastic metamaterial-based phononic crystal. In this crystal, we achieved degenerate linear dispersion for two sets of modes, classified by one of the system’s symmetries. Then, by relaxing and removing that symmetry by deliberately engineering a gauge field emulating a strong spin-orbit coupling of QSH, we observe opening a complete topological bandgap. Finally, the hallmark of the topological order, namely the presence of one-way chiral edge waves insensitive to nonmagnetic defects and disorders, is demonstrated in such elastic metacrystals. We illustrate property of these elastic edge waves to flow around sharp corners without back-reflection or localization.

5:18PM J7.00013 Thickness tunable quantum interference between surface phonon and Dirac plasmon states in thin-films of the topological insulator Bi$_2$Se$_3$1, YURI GLINKA, SERCAN BABAKIRAY, TRENT JOHNSON, DAVID LEDERMAN, Department of Physics and Astronomy, West Virginia University — Raman scattering has been applied to study thin films of the topological insulator Bi$_2$Se$_3$. We observed a more than 100-fold enhancement of Raman responses as laser photon energy switches from 2.33 eV (532 nm) to 1.58 eV (785 nm), which is due to direct optical coupling to Dirac surface states (SS) at the resonance energy of about 1.5 eV (a thickness-independent enhancement) and due to nonlinearly excited Dirac plasmon (a thickness-dependent enhancement). Owing to the direct optical coupling, we were able to monitor an in-plane phonon mode of hexagonally arranged Se-atoms associated with a continuous network of Dirac SS. This mode revealed a Fano lineshape for films below 15 nm thick, resulting from quantum interference between surface phonon and Dirac plasmon states.

1This work was supported by a Research Challenge Grant from the West Virginia Higher Education Policy Commission (HEPC.dsr.12.29).

2:42PM J8.00002 Melting of colloidal crystals in small cavities1, YAFEI YANG, Hong Kong University of Science & Tech — We studied the melting behaviors of small colloidal crystals in different sized and shaped small cavities by video microscopy. The crystals were composed of temperature-sensitive N-isopropyl acrylamide (NIPA) microgel spheres. The cavity shape and defects can dramatically alter the melting kinetics and the vibration modes. The melting point can increase or decrease with size of colloid crystal, depending on the shape of the cavity. Single defect-free crystals melt from edges via nucleation mechanism in large hexagonal cavities, but melt catastrophically without nucleation when the cavity is smaller than a threshold. The smaller-angled cavity better promotes the melting.

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1This work was supported by NSF grant DMR12-05463, Penn MRSEC grant DMR11-20901, and NASA grant NNX08AO0G.

2:54PM J8.00003 Born melting of three dimensional crystals, JORIS SPRAKEL, Wageningen University, ALESSIO ZACCONI, Technical University Munich, PETER SCHALL, University of Amsterdam, DAVID A. WEITZ, Harvard University — While the microscopic nature of melting in 1 and 2 dimensions has been elucidated both theoretically and experimentally, this has proven elusive for three-dimensional crystalline solids. Max Born hypothesized that melting can be described as a rigidity catastrophe where the crystal’s shear elastic constant vanishes at melting. Here we show experimental evidence, using three-dimensional imaging of soft colloidal crystals, for such a mechanical instability underlying melting. Our results reveal how non-affine fluctuations govern the mechanical instability which precipitates melting; modification of Born’s theory to take non-affinity into account accurately describes our experimental data. Moreover, we show how the continuous weakening of the crystal’s resistance to shear leads to the emergence of collective fluctuations who’s size diverges at the melting point.

3:06PM J8.00004 Grain Boundary Roughening in Colloidal Crystals1, YILONG HAN, MALIJA LIAO, XIAO XIAO, Hong Kong University of Science and Technology, TOM LUBENSKY, University of Pennsylvania — We studied the grain-boundary roughening transition inside the bulk of thermal-sensitive thin-film colloidal crystals by video microscopy and phase-field simulations. As the volume fraction of the microgel colloidal polycrystals decrease, we observed that the large-angle grain boundaries become rough with the strongest shape fluctuations at the roughening transition point below the premelting point. The roughening transition exhibits critical behaviors. We discovered the structural change responsible to the exotic decrease of the shape fluctuation and the mobility change of the grain boundary as approaching the premelting point. Small-angle grain boundaries do not have the roughening transition and exhibit different melting behaviors.

1The project was supported by GRF grants 601911 and 1630154.
3:30PM J8.00006 Quantifying Stress Fields of Defects in 3D Colloidal Crystals. MATTHEW BIERBAUM, NEIL Y.C. LIN, CORNELL UNIVERSITY, PETER SCHALL, UNIVERSITY OF AMSTERDAM, JAMES P. SETHNA, ITAI COHEN, CORNELL UNIVERSITY — We introduce the “Stress Assessment from Local Anisotropy” (SALSA) method and use it to directly measure the local stress fields of defects including vacancies, dislocations, and polycrystals in 3D colloidal suspensions. In this technique, we extract a time-series of particle positions from confocal images from which we determine stresses on the particle scale. In the case of both bulk voids and the particle scale, we find a nonlinear pressure ring which is well described by linear elastic theory with a geometric nonlinearity. We next measure the stress fields in a polycrystal before and after cyclic shear. We find that the normal stresses in the grain boundaries are about 10%-20% lower than in the grains. This provides a more detailed, particle level measurement of polycrystalline stresses that is consistent with analogous X-ray experiments as well as previous simulations.

3:42PM J8.00007 Stripe Systems with Competing Interactions on Quasi-One Dimensional Periodic Substrates, DANIELLE MCDERMOTT, WABASH COLLEGE, CYNTHIA J. OLSON REICHHARDT, CHARLES REICHHARDT, THEORETICAL DIVISION, LOS ALAMOS NATIONAL LABORATORY — We numerically examine the two-dimensional ordering of a stripe forming system of particles with competing long-range repulsion and short-range attraction in the presence of a quasi-one-dimensional corrugated substrate. As a function of increasing substrate strength or the ratio of the number of particles to the number of substrate minima, we show that a remarkable variety of distinct orderings can be realized, including modulated stripes, prolate clump phases, two dimensional ordered kink structures, crystalline void phases, and smectic phases. Additionally in some cases the stripes align perpendicular to the substrate troughs. Our results suggest that a new route to self assembly for systems with competing interactions can be achieved through the addition of a simple periodic modulated substrate.

3:54PM J8.00008 Conformal Crystals, VISHAL SONI, UNIVERSITY OF CHICAGO, LEOPOLDO GOMEZ, UNIVERSIDAD DEL SUR - CONICET, WILLIAM IRVINE, UNIVERSITY OF CHICAGO — Interacting particles which would otherwise form a perfect crystal arrange into fascinating structures when immersed in spatially varying potentials. Using colloidal experiments and molecular dynamics simulations, we explore the two dimensional ordering of repulsive particles confined by external potentials. By relating the resulting inhomogeneous structures to a lattice frustrated by Gaussian curvature, we investigate the role of topological defects in organizing the conformal crystal-like ground states.

4:06PM J8.00009 Self-Healing Colloidal Crystals: Why Soft Particles Feel the Squeeze, ANDREA SCOTTI, URS Gasser, LNS, Paul Scherrer Institut, EMILY HERMAN, Ultraink Inc., MIGUEL PELAEZ-FERNANDEZ, SCHOOL OF PHYSICS, GEORGIA INSTITUTE OF TECHNOLOGY, ANDREW LYON, SCHMID COLLEGE OF SCIENCE AND TECHNOLOGY, ALBERTO FERNANDEZ-NIEVES, SCHOOL OF PHYSICS, GEORGIA INSTITUTE OF TECHNOLOGY — Point defects in crystalline materials disturb the crystal structure and often prevent crystallization. In particular, this is the case for too big particles that are put into a crystal. In metal melts, a size mismatch of 15% of the atoms in the melt suppresses crystallization. Furthermore, hard spheres with a polydispersity greater than 12% do not form crystals, and the polydispersity in the crystal state does not exceed 5.7%, as local segregation occurs. These restrictions do not necessarily apply for soft microgels. Lyon et al. (A. St. J. Iyer and L. A. Lyon, Angew. Chem. Int. Ed., 48, 2009) find bigger microgels to shrink and fit into the lattice formed by smaller ones. We find that charged groups in the microgel and their counter-ions are the key to explain this remarkable spontaneous deswelling of microgels. Using small-angle neutron and X-ray scattering, we directly observe the deswelling of bigger particles with increasing volume fraction and the effect of the bigger particles on the phase behavior of the suspension. Furthermore, we determine the osmotic pressure using osmometry and present a model for the selective deswelling of the big particles.

4:18PM J8.00010 Self-Assembly of an Icosahedral Quasicrystal Network, MICHAEL ENGEL, PABLO F. DAMASCENO, UNIVERSITY OF MICHIGAN, CAROLYN L. PHILLIPS, ARgonne national laboratory, SHARON C. GLOTZER, UNIVERSITY OF MICHIGAN — Icosahedral quasicrystals (IQC) are a form of matter that is ordered but not periodic in any direction. IQCs have the highest symmetry of all crystals and therefore exhibit orientationally highly uniform properties. This makes them candidates for materials with a complete photonic bandgap or as specialized alloys. Unlike axially-symmetric quasicrystals, which have been reported experimentally in micellar or nanoparticle systems and suggested in bi-layer water, silicon, and mesoporous silica, IQCs have not been observed in the context of non-intermetallic systems. Here, we demonstrate the self-assembly of an IQC by means of molecular dynamics simulations. The IQC is a predominantly tetrahedral, body-centered-icosahedral network and is structurally related to clathrates and other tetrahedrally coordinated crystalline networks. The IQC self-assembles rapidly and reproducibly from a fluid phase in a one-component system of particles. We provide a crystallographic structure model and show the presence of a diffusion mechanism not available in periodically ordered solids. [1] M. Engel, P.F. Damasceno, P.L. Phillips, S.C. Glotzer, Nature Materials, in press (2014).

4:30PM J8.00011 Particle dynamics in dense colloidal suspensions with short-range attraction, PIOTR HABDAS, ZACHERY BROWN, DEPARTMENT OF PHYSICS, SAINT JOSEPH’S UNIVERSITY, MATTHEW GRATALE, ARJUN G. YODH, DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF PENNSYLVANIA — We study single particle dynamics and dynamical heterogeneity in colloidal suspensions with tunable short-range attraction as a model for particles confined near an attractive glass. Short-range (MSD) forces induce the transition. Using direct optical microscopy, we identify colloidal particles that exhibit substantial motional events. We observe that these particles demonstrate heterogeneous dynamics which is manifested by non-Gaussian distribution of the particle displacements. Maximum dynamical susceptibility is determined systematically over a range of probe length and time scales. Preliminary results show that at volume fractions just above the colloidal glass transition the intensity of spatial heterogeneities decreases as the interparticle attraction strength is increased suggesting the system enters the ergodic fluid state.

1 Acknowledgement: Marie Curie International Outgoing Fellowship within the European Union (EU) Seventh Framework Program
2 School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA, FRANS SPAEPEN, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA. — A comparative study has been made to explore melt transition for two different types of soft colloids: sterically stabilized aqueous core-shell (CS) microgels and charge stabilized PMMA particles. The shell component made of polymer network stabilize the CS suspension whereas the PMMA particle suspension is stabilized by the surface charge on each particle. Both types of particles form stable three dimensional crystal structures at higher volume fractions. We locate individual particles to construct 3D pair-correlation function and mean-square-displacements (MSD). We explore the melting transition in equilibrium for both the systems by changing the inter-particle separation i.e by changing volume fraction. Different melting criterions have been used to identify melting point. The result shows that melting transition for sterically stabilized CS microgel is fundamentally different from that of charge stabilized PMMA particles.

3 NSF MRSEC Grant DMR-1120901, and NASA Grant NNX08AO0G.
4:42PM J8.00012 Jamming and Phase Transition in Binary Soft Colloids

AKANKSHA AGRAWAL, School of Chemical and Biomolecular Engineering, Cornell University, HSU-YU YU, School of Chemical and Biomolecular Engineering, University of Pennsylvania, SAMANVAYA SRIVASTAVA, LYNDEN A. ARCHER, School of Chemical and Biomolecular Engineering, Cornell University, SURESH NARAYANAN, Advanced Photon Source, Argonne National Laboratory — We report on jamming, yielding, and flow of binary mixtures of self-suspended silica nanoparticles densely grafted with Polyethylene glycol (PEG)(MW ~ 5000g/mol). The ratio of volume fraction of the larger particles to the total volume fraction of the silica cores, \( x_c \), is shown to sensitively affect both the yielding and jamming transitions of these systems. For all the binary systems a two-step yielding is observed in oscillatory shear measurements, which we discuss in terms of the breaking of small and big particle cages. We find that addition of larger particles to a suspension of smaller ones softens the suspensions and, for small values of the particle radius ratio \( r = R_1 / R_2 \), the larger particles produce complete fluidization of their smaller counterparts. We show that these behaviors coincide with a speeding-up of de-correlation dynamics of all particles in the suspensions using XPCS measurements and are preceded by an abrupt transition in the average inter-particle spacing, similar to behavior predicted for a semi-dilute binary hard sphere suspension model as observed from SAXS experiment.

1 Supported by U.S. Department of Energy (DOE) grant DE-FG02-08ER46512

4:54PM J8.00013 Anisotropic stress correlations in 2D liquids

BIN WU, TAKUYA IWASHITA, TAKESHI EGAMI, Univ of Tennessee, Knoxville — We demonstrate the presence of anisotropic stress correlations in the simulated 2D liquids. Whereas the temporal correlation of macroscopic shear stress is known to contribute to viscosity via the Green-Kubo formula, the general question regarding angular dependency of the spatial correlation among atomic level stresses in liquids without external shear has not been explored. Besides the apparent anisotropy with well-defined symmetry, we found that the characteristic length of shear stress correlation depends on temperature and follows the power law, suggesting divergence around the glass transition temperature. The anisotropy of the stress correlations can be explained in terms of the inclusion model by Eshelby, based upon which we suggest that the mismatch between the atom and its nearest neighbor cage produces the atomic level stress as well as the long-range stress fields.

5:06PM J8.00014 Frustrated packing of monodisperse spheres in a flat container

RALF STANNIARIUS, KIRSTEN HARTH, Otto von Guericke University, Magdeburg — We study the packing of monodisperse spheres in a flat vertical box with cell gap slightly larger than the particle diameter, and evaluate the statistics of the particle arrangements. After ‘gravitational’ filling of the container and appropriate agitation, the particles form a nearly regular triangular lattice in the cell plane. The additional freedom of a displacement normal to the cell plane places the particles either at the front or rear cell plate. This leads to a denser arrangement in the cell plane, but at the same time causes frustrated states. Two of three neighboring beads in a local triangle have to occupy the same cell wall. Analogies to order in antiferroelectric Ising spin systems on a triangular lattice and to colloidal assemblies in thin layers are evident. We analyse experimental packings statistically and compare them to the predictions of models and Monte Carlo simulations. When the container is tilted from the vertical, the gravitational field mimics an external force similar to a magnetic field in spin systems. The experiment both offers insights into the influence of geometrical constraints on random packing, and provides a descriptive example of frustrated ordering.

Tuesday, March 3, 2015 2:30PM - 5:30PM —
Session J9 DMP: Focus Session: van der Waals Bonding in Advanced Materials: Layered Materials

2:30PM J9.00001 Hexagonal Boron Nitride-Water Non-bonded Interaction from First Principles

YANBIN WU, LUCAS K. WAGNER, NARAYANA R. ALURU, Univ of Illinois - Urbana — The interaction between water and h-BN is estimated using the Muller-Plesset perturbation theory of the second order (MP2) and diffusion Monte Carlo (DMC) method. The MP2 and DMC results are verified using coupled cluster treatment with single and double excitations and perturbative triples at the complete basis set limit (CCSD(T)/CBS) using B3N3H6-water as a proxy. The water-h-BN binding energy is estimated as 1.9 \( \pm \) 0.2 kcal/mol. Boron/nitride (BN)-water non-bonded interaction parameters are developed based on the MP2 energies. The B/N-water parameters predict the water contact angle on bulk h-BN surface that is in good agreement with experimental measurements.

2:42PM J9.00002 Role of weak interactions in phase transitions of layered transition metal dichalcogenides: An ab initio study

NILADRI SENGUPTA, ADRIENN RUZSINSZKY, JOHN P. PERDEW, Temple Univ — Phase transitions of layered materials are not often clearly explained and captured by the GGA level density functional calculations. Weak interactions might play an important role in these phase transitions. Now GGA can not describe well weak interactions. So we intend to use several new meta GGAs (TPSS, RevTPSS, MS family etc.), many body VDW corrected meta GGAs and RPA to study phase transitions of layered transition metal dichalcogenides (ME\( _2 \); M = Ti, V, Cr, Ta, Mo, W ; E = Se, S, Te) and investigate the role of weak interactions in those cases.

2:54PM J9.00003 Dispersion Forces of Adatoms on Deformed Graphene

VALERI KOTOV, University of Vermont — van der Waals (vdW) forces are especially important near atomically-thin materials, such as graphene, boron nitride (h-BN) and transition metal dichalcogenides (e.g. MoSe2), which form the building blocks of the so-called van der Waals heterostructures. These systems can also exhibit strong deformations in their structure due to stress, either applied externally, or induced by the presence of a substrate. A problem of fundamental and technological importance is how the vDW forces, which reflect Coulomb interactions and polarization effects, depend on electronic and mechanical material properties. I will show that strain fields can greatly enhance the vDw interactions of neutral adatoms near graphene and structurally similar surfaces, thus substantially affecting adsorption properties and altering the dissipative dynamics associated with atomic motion. For the case of two strained graphene sheets similar enhancement was predicted by A. Sharma et.al., PRB 89, 235425 (2014). I will consider several aspects of the adatom-graphene problem: (1) Variation of the vDw force as a function of uniaxial and more general strain fields, (2) Dependence on electron-electron interactions, including renormalization effects near the Dirac point, (3) Implications for dissipative atom dynamics.
3:06PM J9.00004 RPA and beyond-RPA total energy methods for strongly and weakly bonded materials, KRISTIAN THYGESEN, Center for Atomic-scale Materials Design (CAMD), Technical University of Denmark — The random phase approximation (RPA) is attracting renewed interest as a universal and accurate method for first-principles total energy calculations. The RPA naturally accounts for long-range dispersive forces making the RPA superior to density and hybrid functionals in systems dominated by weak van der Waals or mixed covalent-dispersive interactions. We have applied the RPA to calculate the potential energy surfaces of graphene on various metal surfaces. For some of the metals, the RPA binding energy curve shows two distinct minima which arise from a delicate balance between covalent and dispersive forces that are not captured by standard semilocal or van der Waals density functionals [1]. We benchmark the RPA by calculating cohesive energies of graphite and a range of covalently bonded solids and molecules as well as the dissociation energies of H2 and H2+—The results show that the RPA with orbitals from the local density approximation suffers from delocalization errors and systematically understimates covalent bond energies yielding similar or lower accuracy than the Perdew-Burke-Ernzerhof (PBE) functional for molecules and solids [1]. Inclusion of an adiabatic xc-kernel defined through a renormalization of the LDA kernel is found to significantly improve the RPA description of short range correlations yielding essentially exact results for the homogeneous electron gas [2]. By generalizing this renormalized LDA xc-kernel to inhomogeneous systems we find a fourfold improvement of RPA binding energies in both molecules and solids. We also consider examples of barrier heights in chemical reactions, molecular adsorption, and graphene interacting with metal surfaces, which are three examples where the RPA has been successful. In these cases, the renormalized kernel provides results that are of equal quality or even slightly better than the RPA, with a similar computational cost [3].


3:42PM J9.00005 The Quantum Monte Carlo studies of Van der Waals interaction in bilayer systems, CHING-MING WEI, CHENG-RONG HSING, Institute of Atomic and Molecular Sciences, Academia Sinica, CHING CHENG, Department of Physics, National Cheng Kung University, CHUN-MING CHANG, Department of Physics, National Dong Hwa University — Van der Waals (vdW) interaction is one of the most fundamental physical quantities resulted from the quantum fluctuation of charges. However, it remains a challenge to account for this interaction quantitatively in both theory and experiment. For example, vdW interaction is one of the physical properties that the LDA and GGA of Density Functional Theory (DFT) fail to describe correctly. In recent years, there have been many proposals of DFT-vdW to overcome this deficiency. However, discrepancies in binding energy among these DFT-vdW results are usually apparent. In this talk, we present the Quantum Monte Carlo (QMC) and DFT studies of various bilayer systems: BN/BN [New. J. Phys. 16, 113015 (2014)], Silicene/Graphene, Silicene/BN and MoS2/Graphene. The calculations show large discrepancies among various DFT functionals. The QMC calculated binding energy was found to be larger than that obtained by the LDA calculation and smaller than those using DFT-vdW correction. Moreover, the QMC calculated interlayer interaction was found to have a longer-range behavior than all the available DFT schemes. The outcome of the present QMC study would provide a benchmark for future generation of various DFT xc-functionals and guidance for prospective experiments.

In these cases, the renormalized kernel provides results that are of equal quality or even slightly better than the RPA, with a similar computational cost [3].

1 work supported by MOST, NCHC, NCTS and the Academia Sinica Computing Center of Taiwan.

3:54PM J9.00006 Ni(111)-graphene interface: the importance of screened van der Waals interactions, PIER LUIGI SILVESTRELLI, ALBERTO AMBROSETTI, Università degli Studi di Padova — Due to the direct applicability of Ni(111) surfaces in high-quality graphene production, the Ni(111)-graphene interface has recently been the object of extensive experimental and theoretical investigations. Achieving an accurate and efficient theoretical description of the Ni(111)-graphene interaction, however, still represents a major theoretical challenge, due to the complex interplay between van der Waals (vdW) and hybridization effects. Here we apply the DFT/vdW-WF2s method [1], augmenting semi-local Density Functional Theory with the inclusion of screened vdw interactions. Interestingly, we show that a reliable description of the vdw energy in Ni(111)-graphene requires an appropriate modeling of the metal-screening, which should not only account for the p- and s-like quasi-free electrons, but should further include the effect of the more localized d-like states. Good agreement is found with experiment and highly accurate theoretical predictions. Moreover, being the DFT/vdW-WF2s method based on Maximally Localized Wannier Functions, it permits an intuitive understanding of the complex physics underlying transition metals-graphene interactions.


4:06PM J9.00007 ZnO-Graphene Interfacial Binding Strength: Dependence on Surface Orientation, HAIYING HE, KELSEY LARSON, ADAM CLARK, ALLYSE APPEL, STAN ZYGMUNT, Valparaiso University — There is an increasing interest of hybridized materials with impacts such as improving structural integrity of known and commonly used materials. Recent experiments have suggested that the adhesion of zinc oxide (ZnO) nanowires with carbon fibers can significantly improve interfacial shear strength of fiber reinforced composites. We have carried out a systematic study of the interaction between ZnO and graphene based on density functional theory, through the inclusion of screened vdw interactions. Interestingly, we show that a reliable description of the vdw energy in Ni(111)-graphene requires an appropriate modeling of the metal-screening, which should not only account for the p- and s-like quasi-free electrons, but should further include the effect of the more localized d-like states. Good agreement is found with experiment and highly accurate theoretical predictions. Moreover, being the DFT/vdW-WF2s method based on Maximally Localized Wannier Functions, it permits an intuitive understanding of the complex physics underlying transition metals-graphene interactions.

4:18PM J9.00008 Structural and Electronic Properties of BC 3 with Van der Waals Density Functional Theory, BURAK OZDEMIR, VERONICA BARONE, Central Michigan Univ — Layered materials have attracted a lot of attention recently due to their unique properties that can be optimized for technological applications such as energy storage and transparent conductors. Among these materials, a graphite-like BC3 (g-BC3) structure has been recently under investigation as it provides a similar morphology than graphite but with a large concentration of electron deficient B atoms. Despite the recent experimental and theoretical works, the morphology of this materials is still not well understood. In this work, stable stacking configurations of g-BC3 has been determined using different exchange-correlation functionals that include dispersion corrections. We identify the most stable structures and characterize their electronic properties.

4:30PM J9.00009 Measurement of the long range van der Waals force in graphene, JUN XU, University of California, Riverside, ALEXANDR BANISHEV, University of Illinois at Urbana-Champaign, UMAR MOHIDEEN, University of California, Riverside — The gradient of the long range van der Waals force between a Si-SiO2-graphene substrate and an Au-coated sphere is measured by means of a dynamic atomic force microscope operated in the frequency shift technique. It is shown that the presence of graphene leads to up to a 9% increase in the force gradient at the shortest separation considered. The experimental results are compared to a theory of the long range thermal van der Waals interaction for multilayered test bodies coated with a graphene sheet and found to be in good agreement. References: [1] A.A. Banishev, H. Wen, J. Xu, R.K. Kawakami, G.L. Klimchitskaya, V.M. Mostepanenko, U. Mohideen, Measuring the Casimir force gradient from graphene on a SiO2 substrate, Phys. Rev. B, 87 (2013) 5. [2] G.L. Klimchitskaya, U. Mohideen, V.M. Mostepanenko, Theory of the Casimir interaction from graphene-coated substrates using the polarization tensor and comparison with experiment, Phys. Rev. B, 89 (2014) 8.

The authors thank G.L. Klimchitskaya and V.M. Mostepanenko for help with the theory and the US Department of Energy for funding the research.
Ab-stacking mode is slightly favored than the AB mode but the binding energy difference is very small, only about 0.3 meV/atom. It is also found that vdW interactions allow accurate description of the van der Waals interaction between two graphyne layers. The QMC results for the interlayer binding energies have revealed that the multiplet structure of SmB$_6$ samarium hexaboride (SmB$_6$) without Kondo physics substrates, in good agreement with recent experimental measurements by quartz crystal microbalance technique. The calculated activation energies indicate that Xe becomes movable on pure Au(111) surface at a temperature of around 30 K, whereas its motion can be activated only at a high temperature of 50 K on graphene and on graphene-coated Au(111) substrate. The van der Waals force from graphene determined per layer was found to decrease with the number of layers. In addition, increased hole doping of graphene enhanced the force. The screening was lifted in the single-layer graphene upon its fluorination, which rendered it electrically insulating. Finally, we also demonstrated strong screening of the van der Waals forces of the silicon oxide substrate by single- and double-layer molybdenum disulfide. Analysis of the experimental results was aided by density functional theory calculations.

4:54PM J9.00011 Interlayer Binding of Bilayer $\alpha$-graphyne : Quantum Monte Carlo Study
YONGKUN H Kwon, HYEONDEOK SHIN, HOONKYUNG LEE, Konkuk University, JEONGNIM KIM, Oak Ridge National Laboratory — Graphynes have recently received considerable attention because of their intriguing potential as new Dirac materials. Recent DFT calculations of Leenaerts et al. [1] predicted two stable stacking modes of bilayer $\alpha$-graphyne, while a AB-stacked configuration was found to possess a gapless parabolic band structure, the other stable mode of Ab-stacked graphyne exhibits a double Dirac cone spectrum. On the other hand, more accurate DFT calculations predicted different ground-state configurations for bilayer $\alpha$-graphyne, depending on the van der Waals (vdW)-corrected exchange-correlation functional used. In order to determine the most stable configuration of bilayer $\alpha$-graphyne along with accurate computation of its interlayer binding energy, we here employ quantum Monte Carlo method which allows accurate description of the vdW interaction between two graphyne layers. The QMC results for the interlayer binding energies have revealed that the Ab-stacking mode is slightly favored than the AB mode but the binding energy difference is very small, only about 0.3 meV/atom. It is also found that the DFT results with vdW-DF2, based on the non-local vdW functional proposed by Lee et al. [2], are in good agreement with the QMC results. This leads us to conclude that within the DFT formalism the interlayer binding of the graphyne structures is best described by the vdW-DF2 functional. [1] O. Leenaerts et al., Appl. Phys. Lett. 103, 013105 (2013). [2] K. Lee et al., Phys. Rev. B 82, 081101R (2010).

5:06PM J9.00012 Adapting DFT C6-corrections for modeling graphene on metal surfaces
PETER SCHULTZ, Sandia National Laboratories, Albuquerque, NM, USA, MICHAEL FOSTER, Sandia National Laboratories, Livermore, CA, USA — Modeling graphene on metals accurately presents a challenge for first principles due to difficulties modeling non-local electron correlation. An effective model must resolve small van der Waals (vdW) binding of graphene to the surface from the large cohesive energy in the metal and chemical bond energies in the graphene. Conventional density functional theory (DFT) such as GGA/PBE fails to describe vdW effects accurately. More sophisticated non-local vdW functionals, still in their infancy, produce inconsistent results, and there is a shortage of experimental data to assess which of these is more reliable. Moreover, computational expense limits their general application. We adopt DFT plus C6-corrected methods in concert with non-local vdW functionals to study graphene on Cu(111), Ni(111), and Ir(111). The known strengths of vdW-functionals and limited experimental data are used to constrain the definition of the C6-corrections (which in turn provides guidance as to which vdW-enhanced functionals are most suitable for accurate simulations of graphene adsorption on metals). The less expensive DFT+C6 and vdW-DFT are shown to give consistent results, and agree with known experimental data for these three metal surfaces.

1 Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy’s NNSA under contract DE-AC04-94AL85000.

Tuesday, March 3, 2015 2:30PM - 5:30PM — Session J10 DCMP: Topological Kondo Insulators
007A - Nicholas Butch, National Institute of Standards and Technology

2:30PM J10.00001 A new theoretical approach to SmB$_6$ and related mixed valence compounds without Kondo physics
ALFRED CHEUNG, MONA BERCIU, ILYA ELFIMOY, GEORGE SAWATZKY, Univ of British Columbia — Currently, samarium hexaboride (SmB$_6$) is widely thought of as a Kondo insulator with the formation of its hybridization gap being attributed to Kondo physics. This is in spite of the fact that Sm is strongly mixed valent and is hence incompatible with the Kondo scenario of fixed spins undergoing spin fluctuations. In this talk, we summarize arguments for why Kondo physics is inappropriate for the case of SmB$_6$. We then present a new model in which the low energy scale atomic multiplet structure of SmB$_6$ and the strong Sm 4f valence fluctuations are properly taken into account, replacing Kondo lattice physics as the principal player in SmB$_6$.

2:42PM J10.00002 30 MHz Self Oscillator using Topological Kondo Insulator SmB$_6$
ALEXANDER STERN, DAEJEONG KIM, SEAN THOMAS, ZACHARY FISK, JING XIA, University of California, Irvine, Department of Physics and Astronomy — We are studying electrical properties of SmB$_6$ (or Samarium Hexaboride), which is a topological insulator material. By applying a DC current to a tiny crystal of SmB$_6$ and a capacitor, we were able to generate 30 MHz oscillation voltage across the crystal. The frequency range is set by the crystal size and quality and the frequency can be fine-tuned by the amount of DC current. With varying crystal size, we have achieved the frequencies from 20Hz to 30MHz with amplitudes up to 50mV. The DC current driven oscillation is induced by thermal oscillation between topological surface and the bulk states. We will present a theoretical model for this intriguing behavior. This work is supported by DARPA/Air force grant FA 8650-14-1-7407.

3 This work is supported by DARPA/Air force grant FA 8650-14-1-7407.
Emergent photovoltage on SmB$_6$ surface upon bulk-gap evolution revealed by pump-and-probe photoemission spectroscopy

YUKI AKIMURA, TOSHIO OTSU, TOMOKO SHIMADA, MARIO OKAWA, YOHEI KOBAYASHI, ISSP, University of Tokyo, FUMITOSHI IGA, Ibaraki University, TOSHIRO TAKABATAKE, Hiroshima University, SHIK SHIN, ISSP, University of Tokyo — Recent studies suggest that an exemplary Kondo insulator SmB$_6$ belongs to a new class of topological insulators (TIs), in which non-trivial spin-polarized metallic states emerge on surface upon the formation of Kondo hybridization gap in the bulk. Remarkably, the bulk resistivity reaches more than 20 $\Omega$ cm at 4 K, making SmB$_6$ a candidate for a so-called bulk-insulating TI. We here investigate optical-pulse responses of SmB$_6$ by pump-and-probe photoemission spectroscopy. Surface photovoltage effect is observed across $\sim$ 90 K. This indicates that an optically-active band bending region develops beneath the novel metallic surface upon the bulk-gap evolution. The photovoltaic effect persists for $>200 \mu$s, which is long enough to be detected by electronics devices, and could be utilized for optical gating of the novel metallic surface.

Supported by JSPS through FIRST program, by Photon and Quantum Basic Research Coordinated Development Program from MEXT, and by JSPS KAKENHI (20102004, 23540413, and 26800165).

Also at Hiroshima University

Surface damage of SmB$_6$ through ion-irradiation

NICHOLAS WAKEHAM, YONGQIANG WANG, Los Alamos National Laboratory, ZACHARY FISK, University of California, Irvine, FILIP RONNING, JOE THOMPSON, Los Alamos National Laboratory — SmB$_6$ is a Kondo insulator, but there is strong evidence for an intrinsic conductive surface state at low temperatures. Theoretical work indicates that SmB$_6$ may be a topological Kondo insulator with a topologically protected surface state that is robust against time-reversal invariant perturbations. To investigate this robustness, we have used non-magnetic ion-irradiation to damage the (001) surfaces of SmB$_6$ single crystals to varying depths, and have measured the resistivity as a function of temperature for each depth of damage. We observe a reduction in the residual resistivity with increasing depth of damage. Our data are consistent with a model in which the surface state is not destroyed by the ion-irradiation, but instead the damaged layer is poorly conducting and the initial surface state is reconstructed below the damage. This behavior is consistent with a surface state that is topologically protected. Investigations of time-reversal symmetry breaking perturbations of the surface layer, with magnetic ion-irradiation, will also be discussed.

Ultrafast quasiparticle dynamics of Kondo insulator SmB$_6$ using THz spectroscopy

JINGDI ZHANG, Department of Physics, University of California, San Diego, JIE YONG, Department of Physics, University of Maryland, College Park, ICHIRO TAKEUCHI, Department of Materials Science & Engineering, University of Maryland, College Park, RICHARD GREENE, Department of Physics, University of California, San Diego, RICHARD AVERITT, Department of Physics, University of California, San Diego — Samarium Hex boride (SmB$_6$) is a prototype Kondo insulator with a hybridization gap of 19 meV at low temperatures. It has been theoretically predicted to be the first topological insulator involving electron-electron correlations that are truly insulating in bulk. Recent progress in fabricating thin film SmB$_6$ [1] enables using terahertz spectroscopic methods to investigate topological surface states and carriers adjacent to the hybridization gap, potentially distinguishing these distinct contributions to the optical conductivity. We report on the photo-excited quasi-particle (QP) dynamics of the Kondo insulator SmB$_6$, using ultrafast terahertz spectroscopy. The amplitude of the transient change in transmission increases with decreasing temperature, exhibiting a single-exponential decay that significantly decreases below the damage temperature. This phonon bottleneck originates from competition between QP recombination and re-excitation of QP across the hybridization gap by phonons.


Thin films synthesis and transport properties of the topological Kondo insulator candidate SmB$_6$

CHRISTOPHER M. MORRIS, N.J. LAURITA, S. KOOPAYEH, P. COTTINGHAM, W.A. PHELAN, L. SCHOOP, T.M. MCQUEEN, N.P. ARMITAGE, The Institute for Quantum Matter, Department of Physics & Astronomy, The Johns Hopkins University, Baltimore, MD 21218 — The Kondo insulator SmB$_6$ has long been known to display anomalous transport behavior at low temperatures (T < 10 K) and high pressures. At low temperatures, a plateau is observed in the resistivity, contrary to the logarithmic divergence expected for a normal Kondo insulator. Recent theoretical calculations suggest that SmB$_6$ may be the first topological Kondo insulator, a material with a Kondo insulating bulk, but topologically protected metallic surface states. Here, time domain terahertz spectroscopy (TDS) is used to investigate the temperature dependent optical conductivity of single crystals of SmB$_6$. A secondary bulk conduction mechanism is observed associated with the resistance plateau as the bulk becomes insulating. A secondary bulk conduction mechanism remains down to the lowest measured temperature, 1.6 K. Additionally, FTIR measurements have been performed that show the Kondo gap of SmB$_6$ opening at low temperatures.

Thin films synthesis and transport properties of the topological Kondo insulator SmB$_6$

YUFAN LI, SUNXIANG HUANG, C.-L. CHIEN, Department of Physics and Astronomy, Johns Hopkins University — SmB$_6$, the candidate of the newly proposed topological Kondo insulator, has attracted great research interest in its physical properties. Evidence supports the presence of the topologically protected surface state that was obtained from several experimental studies. However, recently, many researchers have focused on the bulk SmB$_6$ rather than the surface. Here, we report on the synthesis and transport properties of thin films of SmB$_6$. SmB$_6$ thin films are deposited on Si (100) substrates by RF magnetron sputtering. The resistivity decreases below 10 K and forms a plateau, while at higher temperatures the insulating behavior manifests a band gap $\sim$ 3 meV consistent with the reported value of bulk samples. A sign change of the normal Hall coefficient may indicate the formation of the hybridization energy gap.

Thin films synthesis and transport properties of the topological Kondo insulator SmB$_6$

W. K. PARK, L. SUN, L. H. GREENE, University of Illinois at Urbana-Champaign, D. J. KIM, Z. FISK, University of California, Irvine — Topological insulators are a new class of materials harboring topologically protected surface states. SmB$_6$, a well-known Kondo insulator, has attracted much interest recently due to its possibility to be topological as a system with strong interaction. Despite intensive investigations in recent years, the nature of the surface states in SmB$_6$ still remains intriguing. We adopt planar tunneling spectroscopy to study the electronic density of states in topological insulators and superconductors. As a surface-sensitive technique, it should be able to detect the surface states in SmB$_6$. Planar tunnel junctions are made on both (100) and (110) surfaces of high-quality single crystals. Crystal surfaces are prepared by polishing (with sub-nm scale smoothness) and ion-beam cleaning/etching. AlO$_x$ tunnel barrier of varying thickness is formed by sputter deposition of Al and subsequent oxidation. Differential conductance is measured as a function of temperature down to 1.7 K and magnetic field up to 9 T. Our tunneling conductance spectra show asymmetric gap-like features, reminiscent of a Fano resonance in a Kondo lattice, up to 40–50 K, close to the temperature below which the band renormalization and hybridization is known to occur. We’ll discuss how the contributions from the bulk and the surface states can be identified in our conductance data. * The work at UIUC is supported by the NSF DMR 12-06766.

Thin films synthesis and transport properties of the topological Kondo insulator SmB$_6$

T.M. MCQUEEN, N.P. ARMITAGE, The Institute for Quantum Matter, Department of Physics & Astronomy, The Johns Hopkins University, Baltimore, MD 21218 — Topological insulator candidate SmB$_6$ has long been known to display anomalous transport behavior at low temperatures (T < 10 K) and high pressures. Here, time domain terahertz spectroscopy (TDS) is used to investigate the temperature dependent optical conductivity of single crystals of SmB$_6$. A secondary bulk conduction mechanism is observed associated with the resistance plateau as the bulk becomes insulating. A secondary bulk conduction mechanism remains down to the lowest measured temperature, 1.6 K. Additionally, FTIR measurements have been performed that show the Kondo gap of SmB$_6$ opening at low temperatures.

Thin films synthesis and transport properties of the topological Kondo insulator SmB$_6$

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Thin films synthesis and transport properties of the topological Kondo insulator SmB$_6$

W. K. PARK, L. SUN, L. H. GREENE, University of Illinois at Urbana-Champaign, D. J. KIM, Z. FISK, University of California, Irvine — Topological insulators are a new class of materials harboring topologically protected surface states. SmB$_6$, a well-known Kondo insulator, has attracted much interest recently due to its possibility to be topological as a system with strong interaction. Despite intensive investigations in recent years, the nature of the surface states in SmB$_6$ still remains intriguing. We adopt planar tunneling spectroscopy to study the electronic density of states in topological insulators and superconductors. As a surface-sensitive technique, it should be able to detect the surface states in SmB$_6$. Planar tunnel junctions are made on both (100) and (110) surfaces of high-quality single crystals. Crystal surfaces are prepared by polishing (with sub-nm scale smoothness) and ion-beam cleaning/etching. AlO$_x$ tunnel barrier of varying thickness is formed by sputter deposition of Al and subsequent oxidation. Differential conductance is measured as a function of temperature down to 1.7 K and magnetic field up to 9 T. Our tunneling conductance spectra show asymmetric gap-like features, reminiscent of a Fano resonance in a Kondo lattice, up to 40–50 K, close to the temperature below which the band renormalization and hybridization is known to occur. We’ll discuss how the contributions from the bulk and the surface states can be identified in our conductance data. * The work at UIUC is supported by the NSF DMR 12-06766.
4:06PM J10.00009 Effects of Surface Morphology on the 3D Topological Insulator Samarium Hexaboride

Steven Wolgast, Yun Su Kwon, Cagliyan Kurda, Dept. of Physics, University of Michigan, Dae-Jeong Kim, Zachary Fisk, Dept. of Physics and Astronomy, University of California, Irvine

The recent verification of a topologically-protected surface state in SmB₆ at low temperatures has led to several transport studies of the surface states. This task is complicated because current can flow on all surfaces of a topological insulator, each of which can have different transport characteristics. Our own measurements using a Corbino disk geometry overcome this difficulty, limiting the conduction to individual surfaces. However, the sheet conductivities of our samples counter-intuitively decrease with finer surface polishing. We therefore investigate surface and sub-surface morphology as a factor affecting the surface conductivity. Specifically, surface cracks may themselves harbor surface states and contribute to the total electrical conduction, yielding a higher measured sheet conductivity than that of a flat surface. This situation may contribute to the (sometimes unphysically) large surface conductivities already observed in SmB₆.

4:18PM J10.00010 Ultrafast carrier dynamics of SmB₆

Sanjay Adhkari, West Virginia University, Yanjun Ma, Chang-Beom Eom, UWM, Jing XIA, UCI, Cheng Cen, West Virginia University

We report femtosecond pump-probe experiment performed in SmB₆ single crystals and epitaxial thin films at variable temperatures. The observed carrier relaxations as well as different collective oscillation modes in GHz - THz range allow us to study the hybridization gap and the carrier coherence in different samples.

4:30PM J10.00011 ARPES investigation on the surface vs bulk electronic structures of correlated topological insulators YbB₆ and other rare earth hexaborides


Using ARPES performed in wide photon energy range we systematically studied the bulk and surface electronic structures of a topological mixed-valence insulator candidate, YbB₆. The bulk B-2p states are probed with bulk-sensitive soft X-ray ARPES, exhibiting strong three-dimensionality with the band top locating 80 meV below the EF at the X point. The measured bulk Yb-4f states are located at 1 and 2.3 eV below EF, which hybridize with the dispersive B-2p states. The bulk band structures obtained by experiments are substantially different from the first principle calculations, but it can be better described by adding a correlation parameter U = 7 eV, indicating YbB₆ is a correlated system. Using surface-sensitive VUV ARPES, we revealed two-dimensional surface states which form three-electron-like FSs with Dirac-cone-like dispersions. The odd number of surface FSs gives the first indication that the surface states are topological non-trivial. The spin-resolved ARPES measurements provide further evidence that these surface states are spin polarized with spin locked to the crystal momentum. Recent results on the TI phase in other rare earth hexaborides will also be shown.

4:42PM J10.00012 Observation of a non-Kondo-like topological insulator state in the correlated rare-earth hexaboride YbB₆

Madhab Neupane, S.-Y. Xu, N. Alidoust, G. Bian, C. Liu, I. Belopolski, Princeton University, USA, T.-R. Chang, National Tsing Hua University, Taiwan, H.T. Jeng, National Tsing Hua University & Institute of Physics, Academia Sinica, Taiwan, T. Durakiewicz, Los Alamos National Laboratory, USA, H. Lin, National University of Singapore, Singapore, A. Bansil, Northeastern University, USA, D.J. Kim, Z. Fisk, University of California at Irvine, USA, M.Z. Hasan, Princeton University, USA

We present angle-resolved photoemission study on the rare-earth hexaboride YbB₆, which has recently been predicted to be a topological Kondo insulator. Our data do not agree with the prediction and instead show that YbB₆ exhibits a novel topological insulator state in the absence of a Kondo mechanism. We find that the Fermi level electronic structure of YbB₆ has three 2D Dirac cone surface states enclosing the Kramers’ points, while the f-σ orbital which would be relevant for the Kondo mechanism is about 1 eV below the Fermi level. Our first-principles calculation shows that the topological state which we observe in YbB₆ is due to an inversion between Yb d and B p bands. I will also present some of our recent results on other member of hexaborides. These experimental and theoretical results provide a new approach for realizing novel correlated topological insulator states in rare-earth materials.

4:54PM J10.00013 Non-topological 2DEG at the surface of YbB₆ and Divalent Hexaborides

J.D. Denlinger, Lawrence Berkeley Nat’l Lab, C.H. Min, F. Reinert, U. Wuerzburg, Boyoun Kang, D.J. Kim, Z. Fisk, UC Irvine, K. Gottlieb, A. LANZARA, UC Berkeley, C.-J. Kang, B.I. Min, Postech, J.W. Allen, U. of Michigan—A recent theoretical prediction of YbB₆ being an f-d band-inverted mixed-valent topological insulator very similar to SmB₆ [1] and subsequent angle-resolved photoemission studies of the rare-earth hexaboride YbB₆, which has recently been predicted to be a topological Kondo insulator due to an orbital which would be relevant for the Kondo mechanism is about 1 eV below the Fermi level. Our first-principles calculation shows that the topological state which we observe in YbB₆ is due to an inversion between Yb d and B p bands. I will also present some of our recent results on other member of hexaborides. These experimental and theoretical results provide a new approach for realizing novel correlated topological insulator states in rare-earth materials.

5:06PM J10.00014 Scanning Tunneling Microscopy Studies of the Topological Insulator Candidate YbB₆

Zhihua Zhu, Y. He, Department of Physics, Harvard University, Cambridge, MA 02138, USA, D.-J. Kim, Z. Fisk, Department of Physics and Astronomy, University of California, Irvine, California 92697, USA, J. E. Hoffmann, Department of Physics, Harvard University, Cambridge, MA 02138, USA

We report scanning tunneling microscopy studies of YbB₆, a proposed topological insulator candidate with moderate correlation. The in-situ cleaved sample surface has two dominant morphologies: atomic scale terraces and disordered rows, which likely correspond to Yb and B terminations, respectively. Spatially resolved dI/dV maps show enhanced tunneling due to the local perturbation of the tip-induced band bending. The dI/dV spectra reveal a bulk gap with distinct in-gap features near the Fermi level on different terminations. Our study presents nanoscale evidence for the interplay between surface structure, correlation and topological properties.

The work at Harvard was supported by NSF-DMR-1410480 and NSERC (ZHZ).
5:18PM J10.00015 Is the black phase of SmS a topological Kondo insulator? — ERIC BAUER, N. J. GHIMIRE, F. RONNING, C. BATISTA, D. BYLER, J. D. THOMPSON, Los Alamos National Laboratory, A. RAHMANISIAN, University of British Columbia, Z. FISK, University of California, Irvine — SmS is a prototypical Kondo insulator where electronic correlations drive a system insulating that would otherwise be metallic. Whether or not such a system is also a topological insulator that hosts a protected metallic surface state, depends on the parity of the wavefunction of the occupied states. However, unlike weakly correlated materials, it is unclear whether state-of-the-art electronic structure calculations accurately predict the parity of the occupied wavefunctions of correlated insulators. Nevertheless, Dzero and collaborators suggest that Kondo insulators such as SmB6 can be topological. Like SmB6, Cubic SmS is a non-magnetic semiconductor with an insulating behavior at ambient pressure and low temperatures driven by hybridization with the Sm f-electrons. At 6 kbar, SmS undergoes a phase transition into a valance fluctuating phase accompanied by a visible color change from black to gold. It then undergoes a second phase transition at about 20 kbar to an antiferromagnetic order at low temperatures. We will discuss whether electronic structure calculations indicate a topological state of SmS at P = 0. We will also discuss whether or not the magnetic, thermal and transport properties of the black phase of SmS are consistent with the existence of a topologically protected surface state.

Tuesday, March 3, 2015 2:30PM - 5:30PM —
Session J11 DMP: Focus Session: Engineering Vortex Matter in Superconductors

2:30PM J11.00001 Observing real time motion of nano-scale objects — JORIS VAN DE VONDEL, MATIAS TIMMERMANS, KU Leuven, Belgium, TOMÁS SAMUELY, P. J. Šafářík University, BART RAES, Catalan Institute of Nanotechnology, LISE SERRIER-GARCIA, VICTOR MOSHCHELKOV, KU Leuven, Belgium — The dynamics of nanoscale objects is a very interesting field of research with a strong technological impact. Still, the combination of a technique resolving (sub)nanometer particles within a time frame relevant to observe dynamics is a very challenging task. Due to the inherent atomic-scale resolution, scanning tunneling microscopy (STM) is an ideal candidate to achieve this goal. Nevertheless, in most physical systems the dynamic events of the objects under investigation cannot be resolved by conventional STM image acquisition and will only reveal an average trace of the moving object. This is why a strong drive exists to develop new functionalities of STM, which allow studying dynamic events at the nanoscale. We address this issue, for vortex matter in NbSe2, by driving the vortices using an ac magnetic field and probing the induced periodic current modulations [1]. Our results reveal different dynamical modes of the driven vortex lattice. In addition, by extending a known functionality of STM, (i.e. the ‘Lazy Fisherman’ technique) we can use single pixel information to obtain the overall dynamics of the vortex lattice with submillisecond time resolution and subnanometer spatial resolution.


This work is supported by the FWO and the Methusalem funding of the Flemish government.

2:42PM J11.00002 Vortex cutting in superconductors — VITALII K. VLASKO-VLASOV, ALEXEI E. KOSHELEV, ANDREAS GLATZ, ULRICH WELP, WAI-K. KWOK, Argonne National Laboratory — Unlike illusive magnetic field lines in vacuum, magnetic vortices in superconductors are real physical strings, which interact with the sample surface, crystal structure defects, and with each other. We address the complex and poorly understood process of vortex cutting via a comprehensive set of magneto-optic experiments which allow us to visualize vortex patterns at magnetization of a nearly twin-free YBCO crystal by crossing magnetic fields of different orientations. We observe a pronounced anisotropy in the flux dynamics under crossing fields and the filamentation of induced supercurrents associated with the staircase vortex structure expected in layered cuprates, flux cutting effects, and angular vortex instabilities predicted for anisotropic superconductors. At some field angles, we find formation of the vortex domains following a type-I phase transition in the vortex state accompanied by an abrupt change in the vortex orientation. To clarify the vortex cutting scenario we performed time-dependent Ginzburg-Landau simulations, which confirmed formation of sharp vortex fronts observed in the experiment and revealed a left-handed helical instability responsible for the rotation of vortices.

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

2:54PM J11.00003 Detecting vortices in superconductors: Extracting one-dimensional topological singularities from a discretized complex scalar field — CAROLYN PHILLIPS, TOM PETERKA, DMITRY KARPEYEV, Mathematics and Computer Science Division, Argonne National Laboratory, ANDREAS GLATZ, Materials Science Division, Argonne National Laboratory — In type-II superconducting material, the dynamics of the vortices play a critical role in determining the performance of the material. In Ginzburg-Landau simulations of superconducting materials, vortices correspond to topological singularities in a discretized complex scalar field. Visualizing the vortices to understand their behavior is a key step in using simulations to engineer optimized pinning landscapes. In the past, vortices have been visualized by examining contour plots and isosurfaces of the magnitude of the field. However, these methods, primarily used for small-scale simulations, blur the fine details of the vortices, scale poorly to large-scale simulations, and do not easily enable isolating and tracking individual vortices. We present a method for exactly finding the vortex core lines from a complex order parameter field. With this method, the vortices can be easily described at a resolution even finer than the mesh itself. The precise determination of the vortex cores allows the interplay of the vortices inside a model superconductor to be visualized in higher resolution than has previously been possible.

Research supported by the U.S. DOE, Office of Science, DE-AC02-06CH11357

3:06PM J11.00004 Improved critical current in confined superconductors in parallel field configuration — ANDREAS GLATZ, IGOR ARONSON, YONGLEI WANG, ZHILI XIAO, Argonne National Laboratory — We present results on the re-entrance of the superconducting state in systems placed into a magnetic field parallel to the applied current. In experiments it was observed that the magneto-resistance first increases with magnetic field, but at higher field drops again such that superconductivity is recovered. This effect is strongly temperature dependent and can lead to a suppression of resistance below the measurable threshold over a range of a few K. We study the vortex dynamics and magneto-resistance in this situation in the framework of a large-scale time-dependent Ginzburg-Landau simulation. A small external current as well as the magnetic field are applied in the x-direction, the latter is then ramped up. Our simulations reproduce this effect and reveal the mechanism for the observed behavior: the intermediate resistive state is due to a vortex instability leading to an unwinding of twisted vortex configurations. This leads to a periodic dynamic resistive state. When the field increases these instabilities get stabilized due to a higher vortex density and the resistance drops upon increasing the magnetic field.

Work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences, and by the Office of Science, Materials Scie...
3:18PM J11.00005 Interplay between vortex matter phases and arrays of pinning centers in low temperature superconductors \(^1\). JOSE L. VICENT, JAVIER DEL VALLE, ALICIA GOMEZ, Universidad Complutense Madrid, MANUEL RODR\'\'GUEZ, DANIEL GRANADOS, IMDEA-Nanociencia, Madrid. FERNANDO GALVEZ, ELYRVA M. GONZALEZ, Universidad Complutense Madrid. We have studied vortex matter phases in Nb films grown on Si substrates with arrays of Cu nanodots. The symmetry of the pinning arrays rules the presence of vortex matter phases. Four-fold symmetry arrays enhance the vortex glass transition temperature, at matching fields, in comparison with plain Nb films. This is a similar effect that obtained using arrays of magnetic pinning centers (Villegas et al. PRB72, 174512). Breaking the symmetry of the pinning array, such that the array mimic a smectic crystal, leads to a new phase, in a very narrow temperature window between the liquid and glassy phases, which can be identified with a vortex smectic phase. Remarkably, the smectic vortex phase is enhanced increasing the array symmetry. Increasing the number of vortices vanishes this smectic phase. (H,T) phase diagrams will be presented for different types of arrays.

\(^1\)We thank Spanish MINECO and CM.

3:30PM J11.00006 Vortex-Antivortex coexistence in Nb based Superconductor/Ferromagnet heterostructures. C. DI GIORGIO, E.R. Caianiello Physics Department, University of Salerno, IT; Physics Department, Temple University, Philadelphia, PA; F. BOBBA, E.R. Caianiello Physics Department, University of Salerno, IT; A. SCARPATI, M. LONGOBAIRD, Department of Condensed Matter Physics, University of Geneva, CH. M. IAVARONE, S.A. MOORE, Physics Department, Temple University, Philadelphia, PA. G. KARAPETROV, Physics Department, Drexel University, Philadelphia, PA; V. NOVOSAD, V. YEFREMEMKO, Materials Science Division, Argonne National Laboratory, Argonne, IL, A.M. CUCULO, E.R. Caianiello Physics Department, University of Salerno, IT. Superconductor/Ferromagnet thin film heterostructures, based on Niobium/Permalloy (Nb/Pt), have been studied by low temperature Magnetic Force Microscopy. The experimental observation of spontaneous Vortex-Antivortex in these systems depends on the Nb penetration depth and thickness, on the intensity of the Py stray field induced by the small, alternating up-and-down, out-of-plane component of the magnetic moment. Comparison with the available theoretical models allows to estimate the threshold of the local \(M_s\) for different Py thicknesses.

3:42PM J11.00007 Development of strong vortex pinning and very high \(J_c\) in iron based superconductors. CHIARA TARANTINI, National High Magnetic Field Laboratory - Florida State University — Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\) (Ba122) is the most tunable of the Fe-based superconductors (FBS) in terms of its acceptance of high densities of secondary phases capable of acting as effective pinning centers without depressing the properties of the superconducting matrix. It has been demonstrated that self-assembled nanorods made of Ba-Fe-O generate a strong correlated pinning along the c-axis, enhancing the critical current density, \(J_c\), in this direction and reducing the \(J_c\) anisotropy \([1, 2]\). However, when 20% of secondary phases are introduced, the reduction of the cross-section becomes significant, decreasing the low field performance. In order to overcome this issue, artificially introduced pinning centers can be added by multilayer deposition producing an anisotropy increase of \(J_c\) \([2]\). Moreover, FBS are especially sensitive to strain, allowing an important enhancement in the critical temperature, \(T_c\), of the material. It will be shown that strain induced by the substrate can further improve \(J_c\) of both single and multilayer films by more than expected because of the \(T_c\) increase. The multilayer deposition of Ba122 on CaF\(_2\) increases the pinning force density, \(F_p\), by more than 60% compared to a single layer film, reaching a maximum of 84 GN/m\(^2\) at 22.5T and 4.2 K, the highest value ever reported in any 122 phase. This work shows that the in-field performance of Ba122 widely exceeds that of Nb3Sn above 10T, attracting attention for possible applications.\[1\] C. Tarantini, S. Lee, Y. Zhang, J. Jiang, C.W. Bark, J.D. Weiss, A. Polyaniskii, C.T. Nelson, H.W. Jiang, C.M. Folkman, S.H. Baek, X.Q. Pan, A. Gurevich, E.E. Hellstrom, C.B. Eom, D.C. Larbalestier, Appl.Phys.Lett. 96, 142510 (2010)\[2\] C. Tarantini, S. Lee, F. Kametani, J. Jiang, J.D. Weiss, J. Jaroszynski, C.M. Folkman, E.E. Hellstrom, C.B. Eom, D.C. Larbalestier, Phys.Rev.B 86, 214504 (2012)\[3\] C. Tarantini, F. Kametani, S. Lee, J. Jiang, J.D. Weiss, J. Jaroszynski, E.E. Hellstrom, C.B. Eom, D.C. Larbalestier, Scientific Reports (2014)

4:18PM J11.00008 Defects and critical current in REBCO films by ion irradiation. QIANG LI, TOSHINORI OZAKI, CHENG ZHANG, Brookhaven National Lab, BROOKHAVEN NATIONAL LAB TEAM — We will present our recent studies on the defects and critical current density \(J_c\) in superconducting ReBa\(_2\)Cu\(_3\)O\(_7\) films (Re = Y, or rare earth element) irradiated by several types of ions at energy level between hundreds of KeV and tens of MeV. We observed remarkable enhancement of \(J_c\) in some of the irradiated films at low temperature and at high magnetic fields up to 35T. We examined the ion irradiation induced defects by using advanced transmission electron microscopy. It was found that the ion irradiation at this kinetic energy range produces defects that are rather small (~ a few nanometers) in physical size. However, these defects were found to create a substantially large strain field in the vicinity that depresses the pair potential and produce effective flux pinning at low temperatures. As the temperature approaching \(T_c\), the irradiation induced pinning was found less effective, presumably due to the softening of vortex line. A correlation between the nano-structures of the defects and critical current will be discussed.

4:30PM J11.00009 Enhanced critical currents of commercial 2G superconducting coated conductors through proton irradiation. ULRICH WELP, M. LEROUX, K.J. KIHLSTROM, W.-K. KWOK, A.E. KOSELEV, D.J. MILLER, Argonne National Laboratory, M.W. RUPICH, S. FLESHLER, A.P. MALOZEMOFF, American Superconductor Corp., A. KAYANI, Western Michigan University — We report on magnetization and transport measurements of the critical current density, \(J_c\), of commercial 2G-YBCO coated conductors before and after proton irradiation. The samples were irradiated along the c-axis with 4 MeV protons. Proton irradiation produces a mixed pinning landscape composed of pre-existing rare earth particles and a uniform distribution of irradiation induced nm-sized defects. This pinning landscape strongly reduces the suppression of \(J_c\) in magnetic fields resulting in a doubling of \(J_c\) in a field of ~ 4T. The irradiation dose-dependence of \(J_c\) is characterized by a temperature and field dependent threshold of the local \(M_s\) for different Py thicknesses.

4:42PM J11.00010 Optimization of vortex pinning by nanoparticles using numerical simulations. ALEXEI KOSHELEV, IVAN SADOVSKYY, Materials Science Division, Argonne National Laboratory, CAROLYN PHILLIPS, Mathematics and Computer Science Division, Argonne National Laboratory, ANDREAS GLATZ, Materials Science Division, Argonne National Laboratory and Northern Illinois University — Vortex pinning by self-assembled nanoparticles has been established as an efficient route to enhance current-carrying capability of practical superconductors. We explore vortex pinning by randomly distributed metallic spherical nanoparticles using large-scale numerical simulations of time-dependent Ginzburg-Landau equations. We found optimal size and density of particles at which the highest critical current realizes for fixed magnetic field. For every particle size the critical current reaches maximum value of 15-22% of the volume fraction filled by the particles, which is close to the percolation concentration. This optimal particle density increases with the magnetic field. We also found that the optimal particle diameter is close to 4 coherence lengths. Our results provide guidance for pinning optimization in practical superconductors.\[1\] ALEXEI KOSHELEV, IVAN SADOVSKYY, Materials Science Division, Argonne National Laboratory, CAROLYN PHILLIPS, Mathematics and Computer Science Division, Argonne National Laboratory, ANDREAS GLATZ, Materials Science Division, Argonne National Laboratory. RODRIGUEZ, DANIEL GRANADOS, IMDEA-Nanociencia, Madrid. FERNANDO GALVEZ, ELYRVA M. GONZALEZ, Universidad Complutense Madrid. We have studied vortex matter phases in Nb films grown on Si substrates with arrays of Cu nanodots. The symmetry of the pinning arrays rules the presence of vortex matter phases. Four-fold symmetry arrays enhance the vortex glass transition temperature, at matching fields, in comparison with plain Nb films. This is a similar effect that obtained using arrays of magnetic pinning centers (Villegas et al. PRB72, 174512). Breaking the symmetry of the pinning array, such that the array mimic a smectic crystal, leads to a new phase, in a very narrow temperature window between the liquid and glassy phases, which can be identified with a vortex smectic phase. Remarkably, the smectic vortex phase is enhanced increasing the array symmetry. Increasing the number of vortices vanishes this smectic phase. (H,T) phase diagrams will be presented for different types of arrays.\[2\] The work supported by the SciDAC program funded by U.S. DOE, Office of Science, Advanced Scientific Computing Research and Basic Energy Science.


This effect by measuring the transport properties of three samples with cross sections ranging from 250 µm². H. Takahashi et al., 054708 (2011). H. Takahashi, S. Inoue, and the colossally large 17008 (2007). This compound has a small energy gap of S, HIDEFUMI TAKAHASHI, RYUJI OKAZAKI, HIROKI TANIGUCHI, ICHIRO TERASAKI, Nagoya University — An unusually large - Anindya Roy, John Hopkins University and heavy-ion irradiations in commercial coated conductors. This work well for Bi2Te3, and can be used to guide strategies for suppression of bipolar effects to increase the maximum zT.

The greater mobility of the conduction band compared to the valence band suppresses the bipolar effect of the holes that enables the n-type material to retain high zT for the n-type material but the p-type is not useful. We have explained this phenomena using optical band gap measurements and transport modeling.

Seebeck coefficient) of a typical heavily doped semiconductor rises with temperature until it reaches a maximum value, and then decreases due to the activation function of magnetic field orientation as well as field strength and temperature. Since the films can achieve remarkably high critical current, challenges exist in evaluating these low temperature (down to 4.2 K) properties in high magnetic fields up to 30 T. Therefore both conventional transport, and magnetization measurements in a vibrating coil magnetometer equipped with rotating sample platform were used to complement the study. Our results clearly show an evolution of pinning from strongly correlated effects seen at high temperatures to significant contributions from dense but weak pins that thermal fluctuations render ineffective at high temperatures but which become strong at lower temperatures. Support for this work is provided by the NHMFL via NSF DRM 1157490.

Tuesday, March 3, 2015 2:30PM - 5:30PM —
Session J12 DMP/DCOMP GERA FIAP: Focus Session: Thermoelectric and Coupled Phenomena 007C - Anindya Roy, John Hopkins University

2:30PM J12.00001 Colossal enhancement of the Seebeck coefficient in FeSb2 driven by nearly ballistic phonons. HIDEFUMI TAKAHASHI, RYUJI OKAZAKI, HIROKI TANIGUCHI, ICHIRO TERASAKI, Nagoya University — An unusually large S of ~ 45 mV/K (at 10 K) was discovered in FeSb2 single crystal, which prompted extensive investigations into its physical origin [A. Bentien et al., EPL 80, 17008 (2007). This compound has a small energy gap Δ ~ 5 meV, which may be caused by strong correlations of Fe 3d-electrons, as observed with Kondo insulators, and the unusually low S may be attributed to this unique band structure near the Fermi energy. However, the exceptional value of S has not been clearly explained by electron correlations, suggesting an additional contribution such as the non-equilibrium phonon-drag effect [H. Takahashi et al., JPSJ 80, 054708 (2011), H. Takahashi et al., PRB 84, 205215 (2011), and H. Takahashi et al., PRB 88, 165205 (2013)]. Here, we report on the direct investigation of this effect by measuring the transport properties of three samples with cross sections ranging from 250 × 245 µm² to 80 × 160 µm². S and ∇x show a significant size effect, indicating that nearly ballistic phonons, which have a long mean free path relative to the sample dimensions, are responsible for the colossal S.

2:42PM J12.00002 ABSTRACT WITHDRAWN —

2:54PM J12.00003 Improved Thermoelectric Performance via Piezoelectric Interaction. DAVID MONTGOMERY, Wake Forest University — Presented are the initial findings of enhanced voltage output in a hybrid thermoelectric piezoelectric generator (TPEG). We constructed TPEG by integrating insulating layers of polyvinylidene fluoride (PVDF) piezoelectric films between flexible thin film p-type and n-type thermoelectrics. The piezoelectric bound surface charge modifies the thermoelectric properties of the semiconductor electrodes which facilitates an increase in voltage. The TPEG voltage output has three contributions: traditional thermoelectric and piezoelectric terms, and a unique coupling term. A combined thermoelectric and piezoelectric model can be used to quantitate the expected coupling voltage as a function of stress and thermal gradient. The fabrication, placement, and configuration of this interface allows for different device designs and affects overall performance. Under easily achievable stress and thermal gradient this new coupling effect can increase voltage output by 20%. Because of this piezoelectric modified thermoelectric effect these hybrid generators can out preform equivalent thermoelectric or piezoelectric generators.

3:06PM J12.00004 The Role of Minority Carriers in Thermoelectrics: Why Half Heusler ZrNiSn is a good n-type but poor p-type Thermoelectric. G. JEFFREY SNYDER, California Institute of Technology — The bipolar excitation of minority carriers limits the maximum zT of a typical thermoelectric material. This is because the thermopower (absolute value of the Seebeck coefficient) of a typical heavily doped semiconductor rises with temperature until it reaches a maximum value, and then decreases due to the activation of minority carriers of opposite sign. The temperature of this thermoelectric rollover is determined largely by the band gap which acts as the activation energy of the minority carriers. Julian Goldsmid and Jeff Sharp showed that the a simple relationship, Eg = 2Sm Tm, between the maximum thermopower (Sm) the temperature where the maximum occurs (Tm) and the band gap (Ev, measured in eV) is a good approximation for many materials, particularly when both types of carriers have similar mobilities. The (T, Zr, Hf)NiSn half Heusler compounds, however, demonstrate the limits of this relationship. The Goldsmid-Sharp band-gap for n-type ZrNiSn is several times greater than that for p-type ZrNiSn that ultimately results in high thermopower at high temperature and therefore high zT for the n-type material but the p-type is not useful. We have explained this phenomena using optical band gap measurements and transport modeling. The greater mobility of the conduction band compared to the valence band suppresses the bipolar effect of the holes that enables the n-type material to retain high thermopower to high temperature. The models give quantitative guide to the accuracy of Goldsmid-Sharp band-gap by providing a correction factor that works well for Bi2Te3, and can be used to guide strategies for suppression of bipolar effects to increase the maximum zT.
The effect of thermoelectric contributions in switching dynamics and resistance drift of Phase Change Memory devices. EGECAN COGULU, IBRAHIM CINAR, AISHA GOKCE, Bogazici University, BARRY STIPE, JORDAN KATINE, HGST, A Western Digital Company, GULEN AKTAS, OZHAN OZATAY, Bogazici University — Phase Change Memory (PCM) is a promising non-volatile data storage technology that allows for multiple-bit-per-cell operation due to its high contrast in the resistance levels between 0 and 1 logic states. To visualize the complex nature and the stability of the switching dynamics in PCM devices with or without an intermediate resistance state, 3D finite element simulations were carried out in cells with a single Ge2Sb2Te5(GST) layer incorporating temperature and phase dependent thermal and electrical conductivities as well as thermoelectric effects. We compare our results with the experimental data and with our previous simulations to understand the influence of the thermo-electric effect on the phase switching. In addition, we integrated drift equations into our multiphysics simulation to get a complete picture of structural relaxation in time in amorphous and mixed phases of the GST. We compare our results with experimental resistance drift measurements to calculate a decay rate for defect concentration. Our results yield a complete picture of switching dynamics and post-switching resistance drift phenomena on the microscopic scale.

The thermopower of few-electron quantum dots with Kondo correlations. LVZHOU YE, University of Science and Tech of China — The thermopower of few-electron quantum dots is crucially influenced by on-dot electron-electron interactions, particularly in the presence of Kondo correlations. We present a comprehensive picture which elucidates the underlying relations between the thermopower and the spectral density function of two-level quantum dots. The effects of various electronic states, including the Kondo states originating from both spin and orbital degrees of freedom, are clearly unraveled. With these insights, we have exemplified an effective and viable way to control the sign of thermopower and the spectral density function of two-level quantum dots. The effects of various electronic states, including the Kondo states originating from both spin and orbital degrees of freedom, are clearly unraveled. With these insights, we have exemplified an effective and viable way to control the sign of thermopower and the spectral density function of two-level quantum dots.

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Detection of Carrier Scattering Mechanism by Thermopower, SHUANG TANG, MILDRED DRESSELHAUS, Massachusetts Inst of Tech-MIT — We have developed a new method to detect the carrier scattering mechanism at different temperatures by measuring the maximum values of thermopower (Seebeck coefficient). The graphene system has been studied as a model example. The contribution of short-range interaction scattering, and long-range scattering has been inferred when the temperature varies from low temperature to room temperature. The approach to change the maximum values of thermopower (Seebeck coefficient) is also discussed. This method can not only be used in graphene, but in many novel systems, including MoS2, WS2, and black phosphorus, and other general systems.

Magnon drag thermopower and thermomagnetic properties of single-crystal iron. SARAH WATZMAN, HYUNGYU JIN, Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, Ohio, USA, JOSEPH HEREMANS, Department of Mechanical and Aerospace Engineering and Department of Physics, The Ohio State University, Columbus, Ohio, USA — Lucassen et al. [1] demonstrate that magnon drag involves a spin-transfer mechanism closely related to the recently discovered spin-Seebeck effect. This talk will present first results of experiments mapping out the thermopower and magnetothermopower of single-crystal iron and prove that its thermopower is indeed dominated by magnon drag, as suggested by Blatt et al. in 1967 [2]. Measurements will then be presented on the magnetic field and temperature dependence of the full thermomagnetic tensor of iron’s thermopower in the xxx, xyz, and xyz geometries (the first index gives the direction of the heat flux, the second the direction of the magnetic field, and the third the applied magnetic field). Results of magneto-thermopower and Nernst coefficients will be reported for single-crystal samples oriented with α=100. The Nernst coefficients of elemental iron contain a contribution of a direct spin-transfer mechanism, which should be present in the present experiment as an interface between a ferromagnet and a normal metal. This mechanism could be put to use in high temperature ferromagnetic metallic thermoelectric alloys. 1. M. E. Lucassen et al., Appl. Phys. Lett. 99 262506 (2011) 2. F. J. Blatt et al., Phys. Rev. Lett. 18.11 (1967).

Enhancement of thermoelectric performance in composite materials through locally-modulated doping, MICHAEL J. ADAMS, HYUNGYU JIN, Department of Mechanical Engineering, The Ohio State University, JOSEPH P. HEREMANS, Department of Mechanical and Aerospace Engineering and Department of Physics, The Ohio State University — Composites of organic or inorganic constituents are often considered as a way to yield high thermoelectric figure of merit. The limit of this approach is set by the effective medium theory [1], which demonstrates formally that a composite of two materials A and B cannot have higher figure of merit than the highest of either A or B, in the absence of interaction between A and B. In this work, we show that this limit can be lifted by introducing into a host material a second phase that behaves differently vis-a-vis electrons than vis-a-vis phonons. This phase consists of electrically and thermally insulating islands of material that locally dope the semiconducting host. Doped material near the islands provides electrically conductive volumes for charge carriers. Phonons, unaffected by local doping, are scattered by the islands. Thermopower is less affected by the doped regions than electrical conductivity, by an intrinsic mathematical property of the effective medium theory [1]. We employ this concept in Bi1-xSb x alloys and in p-type (Bi2-xSb x)2Te3 compounds, which are known as good thermoelectric materials at cryogenic and room temperatures, respectively. Experimental transport data and the local microscopic characterizations of the samples are presented. 1. D. J. Bergman and L. G. Fel, J. Appl. Phys. 85 8205-8216, 1999

Enhancement of thermoelectric performance in composite materials through locally-modulated doping, MICHAEL J. ADAMS, HYUNGYU JIN, Department of Mechanical Engineering, The Ohio State University, JOSEPH P. HEREMANS, Department of Mechanical and Aerospace Engineering and Department of Physics, The Ohio State University — Composites of organic or inorganic constituents are often considered as a way to yield high thermoelectric figure of merit. The limit of this approach is set by the effective medium theory [1], which demonstrates formally that a composite of two materials A and B cannot have higher figure of merit than the highest of either A or B, in the absence of interaction between A and B. In this work, we show that this limit can be lifted by introducing into a host material a second phase that behaves differently vis-a-vis electrons than vis-a-vis phonons. This phase consists of electrically and thermally insulating islands of material that locally dope the semiconductor host. Doped material near the islands provides electrically conductive volumes for charge carriers. Phonons, unaffected by local doping, are scattered by the islands. Thermopower is less affected by the doped regions than electrical conductivity, by an intrinsic mathematical property of the effective medium theory [1]. We employ this concept in Bi1-xSb x alloys and in p-type (Bi2-xSb x)2Te3 compounds, which are known as good thermoelectric materials at cryogenic and room temperatures, respectively. Experimental transport data and the local microscopic characterizations of the samples are presented. 1. D. J. Bergman and L. G. Fel, J. Appl. Phys. 85 8205-8216, 1999

Enhancement of thermoelectric performance in composite materials through locally-modulated doping, MICHAEL J. ADAMS, HYUNGYU JIN, Department of Mechanical Engineering, The Ohio State University, JOSEPH P. HEREMANS, Department of Mechanical and Aerospace Engineering and Department of Physics, The Ohio State University — Composites of organic or inorganic constituents are often considered as a way to yield high thermoelectric figure of merit. The limit of this approach is set by the effective medium theory [1], which demonstrates formally that a composite of two materials A and B cannot have higher figure of merit than the highest of either A or B, in the absence of interaction between A and B. In this work, we show that this limit can be lifted by introducing into a host material a second phase that behaves differently vis-a-vis electrons than vis-a-vis phonons. This phase consists of electrically and thermally insulating islands of material that locally dope the semiconductor host. Doped material near the islands provides electrically conductive volumes for charge carriers. Phonons, unaffected by local doping, are scattered by the islands. Thermopower is less affected by the doped regions than electrical conductivity, by an intrinsic mathematical property of the effective medium theory [1]. We employ this concept in Bi1-xSb x alloys and in p-type (Bi2-xSb x)2Te3 compounds, which are known as good thermoelectric materials at cryogenic and room temperatures, respectively. Experimental transport data and the local microscopic characterizations of the samples are presented. 1. D. J. Bergman and L. G. Fel, J. Appl. Phys. 85 8205-8216, 1999

Supported by DOE US-China Clean Energy Research Center SubK 3002041929, and by AFOSR MURI FA9550-10-1-0533

Next Generation Electrocaloric and Pyroelectric Materials for Solid State Electrothermal Interconversion, S. PAMIR ALPAY, University of Connecticut — Storrs, JOSEPH V. MANTESE, United Technologies Research Center, SUSAN TROLIER-MCKINSTRY, QIMING ZHANG, Penn State University, ROGER W. WHATMORE, Imperial College London — Thin film electrocaloric (EC) and pyroelectric (PE) electrothermal interconversion energy sources have recently emerged as viable means for primary and auxiliary solid state cooling and power generation. This emergence is a result of two significant developments: (1) advancements in the formation of high quality polymeric and ceramic thin films with figures of merit that project system level performance as a large percentage of Carnot efficiency, and (2) the ability of these newer materials to support larger electric fields which permit operation at higher voltage; thus making the power electronic architectures more favorable for thermal to electric interconversion. Current research targets to adequately address commercial device needs, include reduction of parasitic losses, increases in mechanical robustness, and the ability to form nearly free-standing element in the range of 1 - 10 microns in thickness. This article will describe the current state-of-the-art materials, thermodynamic cycles and device losses; pointing to potential lines of research that would lead to substantially better figures of merit for electrothermal interconversion.
4:54PM J12.00011 Diameter Dependent Thermoelectric Properties of Individual SnTe Nanowires, E.Z. XU, Indiana University,  Z. LI, Indiana University; Los Alamos National Laboratory, J. MARTINEZ, New Mexico State University, N. SINITSYN, H. STITOO, N. LI, Los Alamos National Laboratory, B. SWARTZCENTRUBER, Sandia National Laboratories, J. HOLLINGSWORTH, J. WANG, Los Alamos National Laboratory, S.X. ZHANG, Indiana University — Tin telluride (SnTe), a newly discovered topological crystalline insulator, has recently been suggested to be a promising thermoelectric material. In this work, we report on a systematic study of the thermoelectric properties of individual single-crystalline SnTe nanowires with different diameters. Measurements of thermopower, electrical conductivity and thermal conductivity were carried out on the same nanowires over a temperature range of 25 - 300 K. While the electrical conductivity does not show a strong diameter dependence, we found that the thermopower increases by a factor of two when the nanowire diameter is decreased from 913 nm to 218 nm. The thermal conductivity of the measured NWs is lower than that of the bulk SnTe, which may be attributed to the enhanced phonon - surface boundary scattering and phonon-defect scattering. We further calculated the temperature dependent figure of merit ZT for each individual nanowire. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science by Los Alamos National Laboratory (Contract DE-AC52-06NA25396) and Sandia National Laboratories (Contract DE-AC04-94AL85000).

3We acknowledge support by the Los Alamos LDRD program.

5:06PM J12.00012 ABSTRACT WITHDRAWN —

5:18PM J12.00013 Towards a high-current triode thermoelectronic generator, GERWIN HASSINK, PATRICK HERLINGER, WOLFGANG BRAUN, CYRIL STEPHANOS, JURGEN SMET, Jochen MANNHART, Max Planck Institute for Solid State Research, Stuttgart, Germany — Thermionic power generation obtains electrical power directly from a temperature gradient by thermionic emission from a hot electrode to a cold electrode. The space charge created by the emitted electrons, however, severely reduces the efficiency of such generators. Recently, a triode setup with supporting magnetic field has demonstrated to greatly reduce the space charge [1]. Based on these results, further development has been started to reach higher output by, e.g., reducing the electrode spacing to 100 µm, and by increasing the electrode area. In addition, new gate electrode materials and geometries are investigated. The importance of the work function not only for the emitter and collector, but also for the gate, is clear from both the theory and experiment. Work function engineering through surface modification is discussed.


Tuesday, March 3, 2015 2:30PM - 5:30PM — Session J13 DMP: Focus Session: Ferroelectric and Multiferroic Oxide Heterostructures 007D - Jayakanth Ravichandran, University of Southern California

2:30PM J13.00001 Complex-oxide multilayers by design: a treasure trove of unusual ferroic functionalities, SERGE NAKHMANSOHN, University of Connecticut - Storrs — While inheriting most of the traits of their parents, layered variations of ABO₃ perovskites allow for a number of additional channels for property manipulation and fine-tuning. Their remarkable flexibility toward structural and chemical modification can be exploited for the design of new and advanced functionalities not originally present in the parent ABO₃ compounds. With the help of first-principles-based computational techniques, we have predicted intriguing electroactive behavior in layered-perovskite compounds of the Ruddlesden-Popper (RP) type. Specifically, we showed that Goldstone-like states (collective, close to zero frequency excitations, requiring practically no consumption of energy) can be induced in a PbSrTiO3-RP superlattice, manifesting themselves as easy rotations of the in-plane polarization vector. Examination of a fictitious epitaxial Bα₂ZrO₄-RP compound demonstrated that it exhibits an assortment of competing incommensurate distortions, including ones that promote in-plane polarization. In this presentation we highlight the unusual behavior of a RP Ba₂ZrO₄ structure, which has already been synthesized as a bulk ceramic. An investigation of the properties of a (fictitious) epitaxial thin-film variant of this material reveals that under compression it undergoes a transition into an incommensurate state, while under tension it shows hints of a Goldstone-like polar instability, which surprisingly occurs without the presence of a lone-pair active ions like Pb or Sn. In both cases, we observe anomalies in the planar static dielectric susceptibility of the system, with large dielectric response predicted for the phase displaying the Goldstone-like instability.

3:06PM J13.00002 Theoretical study of electronic transport properties in pillar-embedded multiferroic transition-metal oxides, YUAN-YEN TAI, JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — Multiferroics show great potential in novel application to nanotechnologies based on well-established experimental techniques. Recently, vertically aligned nanocomposite (VAN) multiferroic thin films have demonstrated a significant amount of research interest owing to their promising results to give more delicate device, such as a larger interfacial area and intrinsic heteroepitaxy in this 3D structure. In order to understand the basic influence of the nano-pillar structure to the bulk multiferroics, we apply scaling theory to study the quasiparticle localization/delocalization effects of this novel nanostructure. With an effective tight-binding model, we apply the transfer matrix method to calculate the wave function behavior throughout its transverse direction. We will also show that the critical behavior varies with various disordered nano-pillar patterns. We will also give a qualitative connection of our results to the transport experiments.

3Work at the LANL was performed under the auspices of the U.S. DOE Contract No. DEAC52-06NA25396 through the LANL-LDRD program.

3:18PM J13.00003 Electric Field and Structural Phase Transition Induced Magnetization Effects in BaTiO3-FeRh Heterostructures Probed using Polarized Neutron Reflectometry, STEVEN BENNETT, THOMAS WARD, MICHAEL BIEGALSKI, Oak Ridge National Laboratory, TONY WONG, The University of Tennessee, ZHIQI LIU, HAILE AMBAYE, ARTUR GLAVIC, VALERIA LAUTER, Oak Ridge National Laboratory — The ability to change the magnetic state of a material with an electric field opens up a plethora of possible devices in spintronics and memory applications. A strong candidate material for such a control is FeRh, whose magneto-structural phase transition from antiferromagnetic (AFM) to ferromagnetic (FM) at T=350K, has shown to be controllably changed by an electric field when grown on ferroelectric BaTiO₃ (BTO). It has been suggested that this shift is largely due to the -0.47% in plane compressive strain induced by the piezoelectric BTO. Here we show a sharp repeatable change in magnetization as the system is heated/cooled through the tetragonal to orthorhombic (280-290K) and orthorhombic to rhombohedral (180-205K) crystalline phase transitions of BTO. To further characterize the effect polarized neutron reflectometry (PNR) was used to evolve the depth profile of magnetization in FeRh within the temperature vicinity of these transitions with and without the application of electric field.

3This work was carried out at the Center for Nanophase Materials Sciences (CNMS) and the Spallation Neutron Source (SNS) supported by the Scientific User Facilities Divisions, Office of Basic Energy Sciences, DOE
3:30PM J13.00004 Emergent phenomena in LaAlO3/GdAlO3 superlattices by breaking inversion symmetry , HAI-TIAN ZHANG, RYAN HAISLMAIER, JASON LAPANO, VENKAT GOPALAN, ROMAN ENGEL-HERBERT, Penn State University — Recently, tremendous interest has been focused on materials by design, where hybrid improper ferroelectricity was proposed from first principles predictions in perovskite superlattices (AB03)/(A'B03)m , which is directly coupled to the oxygen octahedral rotations [1]. Such oxygen octahedron rotations are anticipated stable at high temperatures, thus being a potential materials candidate for high temperature piezoelectric sensor and transducer applications. In this talk we will present the homeopitaxial growth of LaAlO3 and GdAlO3 by hybrid molecular beam epitaxy, where a volatile aluminium alkoxide precursor and elemental La3/Gd (flux 2 × 10−3 cm−2 s−1) were co-supplied in the presence of an oxygen plasma (RF plasma power 250 W). Growth mode, film surface morphology and defect type for films grown under La3/Gd-rich and Al-rich growth conditions will be discussed and directly related to structure and properties characterization of the LaAlO3 and GdAlO3. Changes in the octahedral tilts, probed by scanning transmission electron microscopy in the proximity of GdAlO3/LaAlO3 interface are discussed and compared to first principles predictions.

3:42PM J13.00005 Ferroelectric tunnel junctions with electron doped SrTiO3 electrodes , XIAOHUI LIU, J.D. BURTON, EVGENY TSYMBAL, University of Nebraska-Lincoln — Increasing the tunneling electroresistance (TER) is crucial for the application of ferroelectric tunnel junctions (FTJs) for electronic devices.[1] Normal FTJs are composed of a thin ferroelectric layer sandwiched by two metallic electrodes, where TER results from the ferroelectric polarization dependent electric potential height in the ferroelectric barrier. Since the resistance depends exponentially not only on potential height but also on barrier width, TER is expected to be greatly enhanced by modulation of the polarization dependent barrier width when one of the electrodes is substituted by a semiconductor.[2] Recently, experiment reported sizable (10^4) TER in a FTJ where one electrode is n-type SrTiO3, namely Pt/BaTiO3/Nb/SrTiO3.[3] To reveal the mechanism of this phenomenon, we perform theoretical studies on a representative system SrRuO3/EtaTiO3/n-SrTiO3 using on first-principles modeling. We analyze as a function of doping level the effect of ferroelectric polarization on the electronic structure near the interface, its influence on the barrier width and on the transport properties of such a system. [1] E. Y. Tsymal and H. Kohlstedt, Science, 313, 181 (2006) [2] M. Y. Zhuravlev, et al., Phys. Rev. Lett. 94, 246802 (2005) [3] Z. Wen, et al., Nat. Mater. 12, 617 (2013)

3:54PM J13.00006 Role of interface termination in SrRuO3/PbTiO3/SrRuO3 capacitors under epitaxial strain [1], SIMON DIVILOV, MARIVI FERNANDEZ-SERRA, MATTHEW DAWBER, State Univ of NY- Stony Brook — We perform a DFT analysis of (SrRuO3)/(PbTiO3)/(SrRuO3) with varying PbTiO3 using both LDA and LSDA+U. The goal of the study is to analyze the effects of symmetrical termination along the [001] plane on the magnetic and electric properties of SrRuO3 and PbTiO3, respectively. We observe the electrical polarization of the thin film is highly sensitive to the termination plane, as compared to the bulk. In addition, the termination plane determines the oxygen octahedra tilting (OOT) pattern in the thin film, although the OOT are not coupled to the polarization. Despite having a single layer of SrRuO3, we observe a magnetic polarization dependent on the termination. Our results show the importance of ab initio calculations in the presence of a magnetic parameter space to aid experiments in synthesis of superlattice and thin film capacitors.

4:06PM J13.00007 The road towards the ferroelectric-FET — Carrier density modulation by ferroelectric switching in BaTiO3/Ge , PATRICK PONATH, KURT FREDRICKSON, AGHAM POSADAS, YUAN REN, XIAOYU WU, RAMA VAŞUDEVAN, Univ of Texas, Austin, BĂRÎS OKATAN, STEPHEN JESSE, Oak Ridge National Laboratory, TOSHIHIRO AOKI, MARTHA MCCARTNEY, DAVID SMITH, Arizona State University, SERGEI KALININ, Oak Ridge National Laboratory, KEJI LAI, ALEX DEMKOV, Univ of Texas, Austin, PONATH, FREDRICKSON, POSADAS, DEMKOV TEAM, REN, WU, LAI COLLABORATION, VAŞUDEVAN, OKATAN, JESSE, KALININ COLLABORATION, AOKI, MCCARTNEY, SMITH COLLABORATION — Germanium, with its higher hole and electron mobility is a potential candidate to replace silicon as a channel material in a field effect transistor in the future. The ferroelectric high-k dielectric barium titanate (BTO) can be integrated on germanium (001) due to the small lattice mismatch between BTO and Ge and could therefore be a potential candidate for a ferroelectric memory. We report the epitaxial growth of BTO on a germanium (001) substrate with a thin STO buffer layer, which imposes compressive strain on BTO and causes it to be out of plane polarized. The BTO film crystallizes as-deposited which is monitored by RHEED. XRD measurements of the BTO film indicate an out-of-plane ferroelectric polarization of BTO on a germanium (001) substrate with a thin STO buffer layer, which imposes compressive strain on BTO and causes it to be out of plane polarized. The BTO film crystallizes as-deposited which is monitored by RHEED. XRD measurements of the BTO film indicate an out-of-plane ferroelectric polarization of BTO on a germanium (001) substrate with a thin STO buffer layer, which imposes compressive strain on BTO and causes it to be out of plane polarized. The BTO film crystallizes as-deposited which is monitored by RHEED. XRD measurements of the BTO film indicate an out-of-plane ferroelectric polarization of BTO on a germanium (001) substrate with a thin STO buffer layer, which imposes compressive strain on BTO and causes it to be out of plane polarized. The BTO film crystallizes as-deposited which is monitored by RHEED. XRD measurements of the BTO film indicate an out-of-plane ferroelectric polarization of BTO on a germanium (001) substrate with a thin STO buffer layer, which imposes compressive strain on BTO and causes it to be out of plane polarized. The BTO film crystallizes as-deposited which is monitored by RHEED. XRD measurements of the BTO film indicate an out-of-plane ferroelectric polarization of BTO on a germanium (001) substrate with a thin STO buffer layer, which imposes compressive strain on BTO and causes it to be out of plane polarized. The BTO film crystallizes as-deposited which is monitored by RHEED. XRD measurements of the BTO film indicate an out-of-plane ferroelectric polarization of BTO on a germanium (001) substrate with a thin STO buffer layer, which imposes compressive strain on BTO and causes it to be out of plane polarized. The BTO film crystallizes as-deposited which is monitored by RHEED. XRD measurements of the BTO film indicate an out-of-plane ferroelectric polarization of BTO on a germanium (001) substrate with a thin STO buffer layer, which imposes compressive strain on BTO and causes it to be out of plane polarized.

4:18PM J13.00008 Enhanced ferromagnetism in ferroelectric & ultrathin ferromagnetic digital superlattices[1], HANGWEN GUO, ZHENYU DIAO, WANG ZHEN, MOHAMMAD SAGHAYEZHIAN, LINA CHEN, RONGYING JIN, WARD PLUMMER, JIANDI ZHANG, Louisiana State University, SHUAI DONG, Southeast University — Electric control of magnetism has generated much activity due to both intellectual and technical interests. Epitaxial growth of transition-metal oxides with different ordering parameters offers unique platform to study magnetoelectric effect. In particular, quantum confinement of correlated electrons lead to interesting phenomena such as metal-insulator transition. In this work, we explore such effect in quantum confined regime by growing digital superlattices. We selected ferroelectric BaTiO3 (BTO) and La2/3Sr0.7MnO3 (LSMO) which exhibits ferroelectric to magnetic transition at critical thickness. We explore how confined LSMO behaves when sandwiched by BTO. Superlattices are fabricated in formula [(BTO)m/(LSMO)m]y. BTO thickness is constant & LSMO thickness are varied from 40u.c. to 2u.c. For all samples, total thickness of LSMO remains 40 u.c. Stable RHEED oscillations and sharp patterns ensure layer-by-layer growth and decent structural ordering. We find that LSMO has the ferromagnetic ground state down to 2 u.c. In addition, enhancement of ferromagnetism on ultrathin LSMO samples is observed compared to thicker films. Possible explanation involving interfacial magnetization will be discussed.

3:40PM J13.00009 Strain-mediated SrTiO3/PbTiO3 superlattice: The role of oxygen vacancy [1], MENGLEI LI, WENHUI DUAN, Tsinghua University — Using first-principle calculations, we comprehensively study the oxygen vacancy effects on the ferroelectric (FE) and antiferrodistortive (AFD) properties of the [001]-oriented SrTiO3/PbTiO3 1/1 superlattice at different epitaxial strains. Oxygen vacancies form most easily under intermediate strains while the oxygen on the PbO-plane is more difficult to lose than in other positions. Without vacancies, the superlattice is in the paraelectric phase while promote the rotations along the Ti-V-O chain by inducing local tail-to-tail polarization patterns. Furthermore, the oxygen vacancies suppress the octahedra rotations around the direction of Ti-V-O chain while promote the rotations along the other two orthogonal directions. Therefore, the mediation of the FE and AFD properties in different directions in the superlattice can be achieved by the use of the anisotropic effect of oxygen vacancies. Our results provide a theoretical ground to the various coupling effects in ferroelectric-paraelectric superlattices.

1Supported by U.S. DOE under Grant No. DOE DE-SC0002136.
4:42PM J13.00010 The metallic screening of the interfacial dipole field in multiferroic Bi6Fe2-xCoTi3O18 thin films, XIAOFANG ZHAI, YU YUN, CHAO MA, HAOLIANG HUANG, DECHAO MENG, JIANLIN WANG, ZHENPING FU, RANRAN PENG, YALIN LU, University of Science and Technology of China — The demand for superior room-temperature multiferroic materials pushes high-quality fabrication of novel Aurivillius-type complex oxides with a goal of revealing the intrinsic room temperature multiferroic properties. We have found a new route to fabricate single-crystalline quality multiferroic Bi6Fe2-xCoTi3O18 thin-films utilizing a metallic screening effect. The films exhibit abrupt interfaces and greatly enhanced crystalline quality on conductive bottom layers while mixed types of interfaces on insulating bottom layers. The enhanced single-crystalline quality is explained by a metallic screening effect that compensates the diverging dipole field originating from the symmetry breaking at the interface. The films on the conductive bottom layers also exhibit an enhanced ferromagnetic spin coupling and a strong vertical piezoelectric polarization switching. This study demonstrates that screening the interface dipole can be crucial to fabricate high-quality thin films and then multiferroic devices.

4:54PM J13.00011 Self-modulated growth of a super-large-period BiFeCoTiO33 thin-film, YALIN LU, DECHAO MENG, XIAOFANG ZHAI, CHAO MA, HAOLIANG HUANG, YU YUN, YAN HUANG, ZHENPING FU, RANRAN PENG, University of Science and Tech of China, XIANGYU MAO, XIAOBING CHEN, Yangzhou University — The epitaxial growth of super-large-period Aurivillius thin films has been explored in order to study their period-modulated multiferroic property. BiFeCoTiO33 thin films with a pseudo-period of ten have been grown on SrTiO3 single crystal substrates using pulsed laser deposition. The films are found to be coherently strained to the substrates and atomically smooth. The X-ray diffraction indicates an average layer period of 10. While the high resolution scanning transmission electron microscopy reveals a self-modulated nanostructure in which the period changes as the thickness increases. The modulation to the period is tentatively explained by the volatile bismuth stacking difference between hetero-epitaxial growth and homo-epitaxial growth. Nonetheless, the self-modulated large period films exhibit intrinsic ferromagnetic and ferroelectric properties at room temperature.

5:06PM J13.00012 Reversible MagnetoElectric Control of Exchange Coupling in Monodomain BiFeO3 Heterostructures1, JULIAN IRWIN, W. SAENRANG, M.S. RZCHOWSKI, K.J. REIERSON, Dept. of Physics, Univ. of Wisconsin, J.E. PODKAMINER, S.B. BAEK, C.B. EOM, Dept. of Materials Sci. and Engr., Univ. of Wisconsin, J.W. FREELAND, APS, Argonne National Laboratory, B.A. DAVIDSON, CNR-Istituto Officina dei Materiali, TASC Nat. Lab, Trieste, Italy — We investigate reversible switching of the ferromagnetic properties of a monodomain thin film of the multiferroic BiFeO3 (BFO) [2] and a Co overlayer. For different electric polarization directions of the BFO film we observe changes in the Co layer magnetic anisotropy and coercive field as determined from in-plane and out-of-plane anisotropic magnetoresistance (AMR) and Magneto-Optic Kerr Effect (MOKE) measurements between 30K and 300K. The dependence of these results on BFO layer thickness is also investigated due to the thickness dependence of BFO’s cyclodial magnetic ordering. X-ray linear dichromism (XLD) measurements of the BFO layer indicate a reversible change in the BFO magnetic ordering as a result of polarization switching, verifying the presence of a magnetoelastic effect in the BFO film and suggesting a magnetic coupling between the BFO and Co layers. Weak ferromagnetism and changing surface magnetic anisotropy energy are both explored as possible mechanisms for the observed coupling [2].

1This work is supported by the Army Research Office under Grant No. W911NF-10-0382


5:18PM J13.00013 Spin-orbit engineering in perovskite heterostructures, BYOUNGHAK LEE, Physics Department - Texas State University, GURU KHALESA, NIST - Nati Inst of Stds & Tech — There has been a steadily increasing interest in spin-orbit effects in systems with broken inversion symmetry. These effects may have technological applicability due to recent success in inducing dynamics and switching across heavy metal/ferromagnet interfaces through spin-orbit torque. In addition, broken inversion symmetry and large spin-orbit interactions can lead to novel magnetic and superconducting properties. Little effort has focused on developing a materials platform for studying these effects systematically. The versatility of perovskites along with recent advances in their epitaxial growth may provide such a playground. In this talk we discuss our theoretical efforts to engineer spin-orbit effects in materials systems based on perovskites and contrast results with bare surfaces and interfaces.

Tuesday, March 3, 2015 2:30PM - 5:30PM — Session J14 DMP FIAP: Focus Session: Dopants and Defects in Zinc Oxide 008A - Shengbai Zhang, Rensselaer Polytechnic Institute

2:30PM J14.00001 Shallow acceptor complexes in p-type ZnO1, D.E. ASPNES2, North Carolina State University — ZnO films grown on sapphire substrates by organometallic vapor phase epitaxy exhibit p-type behavior when sufficient N is properly incorporated and followed by an appropriate annealing sequence. While substitutional N on the O sublattice is a deep acceptor, shallow acceptor complexes involving N, H and VZn, can provide useful 1015 cm−2 p-type films. Taking advantage of Raman, SIMS, and Hall-effect data, we establish a two-step growth scheme to form a metastable double donor complex, N2HZn−V(OH)−, then convert it to a single shallow acceptor complex, VZn−N2HZnH+ during in situ annealing in N2O. The VZn−N2HZnH+ complex accepts electrons at ionization energies of 134 meV, rendering it an efficient p-type dopant at room temperature.

1Supported by DARPA through the Extreme Light Sources Project W31P4Q-08-1-0003

2Collaborators: J. G. Reynolds, C. L. Reynolds, Jr., J. E. Rowe (all NC State University); A. Mohanta (AMRDEC, Huntsville, AL); H. O. Everitt (AMRDEC, Huntsville, and Duke University)

3:06PM J14.00002 Hindered rotation of the 3326 cm−1 OH center in ZnO1, PHILIP WEISER, ELLEN FARMER, MICHAEL STAVOLA, W. BEALL FOWLER, Lehigh University — Experiments on H in ZnO have found two OH vibrational lines at 3611 and 3326 cm−1 [1,2]. The IR line at 3611 cm−1 has been assigned to isolated H+ in a bond centered configuration. The band at 3326 cm−1 has been assigned to H+ in an antibonding configuration in the vicinity of another defect, perhaps Ca [3]. The 3326 cm−1 band has a distinctive dependence on temperature, consisting of several overlapping components whose intensities show thermally activated behavior over the temperature range 4K to 50K. This behavior is reminiscent of previous results for the hindered rotation of an off-axis OD-Li center in MgO [4]. Our results suggest that the off-axis motion of OH centers in oxides might be a common occurrence.


1Supported by NSF Grant DMR-1160756.
3:18PM J14.00003 Quantum Monte Carlo models of substitutional point defects in zinc oxide and zinc selenide. JAEHYUNG YU, ELIF ERTEKIN, Univ of Illinois - Urbana — Introducing dopants into semiconductors allows manipulation of electrical and optical properties, useful for applications such as optoelectronics and photovoltaics. While first principles quantitative descriptions of the defects properties in semiconductors are critical to understanding and engineering dopants in semiconductors, obtaining accurate descriptions has proven challenging in the past. Here we demonstrate the use of quantum Monte Carlo (QMC) methods to describing the properties of point defects in zinc oxide and zinc selenide. Due to its direct treatment of electron correlation, the QMC method is capable of accurate calculation of band gaps and defect behaviors. We describe the energetics and potential barrier to forming gallium DX-center defects according to QMC in zinc selenide, and compare the description to those of conventional and hybrid DFT. We also use QMC to determine the defect transition levels for nitrogren defects in zinc oxide, and show that QMC obtains descriptions that are in agreement with GW and beyond-DFT approaches. Our results demonstrate the importance of accurate descriptions of electron correlation in the calculation of defect properties of semiconductors.

3:30PM J14.00004 Structural Stability and Ionic Defects in ZnO from Quantum Monte Carlo. JUAN A. SANTANA, Oak Ridge Assoc Univ, JARON T. KROGEL, JEONGNIM KIM, PAUL R.C. KENT, FERNANDO REBOREDO, Oak Ridge National Laboratory — An accurate method capable of describing atomic, molecular and solid-state systems is required to take a full advantage of computer-aided materials discovery and design. We have studied the atomic, molecular and solid-state properties of the Zn-O system with DMC. In particular, the equation of state of bulk Zn and ZnO in the rock salt, zinc blend and wurtzite phases and the properties of ionic defects in wurtzite ZnO were studied. The first ionization potential of O and Zn, and the atomization energy of O, ZnO dimer, and wurtzite ZnO as well as the band gap of this material were evaluated with DMC, and the results agree with experimental measurements to within 0.2 eV. The DMC atomization energy of bulk Zn, 1.00(1) eV, is also in good agreement with the experimental value, 1.35 eV, considering the complexity of this metallic system. The DMC calculated properties of Zn and ZnO under pressure, and the formation energy for the oxygen vacancy, hydrogen impurities and Zn interstitial defects in ZnO will be discussed in comparison with results from experiments and density functional theory approximations.

3:42PM J14.00005 Intrinsic point defects and their interaction with impurities in monocrystalline zinc oxide. BENGT G. SVENSSON, University of Oslo, Physics Department, Center for Materials Science and Nanotechnology, P.O. Box 1048 Blindern, N-0316 Oslo, Norway — Zinc oxide (ZnO) is a direct and wide band-gap semiconductor with several attractive features, like an exciton binding energy of ~ 60 meV, for light emitting devices, photovoltaics and spintronics. In the past decade, ZnO has received tremendous attention by the semiconductor physics community and many challenging issues have been addressed, especially the "native" n-type conductivity, the role of intrinsic point defects, and the realization of reproducible p-type doping. The latter is, indeed, decisive for a true breakthrough of ZnO-based optoelectronics. In this contribution, recent progress in our understanding of the interaction between intrinsic point defects and impurities in ZnO will be discussed. Aluminum (Al) is often introduced intentionally to accomplish high n-type conductivity since Al on Zn-site (Al\textsubscript{Zn}) acts as a shallow donor. However, Al\textsubscript{Zn}, was recently found to react strongly with Zn vacancies (V\textsubscript{Zn}) and the resulting complex (Al\textsubscript{Zn}V\textsubscript{Zn}) is energetically favorable. The Al\textsubscript{Zn}V\textsubscript{Zn} complex is a deep acceptor limiting the n-type doping efficiency and this finding is expected to hold in general for complexes between V\textsubscript{Zn} and group-III elements. Further, implantation of self-ions (Zn and O) has been demonstrated to affect radically the balance of intrinsic point defects where an excess of Zn interstitials gives rise to a dramatic depletion of residual Li impurities on Zn-site (Li\textsubscript{Zn}) whilst the opposite holds for an excess of O interstitials. In fact, this behavior appears to be of general validity and Li depletion occurs for a wide variety of implanted elements incorporated into the Zn sub-lattice while Li pile-up occurs for elements residing on O-site. Finally, the most prominent deep-level defect in ZnO, labelled E3, will be shown to involve hydrogen. E3 exists in most ZnO materials, irrespective of the growth method used, and evidence for a center formed by reaction between interstitial hydrogen and primary defects on the Zn sub-lattice will be given.

4:18PM J14.00006 Dynamical Interplay Between Intrinsic Defects and Impurity Ions in Very Dilute Ce-doped MgO Thin Films. JUNG JUI WANG, Northeastern Univ. (NU) and ALS, LBNL, MUKES KAPILASHRAMI, ALS, LBNL, XIN LI, ALS, LBNL and KTH, Royal Institute of Technology (KTH), Sweden. — A deep acceptor and donor level is observed in Ce-doped MgO thin films. 2. A strong magnetic moment is observed in high-doped films. 3. The magnetic moment is well described by a combined spin-polarized Stoner model and Hartree-Fock model. 4. The magnetic moment increases with increasing Ce concentration.

4:30PM J14.00007 Exploring Cd-Zn-O-S alloys for optimal buffer layers in thin-film photovoltaics. J. VARLEY, Lawrence Livermore National Laboratory, X. HE, University of Illinois at Urbana-Champaign, N. MACKIE, MiaSole, A. ROCKETT, University of Illinois at Urbana-Champaign, V. LORDI, Lawrence Livermore National Laboratory — The development of thin-film photovoltaics has largely focused on alternative absorber materials, while the choices for other layers in the solar cell stack have remained somewhat limited. In particular, cadmium sulfide (CdS) is widely used as the buffer layer in typical record devices utilizing absorbers like Cu(In,Ga)Se\textsubscript{2} (CIGSe) or Cu\textsubscript{x}ZnS\textsubscript{y}(Cu\textsubscript{2}ZnSnS\textsubscript{3}) (CZTS) despite leading to a loss of solar photocurrent due to its band gap of 2.4 eV. While different buffers such as Zn(S,O,OH) are beginning to become competitive with CdS, the identification of additional wider-band gap alternatives with electrical properties comparable to or better than CdS is highly desirable. Here we use hybrid functional calculations to characterize Cd\textsubscript{x}Zn\textsubscript{1-x}O\textsubscript{y}S\textsubscript{1-y} candidate buffer layers in the quaternary phase space composed by Cd, Zn, O, and S. We focus on the band gaps and band offsets of the alloys to assess strategies for improving absorption losses from conventional CdS buffers while maintaining similar conduction band offsets known to facilitate good device performance. We also consider additional criteria such as lattice matching to identify regions in the composition space that may provide improved epitaxy to CIGSe and CZTS absorbers. Lastly, we incorporate our calculated alloy properties into simulation of typical CIGSe devices to identify the Cd\textsubscript{x}Zn\textsubscript{1-x}O\textsubscript{y}S\textsubscript{1-y} buffer compositions that lead to the best performance.
4:42PM J14.00008 Impact of Mg Content on (Mg,Zn)O Native Point Defects, MOLLY BALL, OSCAR RESTREPO, LEONARD BRILLSON, WOLFGANG WINDL, The Ohio State University, DEPARTMENT OF MATERIAL SCIENCE AND ENGINEERING COLLABORATION, DEPARTMENT OF PHYSICS COLLABORATION — The two most thermodynamically stable defects in ZnO are oxygen vacancies (V\text{O}\text{\textsuperscript{2−}}) and zinc vacancies (V\text{Zn}). These native point defects are electrically charged and can contribute to free carrier densities. Experiment shows that Mg addition to ZnO significantly changes native defect densities. To better understand this dramatic decrease in V\text{Zn} \text{\textsuperscript{2−}} and V\text{O}\text{\textsuperscript{2−}}-related defects with increasing Mg content up to x=0.44 and the subsequent increase, we performed density functional theory (DFT) calculations using PAW potentials within PBE using VASP. The results showed to be very sensitive to DFT method used and potential-energy calculation. For the latter, the literature shows that one can assume that the oxygen chemical potential equals that of the atoms in the oxygen molecules at a given surrounding partial oxygen pressure. However, one can also postulate that the total defect concentrations conserve the stoichiometry, or limiting potentials from elemental equilibrium phases can be used. The experimentally observed dependence helped identify the correct way to reproduce the experimental dependence of formation energy on Mg concentration, which will be discussed in detail in this presentation.

4:54PM J14.00009 A hybrid functional study of oxygen interstitial defects in amorphous In-Ga-Zn-O semiconductors, WOO HYUN HAN, YOUNG JUN OH, KEE JOO CHANG, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Republic of Korea — Amorphous indium-gallium-zinc oxide (a-IGZO) semiconductors have attracted much attention because these materials are considered as the replacement of amorphous Si in high performance thin film transistors (TFTs). Although a-IGZO has been the subject of extensive studies due to its superior properties, problems such as threshold voltage shift have been obstacles for device applications. While O-vacancy defects were suggested to be responsible for the device instability under negative bias illumination stress (NBIS), there is no systematic study for the origin of instability under positive bias stress (PBS). In this work, we reveal the origin of PBS instability by performing hybrid density functional calculations for O interstitials in a-IGZO. The defect configuration of an O interstitial depends on its charge state. While an O-O dimer is stable in neutral state, it is easily broken by capturing electrons, acting as an electron trap. Based on the results for the formation energy and transition level of an interstitial O, we propose that excess O atoms in a-IGZO are responsible for the PBS instability.

5:06PM J14.00010 Ionic liquid gated IGZO thin film field effect transistors, PUSHPA RAJ PUDESAINI, JOO HYON NOH, ANTONY WONG, AMANDA VICTO HAGLUND, Department of Materials Science & Engineering, University of Tennessee, Knoxville, SHENG DAI, Chemical Sciences Division, ORNL, THOMAS ZAC WARD, Materials Science and Technology Division, ORNL, DAVID MANDRUS\textsuperscript{1}, PHILIP D. RACK\textsuperscript{2}, Department of Materials Science & Engineering, University of Tennessee, Knoxville — Ionic liquid gated field effect transistors have been extensively studied due to their low operation voltage, ease of processing and the realization of high electric fields at low bias voltages. Here, we report ionic liquid (IL) gated field effect transistor based on amorphous Indium Gallium Zinc Oxide (IGZO) thin film active layers. Conveniently, our device structure includes a conventional bottom gate SiO\text{\textsubscript{2}} insulator so the transfer characteristics of the IL could be directly compared to an equivalent 100 nm thick SiO\text{\textsubscript{2}} gate insulator. The transport measurement of the IL revealed the intrinsic n-channel property of the IGZO thin film with high ON/OFF ratio ~ 10\textsuperscript{4} and a large field effect electron mobility of 2.54 cm\textsuperscript{2}V\textsuperscript{−1}s\textsuperscript{−1} at 300 K and a threshold voltage of 0.1V. Comparable measurements on the bottom SiO\text{\textsubscript{2}} gate insulator revealed an ON/OFF ratio ~ 10\textsuperscript{3} and field effect electron mobility of 5.24 cm\textsuperscript{2}V\textsuperscript{−1}s\textsuperscript{−1} and a threshold voltage of 0.40V. Interestingly, temperature dependent measurements revealed that the ionic liquid electric double layer can be "frozen-in" when dropped below the glass transition temperature which could lead to new switching and possibly non-volatile memory applications.

5:18PM J14.00011 ALD growth of non-polar ZnO-based heterojunctions for UV lighting: structural, electrical and optical properties, CHANG LIU, Wuhan University — Non-polar, semi-polar, and polar ZnO films can be well controlled to epitaxially grow on different substrates such as p-Si (111), p-GaN, and sapphire substrates by atomic layer deposition at 200 °C by introducing different interlayers of Al\textsubscript{2}O\textsubscript{3}, or InGaN or AlN or even none. The electroluminescence of the n-ZnO/Al\textsubscript{2}O\textsubscript{3}/p-GaN heterojunctions was dominated by a blue emission under forward bias, whereas it was violet emission under reverse biases. Under an ultralow driven current density, a blue emission could be observed from the nanocrystalline ZnO/GaN heterojunctions. Well defined Al nanoparticles (NPs) arrays with different shapes were fabricated on the surface of ZnO by electron-beam lithography. The theoretical analysis based on the finite-difference time-domain method was carried out to show the shape dependence of the localized surface plasmon resonance wavelength. By top excitation of the Al NP arrays coupled with ZnO, a 2.6-fold enhancement in peak photoluminescence intensity was measured. Furthermore, the enhancement strongly depends on the NPs shape, revealing an important way of geometrical tuning of the UV-emission.

Tuesday, March 3, 2015 2:30PM - 5:30PM — Session J15 DMP: Focus Session: Transport and Strong Coupling in Plasmonic Nanostructures

2:30PM J15.00001 Electron and hole dynamics in the electronic and structural phase transitions of VO\textsubscript{2} — RICHARD HAGLUND, Vanderbilt University — The ultrafast, optically induced insulator-to-metal transition (IMT) and the associated structural phase transition (SPT) in vanadium dioxide (VO\textsubscript{2}) have been studied for over a decade. However, only recently have effects due to the combined presence of electron-hole pairs and injected electrons been observed. Here we compare and contrast IMT dynamics when both hot electrons and optically excited electron-hole pairs are involved, in (1) thin films of VO\textsubscript{2} overlaid by a thin gold foil, in which hot electrons are generated by 1.5 eV photons absorbed in the foil and accelerated through the VO\textsubscript{2} by an applied electric field; (2) VO\textsubscript{2} nanoparticles covered with a sparse mesh of gold nanoparticles averaging 20-30 nm in diameter in which hot electrons are generated by resonant excitation and decay of the localized surface plasmon; and (3) bare VO\textsubscript{2} thin films excited by intense near-single-cycle THz pulses. In the first case, the IMT is driven by excitation of the bulk gold plasmon, and the SPT appears on a few-picosecond time scale. In the second case, density-functional calculations indicate that above a critical carrier density, the addition of a single electron to a 27-unit supercell drives the catastrophic collapse of the coherent phonon associated with, and leading to, the SPT. In the third case, sub-bandgap-energy photons (approximately 0.1 eV) initiate the IMT, but exhibit the same sub-100 femtosecond switching time and coherent phonon dynamics as observed when the IMT is initiated by 1.5 eV photons. This suggests that the underlying mechanism must be quite different, possibly THz-field induced interband tunneling of spatially separated electron-hole pairs. The implications of these findings for ultrafast switching in opto-electronic devices — such as hybrid VO\textsubscript{2} silicon ring resonators — are briefly considered.

1Support from the National Science Foundation (DMR-1207407), the Office of Science, U.S. Department of Energy (DE-FG02-01ER45916) and the Defense Threat-Reduction Agency (HDTRA1-10-1-0047) for these studies is gratefully acknowledged.
3:06PM J15.00002 Plasmonic Hot Carrier Transport and Collection in Nanostructures, ADAM JERMYN, RAVISHANKAR SUNDARARAMAN, PRINEHA NARANG, WILLIAM GODDARD, HARRY ATWATER, California Institute of Technology. JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS COLLABORATION — Plasmonic resonances provide a promising pathway for efficiently capturing photons from solar radiation and improving photo-catalytic activity via hot carrier generation. Previous calculations have provided the prompt energy-momentum distributions of hot carriers, but have left open the question of their transport to collection surfaces [Accepted in Nature Communications]. As the overall efficiency of plasmonic devices is dependent not just on how many carriers are collected but also on their energy distribution, a transport model which tracks this distribution is of key importance. Here, we provide a first-principles model of this transport based upon the linearized Boltzmann equation with the diffusive and ballistic regimes handled separately, and investigate the role of geometry on plasmonic hot carrier collection.

3:18PM J15.00003 Controlling the ultrafast hot electron dynamics in hybrid plasmonic nanostructures, HAYK HARUTYUNYAN, Department of Physics, Emory University — Plasmons hold promise for applications in photonic circuitry because of their ability to squeeze light into sub-wavelength dimensions and also for their ultrafast response times. To this end, it is important to fabricate plasmonic systems that can generate large optical signals at ultrafast timescales. This goal has been accomplished using coherent harmonic generation or wave mixing in metallic nanostructures where the femtosecond plasmonic response is attributed to plasmon dephasing. However, the multi-frequency nature of these optical effects makes their practical use challenging. Plasmonic devices based on Kerr-type nonlinear optical effects, on the other hand, can operate at a single, fundamental frequency. However, the ultrafast response of gold nanostructures so far has been measured to be in the picosecond timescales attributed to electron — phonon scattering. By designing and fabricating metal-oxide hybrid nanosystems with ultra-high field enhancements we were able to demonstrate much faster, femtosecond dynamics of the optical response. Moreover, our experiments show that the nonlinear optical response can be further tuned in both electron – phonon scattering. By designing and fabricating metal-oxide hybrid nanosystems with ultra-high field enhancements we were able to demonstrate much faster, femtosecond dynamics of the optical response. Moreover, our experiments show that the nonlinear optical response can be further tuned in both time and spectral domains by tuning the material composition of our hybrid nanomaterials. Use of the Center for Nanoscale Materials was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

3:30PM J15.00004 Plasmonic Drag Effect: Toward Coupling of Electronic and Plasmonic Components in Nano-Circuits, MATTHEW LEPAIN, DAVID KEENE, Georgia Southern Univ, VINCENT RONO, NATALIA NOGINOVA, Norfolk State Univ, MAXIM DURACH, Georgia Southern Univ — Plasmonic Drag Effect (PDE) is a phenomenon of rectification of plasmonic optical fields into dc currents or dc polarization in metal nanostructures. Although being a nonlinear effect, PDE is strongly enhanced by resonance and confinement factors and can produce usable pulsed dc voltages of up to several mV in pulsed laser experiments, promising a path to long-awaited opportunities to couple electronic and plasmonic components in nano-circuits. PDE is produced via plasmonic pressure and plasmonic stricton rectification forces. In this talk we will discuss the similarities and differences between these forces and possible additional mechanisms of PDE proposed by authors. We will describe generation of DC potential profiles by photons in metal nanostructures from both theoretical and experimental perspectives.

3:42PM J15.00005 Exploring Photoswitchable Plasmon-Molecule Interactions at the Single-Molecule and Single-Nanoparticle Levels, MINGSONG WANG, Department of Mechanical Engineering, The University of Texas at Austin, BHARATH BANGALORE RAJEEVA, Materials Science and Engineering Program, The University of Texas at Austin, YUEBING ZHENG, Department of Mechanical Engineering and Materials Science and Engineering Program, The University of Texas at Austin — Through synergizing the responsiveness of functional molecules and the plasmon-assisted nanoscale localization of light, hybrid nanosystems consisting of molecules and metal nanoparticle have important applications in biochemical detection, drug delivery, and energy conversion. Single-molecule and single-nanoparticle studies of the hybrid nanosystems help eliminate the degeneracy from ensemble measurements and provide new insights into the structure-property relations. Along this line, herein, we report our recent advances in designing, measuring and controlling two types of photoswitchable metal-nanoparticle-molecule nanosystems at the single-molecule and single-nanoparticle levels: (1) azobenzene molecules on single metal nanoparticles; and (2) spiropyran molecules on single metal nanoparticles.

3:54PM J15.00006 Multifunctional Diagnostic, Nanothermometer and Photothermal Nano-devices, KORY GREEN, MEGAN O’CONNOR, PARMINDER KAUR, HONG WANG, SHUANG FANG LIM, North Carolina State University — In this study, the known therapeutic capabilities of gold nanorods (AuNRs) have been combined with the diagnostic and nanothermometer abilities of upconversion nanoparticles (UCNPs) to develop a system for simultaneous biological imaging, photothermal therapy, and nanothermal sensing. Both the excitation of UCNPs and the finely tuned longitudinal surface plasmon resonance (LSMR) mode of AuNRs lay in a window of relatively high light penetration of tissue in the infra-red. The nanothermometer property of the UCNPs allows direct quantification of the localized temperature of the photothermally heated AuNRs chemically adsorbed to their surface and is free from the bleeding problems inherent in dye thermal sensing systems, especially at high laser fluences required to kill tissue. Spectroscopy on single particles, verified by transmission electron microscopy (TEM), has been performed at varying temperatures to confirm 1) the thermal sensing properties of UCNPs and 2) to finely tune their upconversion enhancement arising from the LSMP coupling of the AuNRs. Preliminary quantification of the localized AuNR temperatures upon photothermal heating will be confirmed through single particle spectroscopy of the attached UCNPs. HeLa cell viability studies have also been performed.

4:06PM J15.00007 Plasmonic Response of Metallic Nanoparticles by Time Dependent Density Functional Theory, EMILY TOWNSEND, GARNETT BRYANT, Joint Quantum Institute, National Institute of Standards and Technology and Univ of Maryland — Plasmons in metallic nanoparticles (MNPs) hold the potential to carry quantum information. Exploiting this will require a quantum understanding of plasmons in hybrid structures of multiple MNPs and emitters/absorbers. We use real-time, real-space time dependent density functional theory (TDDFT) to examine resonances in the optical response of single and paired MNPs. We consider the character of different resonances (some occur in the core, others near the surface of the MNP) and examine the multiple excitations that constitute these resonances. In both the core and surface resonances we see both plasmon-like sloshing of electrons around the Fermi surface and single-particle-like excitation of electrons from below the Fermi surface to above it. We examine the resonances of a pair of MNPs as a function of their separation distance to see how plasmonic and single-particle excitations mix in these particles. Widely separated pairs behave similarly to individual MNPs, but at closer distances pairs behave like a single, more complicated system.

4:18PM J15.00008 Sweet Plasmonics: Sucrose Macrocryystals of Metal Nanoparticles, PEDRO LUDWIG HERNANDEZ-MARTINEZ, Nanyang Technological University, Bilken University, TALHA ERDEM, ZELIHA SORAN-ERDEM, Bilken University, VIJAY KUMAR SHARMA, Nanyang Technological University, Bilken University, HALIL AKCALI, IBRAHIM AKCALI, Bilken University, NIKOLAI GAPONIK, ALEXANDER EYCHMULLER, TU Dresden, HILMI VOLKAN DEMIR, Nanyang Technological University, Bilken University — We present a new plasmonic crystal device comprising silver nanostructures on sucrose macrocrystals. Moreover, our experiments show that the nonlinear optical response can be further tuned in both electron – phonon scattering. By designing and fabricating metal-oxide hybrid nanosystems with ultra-high field enhancements we were able to demonstrate much faster, femtosecond dynamics of the optical response. Moreover, our experiments show that the nonlinear optical response can be further tuned in both time and spectral domains by tuning the material composition of our hybrid nanomaterials. Use of the Center for Nanoscale Materials was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.
4:30 PM J15.00009 Cross-over from collective strong coupling to quenching in quantum dot-metal nanoparticles assemblies1, PRAVEENA MULLAPUDI, Indian Institute of Science, ARNAB MUKHERJEE, SAI SREESH V, student, J.K. BASU, Associate professor — The optical properties for the hybrid structures consisting of gold nanoparticles and CdSe Quantum Dots (QDs) have been widely studied. Compact hybrid monolayer films of gold nano particles (Au NPs) and cadmium selenide (CdSe QDs) with different ratios are prepared using LB method. Suitable tuning of the ratio of QDs and Au NPs at different surface densities leads to enhancement and attenuation of the emission of QDs which acts like a quantum emitters. The net emission enhancement of QDs is maximum, particularly in the case of 0.143 Au NP number fraction (ϕ) for both OFF - resonant and ON-resonant cases, and it is even more enhanced in the case of OFF- resonance i.e., when the SPR (surface Plasmon resonance) is not spectrally overlapping with the quantum dot PL maxima. We suggest that this behavior is indicative of a crossover from single particle to collective emission from quantum dots mediated by gold nanoparticles. The ability to control the radiative and non-radiative decay rates and the emission intensity from such assemblies using spectrally and spatially tuned plasmonic sources would be very crucial in the applications of photovoltaic’s and nano photonics.

1 DST grant

4:42 PM J15.00010 Controlling decay dynamics of quantum emitters with Plasmonic self assembly templates1, S.R.K. CHAITANYA INDUKURI, IISc, J.K. BASU, Department of Physics, IISc, India — Controlling the emission of quantum dots by tailoring local density of states (LDOS) in self assembled plasmonic template. Using very small diameter gold (Au) spherical nanoantenna within a polymer template randomly dispersed with quantum dots, we show how the photoluminescence intensity and lifetime anisotropy of these dots can be significantly enhanced through LDOS tuning. We also studied the effect of diameter, wider range of geometric and spectral parameters bringing out the versatility of these functional plasmonic templates. We studied the effect of nano antenna distribution on radiative and non radiative decay rates in the templates. We demonstrated that the decay dynamics in the plasmonic templates can be controlled in a facile manner by changing the filling fraction of the Au nanoparticles. This polarization dependent anisotropic decay dynamics for the quantum emitters is determined by polarization dependent LDOS of the plasmonic templates as demonstrated by FDTD simulations. Our work provides a new method to achieve spontaneous emission intensity and anisotropy enhancement with nanoscale plasmon resonators for applications from controlled photon emitters to light harvesting.

1 DST, India Nanomission

4:54 PM J15.00011 Changes of photoluminescence emission from metal/organic hybrid thin films with metal nanoparticle concentration, MEGUMI KIMURA, Japan Women’s Univ-Facul Sci, NAOKI TARUTANI, MASAHIKE TAKAHASHI, Department of Materials Science, Graduate School of Engineering, Osaka Prefecture University, ARUP NEOGI, Department of Physics, University of North Texas, RYOKO SHIMADA, Japan Women’s Univ-Facul Sci, JAPAN WOMEN’S UNIVERSITY COLLABORATION, UNIVERSITY OF NORTH TEXAS COLLABORATION — Metal nanoparticles (NPs) have been attracting research interest in the field of nanophotonics due to the localized surface plasmon (LSP) effect that enhances the electric field around metal NPs. This localization leads to enhancement of light emission from fluorescent molecules in the vicinity of the metal NPs. This study focuses on hybrid thin films consisting of metal NPs (silver: Ag-NPs), organic molecules (anthracene) and a polymer matrix (polyphenylsiloxane glass: PSS) to investigate changes of the enhancement of photoluminescence (PL) emission from anthracene molecules at various Ag-NPs concentration. The integrated PL enhancement factor was reduced at high Ag-NPs concentration due to the aggregation of Ag-NPs, and the LSP resonant energy of Ag-NPs exhibited red-shift for this case.

5:06 PM J15.00012 Coupling between Plasmonic Nanostructures and Nitrogen-Vacancy Quantum Emitters, NATHANIEL STEINSULTZ, JINXIAO GONG, MIN OUYANG, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park, MD 20742 — In this talk, we will discuss the coupling between plasmonic nanostructures and nitrogen-vacancy (NV) center quantum emitters in diamonds at the nanoscale. We have developed a method to achieve tunable coupling between plasmonic metal nanostructures and NV centers. The effects of the metallic surface plasmon modes on the spontaneous emission rate of the NV centers can be evaluated by measuring the fluorescence lifetime of the NV centers. By coupling the NV center to the surface plasmon modes of the metallic nanoparticles, we observe an enhanced fluorescence rate of NV centers in nanodiamonds that may lead to increased sensitivity in nanoscale sensors.

5:18 PM J15.00013 XPS Observations of Crystal Field Splitting in TiO2 Thin Films in Quantum Confinement Approach, NATALYA SUSHKOVA, LAB MKS — Transition metal oxides attract increased interest due to amazing electrical and magnetic properties and their outstanding applications designated by relative d-band redistributions that are shifted in such a way that narrow bands arranged by localized electrons are situated in the vicinity of E_F. Different kinds of lattice distortions caused by doping and/or quantum size confinement of TM oxides are assigned to remarkable phenomenon Mott metal-insulator transitions, when mutual metal-oxide orbital arrangement changes dramatically. There is a widespread consensus that strong electron correlations are responsible for that change and magnetic excitation is one of manifestations of these correlations. Here we are presenting XPS study of titanium dioxide nanocrystal formations on silicon substrate with native oxide. The dynamic changes in XPS spectra were used for analysis of TiO2 thin films with mass thicknesses up to 2 monolayers formed by redox reactions of sputtered Ti on Si(100) substrate with native oxide implemented in situ under UHV conditions. XPS spectra evolution, as a traditional source of information on phase composition, was complemented by the possibility to estimate the morphology and crystal field splitting of formed precipitates. Intensity fluctuations observed for O1s, Si 2p, Ti2p spectra were accompanied by crystal field splitting in Ti2p and on second derivatives of O1s. These fluctuations were followed by noticeable changes in the vicinity of band gap indicating possible Mott metal-insulator transitions.

Tuesday, March 3, 2015 2:30PM - 5:06PM
Session J16 DMP DCOMP: Focus Session: Theory of Magnetism and Correlation in Fe-Based Superconductors
101AB - Ilya Eremin, Theory Physics III University

2:30 PM J16.00001 Itinerancy enhanced quantum fluctuation of magnetic moments in iron-based superconductors1, YU-TING TAM, DAO-XIN YAO, Sun Yat-Sen University, China, WEI KU, Brookhaven Natl Lab — We investigate the influence of itinerant carriers on dynamics and fluctuation of local moments in Fe-based superconductors, via linear spin-wave analysis of a spin-fermion model containing both itinerant and local degrees of freedom. Surprisingly against the common lore, instead of enhancing the double-exchange effect, this talk will also address the strongly asymmetric suppression of magnetic order via electron- and hole-doping.

1Supported by US DOE BES DE-AC02-98CH10886 & Chinese NBRPC-2012CB821400, NSFC-11275279.
2:42PM J16.00002 Spin fluctuations-corrected DFT for Fe-based superconductors - LUCIANO ORTENZI, Institute for Complex Systems (ISC), CNR, U.O.S. Sapienza, v. dei Taurini 19, 00185 Rome, Italy, HLYNUR GRETARSSON, Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany, S. KASAHARA, Y. MATUDA, Department of Physics, Kyoto University, Kyoto 606-8502, J. Carsill, T. SHIBAUCHI, Department of Advanced Materials Science, The University of Tokyo, Japan, K.D. FINKELESTEIN, Cornell High Energy Synchrotron Source, Cornell University, Ithaca, New York 14853, USA, W. WU, S.R. JULIAN, YOUNG-JUNE KIM, Department of Physics, University of Toronto, 60 St. George St., Toronto, Ontario, M5S 1A7, Canada, I.I. MAZIN, code 6390, Naval Research Laboratory, 4555 Overlook Avenue SW, Washington, DC 20375, USA, LILIA BOERI, Institute for Theoretical and Computational Physics, TU Graz, Austria — Alpha density functional theory (DFT) is, at the moment, the most appropriate tool for treating itinerant magnetism, its mean field implementations -local spin density approximation (LSA) with or without gradient corrections- underestimate the effect of non local spin fluctuations. As a result DFT fails in reproducing, at the same time, the crystal structure and the amplitude of local moment in near critical systems. In this talk I will present a simple method for correcting the magnetic properties of itinerant systems in LDA. The method is called reduced Stoner theory (RST). I will apply this method to study the ferromagnetic-paramagnetic transition under pressure in Ni₃Al itinerant ferromagnet and for describing the puzzling temperature behavior of the local moment found in doped-CaFe₂As₂ pnictides.

2:45PM J16.00003 Understanding the Origin of Magnetism in Various Iron-Based Superconductors from Itinerant Limit - YU-ZHONG ZHANG, MING-CUI DING, Tongji University, HAI-QING LIN, Beijing computational science research center. By investigating the band structure from first principles calculations for various iron-based superconductors we can understand the ground state of the particle-hole excitations at (\pi,\pi). Though the excitations in a few compounds show anomalous behaviors, they are not the counterexamples against the itinerant scenario. As long as the orbital degrees of freedom, which can lead to competing tendencies towards different magnetically ordered states, and the interlayer couplings are taken into account, these anomalies can be naturally accounted for from the itinerant limit. Moreover, we find that the particle-hole excitations away from the Fermi level are more relevant to the physical properties of iron-based superconductors than those close to the Fermi surfaces, which resolves the long-standing problem of why the Fermi surfaces alone can hardly explain various magnetic states observed experimentally in different iron-based superconductors. Finally, We predict based on our first principles calculations that K-doped BaFe₂P₂ and La- or Al-doped MgFeGe may be a possible iron-based superconductor.

3:06PM J16.00004 Magnetic, structural and superconducting phase diagram in bulk Fe chalcogenides: role of nematic fluctuations and biquadratic exchange - IGOR MAZIN, Naval Research Lab — It has been recently realized that even the bulk FeSe is distinctly unique, compared to “old” pnictogen-based Fe-based superconductors (FeBS), which may be a clue to understanding more exotic FeSe-derivatives. The mystery starts with the FeSe phase diagram: numerous pnictides experience an orthorhombic transition, likely of spin-"nematic" nature, followed by a magnetic transition; external pressure favors superconductivity if the starting phase is magnetic, and suppresses it otherwise, consistent with pressure suppressing spin fluctuations. FeSe, however, experiences an orthorhombic transition with no apparent sign of magnetic ordering, and its Tc raises rapidly with pressure, before switching to the usual, opposite trend. In this talk I will revisit, based on DFT calculations, magnetic fluctuations in chalcogenides, and show that, by magnetic transition, they, unlike pnictides, demonstrate unusual (and unexpected) frustration, which suppresses magnetic, but not nematic order, and fully explain the non-monotonic Tc(\rho). Specifically, after the discovery of FeBS multiple attempts have been made to map the magnetic interactions in these systems (deemed to be crucial for superconductivity) onto a set of short range pairwise exchange interactions, initially in terms of the J_{i,j},\ i\neq j, Heisenberg model. This approach failed to explain the double-stripe magnetism in FeTe, so the model was extended to include J_{i,j,k}. However, it was soon realized that this HM contradicts both ab initio calculations and neutron experiments in the magnetically ordered state of Fe pnictides. Thus the model was augmented to include a nearest neighbor biquadratic exchange K. It was also appreciated that the same interaction is essential for explaining the splitting between antiferromagnetic and orthorhombic phase transition in Fe pnictides. What has not been appreciated though was that (1) the double-stripe order is never a ground state of the HM, independent of the values of J_{i,j}, J_{i,j,k} and K; (2) the HM model has, in addition to usually considered in FeBS phases, a highly competitive novel antiferromagnetic “staggered stripes” phase, which appears to be the ground state in ab initio calculations for FeSe (but not FeTe or for FeSe under pressure). Applying the full J_{i,j,k}+ K model to the Fe(Se,Te) system demonstrates unusual frustration, not relevant for As-based FeBS, which can explain the phase diagram of the system, nonmonotonic behavior if Tc under pressure and unexpectedly large orthorhombic “nematic” region in the FeSe phase diagram.

3:42PM J16.00005 An energetically competitive \(t_3g B_{1g}\) pairing in a \(t_1g - J_1 - J_2\) model with orbital differentiated exchange couplings: implications for superconductivity in alkaline iron selenides - RONG YU, Department of Physics, Renmin University of China, Beijing 100872, China, EMILIAN MARIUS NICA, QIMIAO SI, Department of Physics and Astronomy, Rice University, Houston, Texas 77005 — The pairing state in the alkaline iron selenides remains a challenge to our understanding. We address this issue in the incipient Mott picture based on the bad-metal behavior [1] of these materials. In conjunction with this picture, the multi-orbital effect is amplified, with two studied possibilities being the orbital-selective Mott transition [2] and the orbital-dependent pairing [3]. Here we carry out calculations in a five-orbital model to the Fe(Se,Te) system demonstrates unusual frustration, not relevant for As-based FeBS, which can explain the phase diagram of the system, nonmonotonic behavior if Tc under pressure and unexpectedly large orthorhombic “nematic” region in the FeSe phase diagram.

3:45PM J16.00006 Effective Exchange Interactions for Bad Metals and Implications for Iron-based Superconductors - WENXIN DING, Rice University, RONG YU, Renmin University, QIMIAO SI, Rice University, ELIHU ABRAMANS, University of California Los Angeles — The experimentally observed bad metal behavior in parent iron pnictides and chalcogenides suggests that these systems contain strong electronic correlations and are on the verge of a metal-to-insulator transition. The magnetic excitations in this bad-metal regime mainly derive from the incoherent part of the electronic spectrum away from the Fermi energy. We present a microscopic study of the exchange interactions in such a regime within a slave rotor approach. Generalizations to the multi-orbital case are discussed, as are the implications for the strength of superconducting pairing amplitudes in the iron-based superconductors.

4:06PM J16.00007 Comparative study of pure and Co doped-BaFe₂As₂ - JACQUES SOULLARD, ILYA G. KAPLAN, Universidad Nacional Autonoma de Mexico, RAUL PÉREZ-ENRIQUEZ, Universidad de Sonora — We present a comparative study of the high critical temperature superconductor Co doped-BaFe₂As₂ at the electron correlation level by the embedded cluster method; the electron correlation is calculated through the second order Møller Plesset perturbation theory. We study successively the pure compound, the Co doped-compound in the antiferromagnetic state and in the non-magnetic state. The Co doping introduces a strong modification of the spin distribution in its neighboring atoms. The analysis of the orbital population reveals that the spin distribution of the Co impurity becomes 3 times greater than that of the central Fe of the pure compound, increase attributed to a orbital correlation increase of the \(d_{2z}\) orbital population; a local antiferromagnetic order along the b axis of the crystal structure appears. The formation mechanism of the local magnetic moments implies a spin transfer from the (n.n) and (n.n.n) atoms to the central Co and is relevant to the \(J_1 - J_2\) Heisenberg model. The orbital population analysis reveals also that, in the doped compound and in both magnetic cases, the electron charge is associated to a singlet state and may correspond to a holon.
that all three mechanisms are necessary to account for the available experimental data. We argue that the "Monte Carlo-Mean Field" (MC-MF) method, to study single and multiband Hubbard models. The focus here is on the single band case at half filling. We start with a mean-field (MF) decomposition of the Hubbard Hamiltonian and then promote the MF parameters to classical variables studied via MC simulations, while fermions are exactly diagonalized in the background of those classical variables. We present the Hubbard $U$ vs. temperature phase diagram on large three and two dimensional clusters. Our MC-MF method can capture the nonmonotonicity of $T_N$ with $U$, local moment physics above $T_N$, and the two peak behavior of specific heat, as compared with Determinantal Quantum Monte Carlo (DQMC). Results for the $t$ vs. $t'$ Hubbard model in two dimensions show that our approach can capture ground state and finite temperature properties reliably where DQMC fails due to sign problems. These one-band results set the stage for extending the MC-MF method to multiband Hubbard models of relevance to the Pnictide superconductors.

This work supported by the Singapore National Research Foundation NRF-NRFF2012-01.

**Tuesday, March 3, 2015 2:30PM - 5:30PM – Session J17 DCMP: Transport in Graphene and its Heterostructures 102AB - Jeanie Lau, University of California, Riverside**

2:30PM J17.00001 Theoretical study of Coulomb drag in graphene, DERK HO, National University of Singapore, SHAFFIQUE ADAM, Yale-NUS College and National University of Singapore — In this theoretical work we examine the problem of Coulomb drag in graphene. We consider the common situation of heterostructures comprising graphene double layers separated by a thin sheet of hexagonal boron nitride in both zero and finite magnetic fields. We study three distinct physical mechanisms, namely the interaction induced energy-transfer between the layers, momentum transfer between the layers, and the contribution due to the hybridization of the layers to the overall transport process. We argue that all three mechanisms are necessary to account for the available experimental data.

2:42PM J17.00002 Magnetotransport in graphene and other two dimensional materials, SHAFFIQUE ADAM, Yale-NUS College, Center for Advanced 2D materials and Graphene Research Center, and Department of Physics, National University of Singapore, INDIRA YUDHISTIRA, Center for Advanced 2D materials and Graphene Research Center, and Department of Physics, National University of Singapore — In this work we address theoretically the classical and quantum magnetotransport in graphene [1] and other two dimensional materials [2]. We demonstrate that at room temperature, the largest contribution to the magnetoresistance arises from the disorder-induced carrier density inhomogeneity that gives a quadratic magnetoresistance at low magnetic fields and linear magnetoresistance at large fields. At lower temperatures, quantum phase-coherent effects can be observed in the magnetotransport, and this provides information about the dominant scattering mechanism in these materials. References: [1] J. Ping, I. Yudhistira, N. Ramakrishnan, S. Cho, S. Adam, M. S. Fuhrer, Phys. Rev. Lett. 113, 047206 (2014); [2] H. Schmidt, S. Wang, L. Chu, M. Toh, R. Kumar, W. Zhao, A. H. Castro Neto, J. Martin, S. Adam, B. Özyilmaz, and G. Eda, Nano Letters, 14, 1909 (2014).

2:54PM J17.00003 I-V characteristics of graphene quantum dots, VENKATA CHAGANTI, APALKOV VADYM, Georgia State University — Quantum dots in graphene-like materials with honeycomb crystal structures are studied numerically within tight-binding model of graphene. The energy spectra and corresponding I-V characteristics are found for both isolated graphene islands, i.e., graphene "atoms," and coupled graphene islands, i.e. graphene "molecules." The results were obtained for different sizes of graphene quantum dot and different values of the coupling constants between the dot and the contacts. The current is found to increase with increase of the size of the graphene quantum molecule and increase of the value of the coupling constant. We also study the dependence of the I-V characteristics of graphene quantum dot on the size and the placement of the contacts. For the same size of graphene quantum "atom" and graphene quantum "molecule" the I-V characteristics is almost the same.

This work supported by the Singapore National Research Foundation NRF-NRFF2012-01.
3:06PM J17.00004 Effects of fluorination on graphene spin transport\(^1\), ZHISHENG LIN, BOWEN YANG, JING SHI, UC Riverside — Although ideal graphene has extremely weak intrinsic spin-orbit coupling (SOC), by introducing adatoms, proximity effect, hydrogenation, etc., SOC in graphene can be effectively enhanced. In this work, we study the effects of fluorination on graphene nonlocal transport which can probe the spin Hall effect and inverse spin Hall effect as SOC is introduced. The nonlocal resistance is compared between the pristine and fluorinated graphene devices. Upon fluorination, the nonlocal resistance rises clearly above the ohmic contribution and increases as the dosage increases, which is interpreted as a consequence of increased SOC in fluorinated graphene. Raman spectroscopy is used to monitor the D-peak intensity as a function of the fluorination. We find that by controlling fluorination, the magnitude of the nonlocal resistance enhancement is correlated with the D-peak in Raman spectra. We will discuss the effects of the enhanced SOC on spin diffusion length in fluorinated graphene devices. This work was supported by DOE/BES and NSF/NEB.

\(^1\)DOE/BES and NSF/NEB

3:18PM J17.00005 Spin injection and transport in graphene via spin Hall effect in Au\(^1\), BOWEN YANG, JING SHI, Department of Physics and Astronomy, Univ of California - Riverside — Graphene is a promising material for spintronics due to its negligible intrinsic spin-orbit coupling (SOC, 1-50 µeV in perfect flat graphene) derived from the light weight of carbon atoms. Experimentally, graphene shows a spin diffusion length greater than 1 µm at room temperature even though it is coupled to a substrate, as demonstrated by nonlocal spin valves. In this work, we investigate the spin injection and transport in graphene using a nonlocal Hall bar geometry with Au strips along the Hall bar arms. When a charge current flows along one Au Hall bar arm, it induces a pure spin current in Au due to the spin-Hall effect (SHE). The spin current is injected into graphene and propagates along the etched graphene channel. As it arrives at the other Au strip, the spin current is detected by the inverse spin-Hall effect (ISHE) in Au. In a 2 µm long, 0.2 µm wide Hall bar, the nonlocal resistance we obtained is 10 MΩ. Considering the small spin-Hall angle (0.01-0.02) of evaporated Au, the magnitude of the nonlocal resistance suggests efficient spin injection from metal directly into graphene. The simplicity and high injection efficiency of this method is suitable for further exploration of spin transport mechanism in graphene.

3:30PM J17.00006 Transport phenomena in deformed graphene: Magnetic field versus curvature . THOMAS STEGMANN, Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, NIKODEM SZPAK, Fakultät für Physik, Universität Duisburg-Essen, Germany — The current flow in deformed graphene nanoribbons is studied theoretically. Using a tight-binding model, we apply the nonequilibrium Green’s function (NEGF) method to investigate how a localized deformation and a perpendicular magnetic field affect the current flow. While a magnetic field acts differently on electrons and holes due to their opposite charges, the deformation treats them equivalently. Applying the eikonal approximation to the Dirac equation, which is effectively satisfied at long wavelengths, we show that the obtained geodesic lines are compatible with the current flow paths of our NEGF calculations. The solution of the Mathisson-Papapetrou equations also shows that the effect of the deformation can be subdivided in two parts. First, a pseudomagnetic field with sixfold symmetry of attractive and repulsive regions, which acts differently on electrons and holes, but changes its sign when going from the K to the K’ point. Second, an attractive force due to the curvature of the ribbon, which treats electrons and holes equivalently. We conclude with an outlook on how to use deformed graphene ribbons for geometrical focusing of the current flow.

3:42PM J17.00007 Two-dimensional metal-insulator transition in functionalized graphene . MICHAEL OSOFSKY, SANDRA HERNÁNDEZ, Naval Research Lab, ANINDYA NATH, George Mason University, VIRGINIA WHEELER, SCOTT WALTON, CLIFFORD KROWNE, KURT GASKILL, Naval Research Lab — Since its discovery, graphene has held great promise as a metal with massless carriers and thus extremely high mobility. This feature is the result of the two-dimensional character of the band structure due to the so-called Dirac cone for the ideal, perfectly ordered crystal structure. One of the implications of this ideal case is that the transport properties of this material should be immune to lattice disorder. In reality graphene, which is subject to varying amounts of disorder that depends on preparation method, environment, impurities and other extrinsic variables, has been shown to exhibit an effective mass. Thus, metallic behavior with a wide range of mobilities has been reported. This situation contradicts the prediction that all two-dimensional systems must be insulating. Furthermore, there have also been reports of damaging graphene so severely that it becomes an insulator. Therefore, graphene, with its single layer structure, is a model system for studying the two-dimensional metal-insulator transition (MIT). In this work, we systematically increase the resistivity of epitaxial graphene via the introduction of chemical moieties using very low temperature plasmas. These results reveal the existence of a two dimensional MIT in epitaxial graphene.

3:54PM J17.00008 Electronic transport in Chemically-doped Graphene . ABDOLLAH DADGAR, Columbia University — Chemical doping is a well-known technique to introduce carriers into semiconductors. Previously, we have studied the atomic and electronic structure of graphene doped with nitrogen, and have shown that the dopants primarily incorporate in the graphitic form. Such graphitic dopants are sources of strong intervalley scattering in graphene. In this work, we will describe the effect of these scattering centers on electronic transport in N-doped graphene films produced on SiO2 and BN substrates. We will discuss the mobility and charge carrier concentration inferred from field effect measurements and will discuss the temperature dependent elastic and inelastic scattering rates obtained from weak localization measurements.

4:06PM J17.00009 Near-field study in graphene/hBN heterostructures . GUANGXIN NI, Department of Physics, University of California, San Diego, La Jolla, California 92093, USA, MICHAEL GOLDFLAM, MARTIN WAGNER, ZHE FEI, ALEX SWINTON MCLEOD, MENGKUN LIU, Department of Physics, University of California, San Diego, La Jolla, California 92093, USA, FRITZ KEILMANN, Ludwig-Maximilians-Universität and Center for Nanoscience, 80539 München, Germany, BARBAROS ÖZYILMAZ, ANTONIO H. CASTRO-NETO, Graphene Research Centre and Department of Physics, National University of Singapore, 117542, Singapore, PHILIP KIM, Department of Physics, Columbia University, New York, NY 10027, USA, FRITZ KEILMANN, Ludwig-Maximilians-Universität and Center for Nanoscience, 80539 München, Germany — Graphene is proposed as one of the most promising candidates for novel plasmonic devices, owning to its versatile tunability and ultrafast operation speed. Although exciting results of graphene plasmonics have been obtained, there is keen interest in improving device quality to explore additional plasmon physics and functionalities. Here we present studies of surface plasmons in graphene/hBN devices using scanning near-field optical microscopy. We find that by using these high quality devices, plasmon dissipation rate can be greatly reduced. Moreover, we demonstrated ultrafast hot carriers induced plasmon dispersion in real space. Our study would be important for novel graphene plasmonic applications.
dependence of the critical current on the channel length, both away from and close to the charge neutrality point. The latter regime is particularly interesting work, we study several junctions of different lengths fabricated in CVD graphene, which allows for wider junctions with larger critical currents. We present the small; many of these junctions also tend to be underdamped, resulting in premature switching to the normal state before the critical current is reached. In this Josephson junctions made of graphene. These measurements are challenging, especially near the Dirac point, where the critical current of long junctions is \( \sim \) junctions as a function of the channel length and gate voltage. Previous works on normal metal SNS junctions have established that the product of the critical

| 4:18PM J17.00010 | Vertical transport through a misoriented graphene / hexagonal boron-nitride / graphene heterostructure | SUPENG GE, DARSHANA WICKRAMARATNE, ROGER LAKE, Univ of California - Riverside, UNIVERSITY OF CALIFORNIA RIVERSIDE TEAM — Hexagonal boron nitride has an atomically smooth self-passivated surface and minimal lattice mismatch with graphene, which makes it an ideal substrate material for achieving high-mobility graphene devices. There is also a growing interest in tunneling devices fabricated by vertically stacking h-BN between two layers of graphene. Mechanical stacking of these individual layers leads to interfaces that are naturally misoriented with respect to each other. Furthermore, the number of layers of h-BN between the graphene layers in such devices can also vary. The combined effect of the twist angle and the thickness of the h-BN layer on the vertical transport properties is still an open question. Using ab-initio calculations we calculate transmission across unrotated and rotated graphene/h-BN/graphene heterostructures. For a single layer of BN, misorientation increases the tunneling transmission. The transmission as a function of h-BN layer thickness and different commensurate rotation angles is discussed. |
| 4:30PM J17.00011 | Nonlinear Hall effect in h-BN/graphene on ferri-magnetic substrates | CHI TANG, BIN CHENG, ZHYONG WANG, ZILONG JIANG, MOHAMMED ALDOSARY, YAFIS BARLAS, MARC BORKRATH, JING SHI, UCR, T. TANIGUCHI, K. WATANABE, Advanced Materials Laboratory Japan — In this work, we present a magnetotransport study of fabricated graphene devices transferred on atomically flat ferri-magnetic insulator yttrium iron garnet (YIG) thin films. The graphene sheet is sandwiched between a hexagonal boron nitride (h-BN) top gate dielectric and YIG. Due to the atomically smooth surfaces of both h-BN and YIG, graphene devices exhibit high mobility. Furthermore, unlike traditional back-gated devices, the h-BN top-gated devices show negligible gate hysteresis and can achieve high carrier densities with relatively small gate voltages. To investigate the magnetotransport properties of graphene arising from the proximity-induced exchange interaction, we explore the behavior of the nonlinear Hall component over a wide range of carrier densities. The shape of nonlinear Hall part tracks the magnetization of the underneath YIG film after removal of the linear background that originates from the ordinary Hall Effect. A sign reversal of nonlinear Hall contribution is observed when graphene is tuned from electron- to hole-dominated transport regimes. The magnitude of the nonlinear Hall decreases as the density increases for both carrier types. The h-BN top gate dielectric enables us to probe the intrinsic proximity interaction of multilayered graphene heterostructures more efficiently. |
| 4:42PM J17.00012 | Controlling the electrostatic accumulation at the graphene edge, and effects on carrier transport | MENEYOUNG LEE, PATRICK GALLAGHER, Stanford University, GRACE PAN, Yale University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, DAVID GOLDBEER-GORDON, Stanford University — In graphene without doping, the local carrier density at any point is directly proportional to the net charge density induced by the electric field effect. For any finite sized sample, this induced charge distribution is inhomogeneous over macroscopic length scales and of a form determined by the actual geometry of the device. In contrast to gate-confined 2DEGs in modulation-doped semiconductor heterostructures, the carrier density accumulated at the boundary is greater than in the 2D bulk [1], and many experiments and potential applications need to take this effect into account. We will discuss experiments on boron nitride-encapsulated graphene devices (with low disorder and high mobility, which are designed to explicitly tune the electrostatic accumulation at the boundary, from over-accumulation (the situation in typical experiments) to a nearly flat band condition, and further into a regime where the 2D bulk and the edge have opposite charge. In clean devices where the mean free path exceeds the sample width and boundary scattering dominates, the effect of the electrostatic accumulation on carrier transport is pronounced. |
| 4:54PM J17.00013 | Gate-tunable Topological Pseudospin Transport in Bilayer Graphene | MENCQIAO SUI, GUORUI CHEN, LIGUO MA, Department of Physics, Fudan University, WENYU SHAN, Department of Physics, Carnegie Mellon University, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, XIAOFENG JIN, Department of Physics, Fudan University, WANG YAO, Department of Physics, University of Hong Kong, DI XIAO, Department of Physics, Carnegie Mellon University, YUANBO ZHANG, Department of Physics, Fudan University — Extra quantum degree of freedom, generally referred to as pseudospin, arises in condensed matter systems when electrons from two sublattices of a crystal form degenerate bands at Fermi level. Here we describe a pseudospin system based on the “which-layer” quantum degree of freedom in bilayer graphene that is fully tuned by top and bottom gates. We detect topological pseudospin current - a result of the broken symmetry induced by the top and bottom gate electric fields - in a nonlocal geometry. The nonlocal pseudospin transport persists up to room temperature owing to the large, tunable band gap in our bilayer graphene devices. The gate-tunable pseudospin quantum degree of freedom in bilayer graphene may lead to future pseudospin-based electronic applications. |
| 5:06PM J17.00014 | All-electrical control of RKKY interaction in graphene P-N junction | SHUHUI ZHANG, WEN YANG, Beijing Computational Science Research Center, KAI CHANG, Institute of Semiconductors, Chinese Academy of Sciences — Graphene is a promising material for spintronic devices. In this development, one way is to dope graphene with magnetic impurity spins. Controllable long-range coupling between different spins is a key ingredient for these applications. The electron-mediated RKKY interaction provides a possible solution. However, there lacks efficient way to control this interaction. Here we demonstrate that by focusing the electron waves across a P-N junction, the long-range RKKY interaction can be controllably amplified by electrical gating. This provides a possible route towards scaling up graphene-based spintronic devices. |
| 5:18PM J17.00015 | Length and density dependence of the critical current in long diffusive graphene-based Josephson junctions | CHUNG-TING KE, Duke Univ. Dept. of Physics, IVAN BORZENETS, Tokyo University, Dept. of Physics, ANNE WATSON, YURA BOMZE, GLEB FINKELSTEIN, Duke Univ. Dept. of Physics — We study the critical current in graphene-based Josephson junctions as a function of the channel length and gate voltage. Previous works on normal metal SNS junctions have established that the product of the critical current, \( I_c \), and normal resistance, \( R_n \), is determined by the Thouless energy \( \Delta t \). Several recent studies have addressed the \( I_c R_n \sim \Delta t/c \) relationship in Josephson junctions made of graphene. These measurements are challenging, especially near the Dirac point, where the critical current of long junctions is small; many of these junctions also tend to be underdamped, resulting in premature switching to the normal state before the critical current is reached. In this work, we study several junctions of different lengths fabricated in CVD graphene, which allows for wider junctions with larger critical currents. We present the dependence of the critical current on the channel length, both away from and close to the charge neutrality point. The latter regime is particularly interesting because the phase coherence should be established through the electron and hole puddles on the length scales of up to 800 nm. |

Tuesday, March 3, 2015 2:30PM - 5:30PM -
Session J18 DCOMP: Invited Session: Phonons and Electron-Phonon Interactions beyond LDA/GGA — Mission Room 103A - David Vanderbilt, Rutgers University
This work was supported by DOE.

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We acknowledge support of the Nanoelectronics Research Initiative’s (NRI’s) Southwest Academy of Nanoelectronics (SWAN).
2:30PM J20.00001 John H. Dillon Medal Lecture: Magnetic Field Directed Self-Assembly of Block Copolymers and Surfactant Mesophases1, CHINEDUM OSUJI, Yale University — Molecular self-assembly of block copolymers and small molecule surfactants gives rise to a rich phase behavior as a function of temperature, composition, and other variables. We consider the directed self-assembly of such soft mesophases using magnetic fields, principally through the use of in situ x-ray scattering studies. Field alignment is predicated on a sufficiently large product of magnetic anisotropy and grain size to produce magnetostatic interactions which are substantive relative to thermal forces. We examine the role of field strength on the phase behavior and alignment dynamics of a series of soft mesophases, outlining the possibility to readily create highly ordered functional materials over macroscopic length scales. We show that magnetic fields as large as 10 T have little discernable impact on the stability of block copolymer systems considered, with shifts in order-disorder transition temperatures of roughly 5 mK or smaller. Consequently, directed self-assembly in these systems proceeds by nucleation of randomly aligned grains which thereafter rotate into registry with the field. We highlight the tradeoff between decreasing mobility and increasing anisotropic field interaction that dictates alignment kinetics while transiting from a high temperature disordered state to an ordered system at lower temperatures.

1 NSF support through DMR-0847534 is gratefully acknowledged.

3:06PM J20.00002 Directed Assembly of Block Polymers, EDWIN THOMAS, Department of Materials Science and NanoEngineering Rice University — Various types of boundary conditions and applied fields can be used to impose constraints on how the micro domain organize. In some cases the constraints serve to remove degenerate patterns which serves to eliminate defects that occur at the boundaries between energetically equivalent patterns. In other cases, either new micro domain patterns emerge or certain types of defects are created at special locations depending on the global and local symmetries of both the imposed constraints and the micro domains themselves. Addition of nano particles to a block polymer brings in additional considerations for the overall pattern of the system. Additive size, shape and surface chemistries relative to those of the block polymer influence their location in the overall pattern. By providing commensuration of block polymer period(s) as well as compatibility of the point group symmetries of both the particle(s) and domain(s), help realize systems where the equilibrium microstructure enables multifunctional physical properties.

3:18PM J20.00003 Failure of Batteries with Block Copolymer Electrolytes and Lithium Metal Anodes, NITASH BALSARA, Univ of California - Berkeley, DIDIER DEVAUX, Lawrence Berkeley National Laboratory, KATHERINE HARRY, Univ of California - Berkeley, DILWORTH PARKINSON, Lawrence Berkeley National Laboratory, RODGER YUAN, Univ of California - Berkeley, DANIEL HALLINAN, Florida A&M University/Florida State University, ALASTAIR MACDOWELL, Lawrence Berkeley National Laboratory — Solid block copolymer electrolytes are promising candidates for the development of high performance rechargeable batteries comprising a lithium metal anode due to their chemical stability toward lithium and their mechanical resistance to dendrite growth. The application of a solid polystyrene-b-poly(ethylene oxide) (SEO) block copolymer electrolyte in lithium symmetric cells permits to study the formation and growth of lithium dendrites by a non-destructive tool, hard X-ray microtomography. All solid-state batteries comprising a Li metal anode and a SEO electrolyte layer and a composite cathode were assembled and cycled. The cathode contains lithium iron phosphate as active material, SEO electrolyte as binder, and carbon black. Hard X-ray microtomography enables to visualize the microstructural changes at the Li/SEO and SEO/cathode interfaces to get insight on the battery failure mechanisms.

3:30PM J20.00004 Polymer Dynamics under Cylindrical Nano-Confinement, KAREN WINEY, WEISHAO TUNG, ROBERT RIGGLEMAN, University of Pennsylvania — Polymer melts under cylindrical confinement have previously been shown to exhibit chain conformations elongated parallel to the cylinder axis and compressed perpendicular to the cylinder. Further, simulations and theory found that the number of entanglements per chain decreases as the cylinder diameter decreases. This talk presents the local dynamics and polymer diffusion under cylindrical confinement using simulations and experiments. For the molecular dynamics simulations, an entangled polymer is confined by an amorphous cylindrical confinement. Local dynamics and local packing of monomers are affected by the cylindrical confinement and an anisotropic mean-squared displacement is observed with faster motion along the cylinder axes that increases with increasing confinement. Using elastic recoil detection experiments, polymer diffusion coefficients along cylindrical nanopores were measured for deuterated polystyrene diffusing into nanoporous membranes infiltrated with polystyrene. The tracer diffusion coefficient increased with decreasing pore size, although the increase is less pronounced than found in the simulations. Results will be discussed in terms of the reptation model.

3:42PM J20.00005 The physical aging of star-shaped macromolecules: role of functionality, PETER GREEN, BRADLEY FRIEBERG, EMMANOUIL GLYNOS, University of Michigan, GEORGIOS SAKELLARIOU, University of Athens — The phenomenon of physical aging, structural relaxations that enable the return of a polymer, quenched to a temperature $T_{eq}$ below its glass transition temperature $T_g$, to equilibrium, was investigated in a series of star-shaped macromolecules. These macromolecules possessed functionalities that varied from $f = 3$ to $f = 64$, and their degrees of polymerization per arm $N$ were all comparable ($N \approx 100$). The aging of these star-shaped macromolecules is qualitatively similar to that of linear chain polymers, with their aging rates exhibiting maxima at threshold temperatures $T_{tr}$. The aging rates of the star-shaped molecules, however, are slower than their linear analogs. Moreover, $T_{tr}$ decreased with increasing $f$, and $K$ increased with increasing $f$ for $T_{eq} < T_{tr}$. Our results are, in part, rationalized in terms of dynamic percolation models.

3:54PM J20.00006 Solvent, Thermal and Solvent-Thermal Methods on Block Copolymer Thin Films, THOMAS RUSSELL, XIAODAN GU1, University of Massachusetts, ILIA GUNKEL2, ALEXANDER HEXEMER, Lawrence Berkeley National Laboratory — Real-time grazing-incidence small-angle X-ray scattering experiments were used to study block copolymer self-assembly in thin films during thermal and solvent vapor annealing, where copolymer thin films were exposed to the vapor of a solvent having near equal interactions with the blocks and to elevated temperature in an inert gas atmosphere, respectively. Similarities between both annealing techniques were identified and advantages and disadvantages of each annealing method were discussed. We show that the product of the effective Flory-Huggins interaction parameter, $\chi$, and the degree of polymerization, $N$, determines the grain size, irrespective of the specific annealing technique. Thermal-solvent annealing, where the thin films were exposed to solvent vapors at elevated temperatures, is also discussed and compared to solvent vapor and thermal annealing.

1 Current Address: Stanford University
2 Current Address: Adolphe Merkle Institute, Fribourg, Switzerland

4:06PM J20.00007 Predicting the distribution of functional nanoparticles in block polymers, ROBERT RIGGLEMAN, University of Pennsylvania — Polymer nanocomposites continue to find new applications, and it has become clear that controlling the dispersion state of the nanoparticles plays a key role in their ultimate performance. For optical properties it is crucial to control the particle spacing and mutual orientation, while mechanical properties seem to be dictated by the size and shape of any aggregates that form. However, predicting the equilibrium structure and assembly of nanoparticles as a function of their size, shape, surface functionality, and interactions with the matrix polymers remains a significant challenge. In this talk, I will describe our recent efforts to extend polymer field theory to describe the thermodynamics of polymer nanocomposite materials. Our approach does not require the mean-field approximation, and we can describe nanoparticles with a wide range of surface functionality, including grafting with various polymer architectures and strong wetting with a matrix polymer.
Conditions

201 - Peter Chupas, Argonne National Laboratory

Physical Crosslinking and Finite Concentration

applications on directed assembly, and propose general guidelines and fabrication strategies that are likely to lead to defect-free assembly of block polymers on lithographically directed copolymer assembly processes. We examine the effects of composition, pattern characteristics, solvent concentration and general material characteristics.

highly unfavorable non-equilibrium states that are stabilized by large free energy barriers. It is therefore of interest to identify the kinetic mechanisms that may lead to elimination of such barriers. In this work we use theory and simulations to determine the pathways through which defects are annihilated or annihilated in directed copolymer assembly processes. We examine the effects of composition, pattern characteristics, solvent concentration and general material characteristics.

on directed assembly, and propose general guidelines and fabrication strategies that are likely to lead to defect-free assembly of block polymers on lithographically patterned substrates.

2:42 PM J20.00010 Polymer stability and function for electrolyte and mixed conductor applications

we have been investigating macromolecular systems that may provide acceptable ion transport properties, but withstand the harsh oxidative environment of lithium air systems. An investigation of different polymeric materials commonly examined for electrochemical applications provides insight into polymer design for these kinds of environments.

4:22 PM J20.00011 Structural evolution of polyelectrolyte-complex-core micelles and ordered-phase bulk materials

The kinetics of formation and structural evolution of novel polyelectrolyte complex materials formed by the assembly of water-soluble di- and tri-block copolymers, with one neutral block and one block either cationic or anionic, have been investigated. The mechanism and speed of the assembly process, and the organization of these domains, were probed using dynamic mechanical spectroscopy and small angle X-ray scattering (SAXS). SAXS revealed that the equilibrium morphology of both the di-block copolymer and the tri-block copolymer materials were generally qualitatively the same with some apparent quantitative differences in phase boundaries, possibly attributable to lack of full equilibration. Slow kinetics and difficulties in reaching equilibrium phase structures, especially in tri-block materials, is a principal message of this article. Detailed analysis of the SAXS data revealed that the tri-block copolymer materials formed ordered phases via a nucleation and growth pathway and that the addition of small amounts (∼20%) of corresponding di-block copolymers increased the rate of structure formation and enhanced several key physical properties.

4:43 PM J20.0010 Thermodynamics and Kinetics of Defect Annihilation in Block Copolymer Assembly

We present a coarse-grained simulation framework to study long-time dynamics of lithium ions in unentangled polymer melts. Effects of strong cation-monomer binding are modelled by formation of reversible bonds, and monomer-specific binding features enter via bond lifetime and coordination number, which can be estimated from atomistic simulations. Two competing mechanisms control the cation transport: successive replacement of dynamic bonds, and motion of the "branched" polymer cluster formed by a cation. Either channel can dominate the long-time diffusion depending on chain lengths and/or the bond lifetime relative to the Rouse time. At high concentrations, cations crosslink the polymers into a transient network, which significantly slows down the relaxation of the polymers, resulting in the non-monicotonic dependence of ion conductivity on concentration, in qualitative agreement with experiment.
2:30PM J21.00001 Multi-faceted characterization of battery reactions: the case of spinel hosts for Mg-ion batteries

JORDI CABANA, University of Illinois at Chicago — Electrochemical energy storage was an important enabler of the wireless revolution and it is touted as a key component of a society that shifts away from its dependence on fossil fuels. Batteries are the primary technology when high energy devices are required. They are complex reactors in which multiple physico-chemical phenomena are concurrent in time and space. As a result, it is increasingly clear that holistic approaches to define such phenomena require a breadth of characterization tools. I will exemplify this need in the context of our quest for hosts that are able to reversibly intercalate Mg$^{2+}$ ions. Systems based on the intercalation of multivalent ions are pushed as next generation devices because, while they can resemble systems using Li$^{+}$ ions, they can store more charge per mol of intercalated species, and adopt metals as the anode. Using a combination of characterization tools, including X-ray diffraction, spectroscopy and scattering, electron microscopy and nuclear magnetic resonance, we ascertained that spinel oxides are able to reversibly and extensively accommodate Mg$^{2+}$. The mechanisms of this reaction were also elucidated. The rationale for the choice of techniques and the key pieces they provided to complete the picture will be discussed.

This work was supported as part of the Joint Center for Energy Storage Research (JCESR), an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences.

3:06PM J21.00002 Atomic-scale roughness of Li metal surface evident in soft X-ray absorption spectroscopy

DAVID PRENDERGAST, LIWEN WAN, YUFENG LIANG, YI-DE CHUANG, Lawrence Berkeley National Laboratory (LBNL), RUIMIN QIAO, LBNL and Shandong University, China, SHISHEN YAN, Shandong University, WANLI YANG, LBNL — Realizing Li metal electrodes depends on fundamental understanding and efficient control of surface properties, which requires reliable characterization of the Li metal surface. Controlled experiments of Li K-edge soft X-ray absorption spectroscopy (XAS) reveal evidence of steady oxidation of the Li metal surface even under ultrahigh vacuum (UHV) conditions. The XAS of the short-lived Li metal surface, prepared by in-situ scratching, exhibits a prominent peak at 55.6 eV, more intense and at a slightly higher energy than the first peak expected for bulk Li metal at 55 eV. First-principles XAS calculations explain the origin of both the increased intensity and energy shift. This required the use of surface structural models with under-coordinated Li atoms and an estimated 4 Å inelastic mean-free-path for Auger electrons, implying extreme surface sensitivity of the measurements to the first 2-3 atomic layers. This work provides a benchmark on both experiment and theory for further studies of Li and other reactive metal surfaces, which are currently under scrutiny for next-generation energy storage devices.

3:18PM J21.00003 Neutron Imaging of Rapid Water Imbibition in Fractured Sedimentary Rock Cores

CHU-LIN CHENG, University of Texas-Pan American, EDMUND PERFECT, BRENDAN DONNELLY, University of Tennessee-Knoxville, HASSINA BILHEUX, Oak Ridge National Laboratory, ANTON TREMSIN, University of California-Berkeley, LARRY MCKAY, VICTORIA DISTEFANO, University of Tennessee-Knoxville, JIANCHAO CAI, China University of Geosciences, LOU SANTODONATO, Oak Ridge National Laboratory — Advances in nondestructive testing methods, such as neutron, nuclear magnetic resonance, and x-ray imaging, have significantly improved experimental capabilities to visualize fracture flow in various important fossil energy contexts, e.g. enhanced oil recovery and shale gas. We present a theoretical framework for predicting the rapid movement of water into air-filled fractures within a porous medium based on early-time capillary dynamics and spreading over rough fracture surfaces. The theory permits estimation of sorptivity values for the matrix and fracture zone, as well as a dispersion parameter which quantifies the extent of spreading of the wetting front. Dynamic neutron imaging of water imbibition in unsaturated fractured Berea sandstone cores was employed to evaluate the proposed model. The experiments were conducted at the Neutron Imaging Prototype Facility at Oak Ridge National Laboratory. Water uptake into both the matrix and fracture zone exhibited square-root-of-time behavior. Both theory and neutron imaging data indicated that fractures significantly increase imbibition in unsaturated sedimentary rock by capillary action and surface spreading on rough fracture faces. Fractures also increased the dispersion of the wetting front.

3:30PM J21.00004 Tuning Fork Oscillators as Downhole Viscometers in Oilfield Applications

MIGUEL GONZALEZ, GREG BERNERO, OLIVIERO ALVAREZ, GREGORY HAM, DEFFENBAUGH MAX, Aramco Services Company; Aramco Research Center - Houston, SENSORS DEVELOPMENT TEAM — The commerciality of oil wells is greatly influenced by the physical properties of the fluids being produced. A key parameter in determining how producible the hydrocarbons are is their viscosity. Pressure and temperature changes in recovering a downhole sample to the surface can alter viscosity while accurate downhole measurement of this critical property remains a rudimentary effort in the industry. In this presentation, we describe the challenges of measuring and quantifying the viscosity of reservoir fluids in situ at downhole conditions, as well as present an overview of some of the different measurement techniques currently used. Additionally, we show our characterization of a piezoelectric tuning fork oscillator used as a viscosity sensor. In an attempt to recreate the environment found in oil wells, its mechanical and electrical properties were studied while the device was immersed in different fluids and, separately, under different conditions of pressure and temperature. This device is a first step toward the development of an inexpensive, integrated, and miniaturized sensing platform for the in situ characterization of reservoir fluids.

3:42PM J21.00005 Detecting the topographic, chemical and magnetic contrast at surfaces with nanometer spatial resolution

H. CABRERA, D.A. ZANIN, L.G. DE PIETRO, A. VINDIGNI, U. RAMSPERGER, D. PESCIA, ETH Zurich, MICROSTRUCTURE RESEARCH TEAM — Since the mid of the 1980s and over the past few decades various conventional electron spectroscopies were combined with electron spin sensitivity to investigate the magnetic properties of surfaces and thin films, evolving into the Scanning-Electron-Microscopy with Polarization Analysis (SEMPA) technique, which made it possible to directly observe the re-entrant transitions of magnetic-domain patterns in thin films of Fe on Cu(001) with several tens of nm resolution. The possibility of resolving magnetic-textures in direct space at atomic scale may trigger both fundamental understanding and efficient control of surface properties, which requires reliable characterization of the Li metal surface. Controlled experiments of Li K-edge soft X-ray absorption spectroscopy (XAS) reveal evidence of steady oxidation of the Li metal surface even under ultrahigh vacuum (UHV) conditions. The XAS of the short-lived Li metal surface, prepared by in-situ scratching, exhibits a prominent peak at 55.6 eV, more intense and at a slightly higher energy than the first peak expected for bulk Li metal at 55 eV. First-principles XAS calculations explain the origin of both the increased intensity and energy shift. This required the use of surface structural models with under-coordinated Li atoms and an estimated 4 Å inelastic mean-free-path for Auger electrons, implying extreme surface sensitivity of the measurements to the first 2-3 atomic layers. This work provides a benchmark on both experiment and theory for further studies of Li and other reactive metal surfaces, which are currently under scrutiny for next-generation energy storage devices.

3:54PM J21.00006 Multifarious apparatus for dynamic measurements in intense magnetic fields

FEDOR BALKIREV, Los Alamos Natl Lab — We describe a versatile apparatus which implements multiple types of measurement techniques suitable for intense magnetic field environment. Our approach capitalizes on recent advances in hardware/software co-design solutions to realize dynamic mapping and tracking of field-dependent phenomena in typically short time frame of pulsed measurements. The apparatus is capable of carrying out simultaneous dissimilar measurements such as resistivity, current-voltage characteristics, magnetic torque etc., both in pulse and continuous mode. The control logic can track and respond to changes in sample properties, such as onset of dissipation or changes in high-frequency oscillatory response, in sub-microsecond timescale.

This research performed under the DOE BES ’Science at 100 tesla’ and supported at the NHMFL by NSF Cooperative Agreement No. DMR-1157490
Field Laboratory to extract the carrier Hall mobility and density as a function of the temperature. We report on the integration of a custom attocube 2-axis rotary stepper positioner, with the ability to rotate a sample over the full 3D sphere with milli-degree precision. In this surface imaging technique the image intensity depends sensitively on the local electron landing energy. Specifically, we probe the in-plane potential distribution between laterally spaced electrical contacts on a layered quasi-two-dimensional (2D) sample (single to triple layer graphene). We make use of the property that incoming electrons are resonant with interlayer graphene states for well-defined (local) landing energies. Our method is straightforwardly extendable to other quasi-2D systems, most prominently to the upcoming class of layered van der Waals materials.

4:30PM J21.00009 Development of a Nonlinear Acoustic Phased Array and its Interaction with Thin Plates1. PAUL ANZEL, CARLY DONAHUE, California Institute Of Technology, CHIARA DARAI, ETH-Zurich, California Institute of Technology — Numerous technologies are based on the principle of focusing acoustic energy. We propose a new device to focus sound waves which exploits highly nonlinear dynamics. The advantages of this device are the capability of generating very highly powerful acoustic pulses and potential operation in high-temperature environments where traditional piezoelectrics may fail. This device is composed of rows of ball bearings placed in contact with a medium of interest and with an actuator on the top. Elastic spherical particles have a contact force that grows with their relative displacement to the three-halves power (Hertzian contact). When several spheres are placed in a row, the particles support the propagation of “solitary waves”—strong, compact stress-wave pulses whose tendency to disperse is counteracted by the nonlinearity of the sphere’s contact force. We present results regarding the experimental operation of the device and its comparison to theory and numerical simulations. We will show how well this system is capable of focusing energy at various locations in the medium, and the limits imposed by pre-compression. Finally, the effects of timing error on energy focusing will be demonstrated.

4:42PM J21.00010 Investigation of acoustically dead materials for resonant ultrasound spectroscopy. JONATHAN BETTS, BORIS MAIOROV, BRAD RAMSHAW, Los Alamos National Laboratory, ARKKADY SHEHTER, NHHFL, ALBERT MIGLIORE, Los Alamos National Laboratory — Resonant Ultrasonic Spectroscopy is used to excite mechanical resonances in solid samples. By precisely knowing the resonant frequency the complete elastic tensor of the sample can be calculated. In practice unwanted resonances are also created in the holder structure, these resonances are not related to the sample and can often confuse the measurement. To reduce this problem we have investigated the use of acoustically “dead” materials. We present data from various natural and synthetic materials. We also present RUS sample holder designs that can be used from <4K up to 700K and in magnet fields up to 45T. The elastic tensor of polycrystal beryllium will be presented as a demonstration of the system performance.

4:54PM J21.00011 Closed cycle refrigeration for routine magnetotransport measurements. BINUKA GUNAWARDANA, TIANYU YE, Georgia State University, WERNER WEGSCHEIDER, ETH-Zurich, RAMESH MANI, Georgia State University — Closed cycle refrigerators are an ideal solution to providing a cool environment for measurement of transport properties at low temperatures. We have developed a single-axis 14 T magnet. We discuss technical details of the rotator unit, refrigerator probe wiring and construction, and proof-of-principle measurements demonstrating precise closed loop control of magnetic field orientation.
2:54PM J22.00003 Evidence for a nematic component to the Hidden Order parameter in URu$_2$Si$_2$ from differential elastoresistance measurements. MAXWELL SHAPIRO, Stanford University, SCOTT RIGGS, National High Magnetic Field Laboratory, AKASH MAHARAJ, SRINIVAS RAGHU, Stanford University, ERIC BAUER, RYAN BAUJBACH, National High Magnetic Field Laboratory, PAULA GIRAŁDO-GALLO, Stanford University, MARK WARTENBE, National High Magnetic Field Laboratory, IAN FISHER, Stanford University — In this work, we use a novel piezo actuator technique to measure the differential elastoresistance of the unconventional heavy fermion superconductor URu$_2$Si$_2$. Prior to the onset of superconductivity ($T_c \sim 1.5$ K), URu$_2$Si$_2$ undergoes a phase transition to a novel “Hidden Order” state which has defied comprehensive understanding for over 30 years. By tracking the temperature dependence of various elastoresistivity coefficients (proportional to the Order parameter is a two-component vector oriented in the [110] crystallographic direction which breaks the underlying four-fold symmetry of the lattice (in to the Hidden Order transition. Understood within a Ginzburg-Landau framework for coupled order parameters, these measurements imply that the Hidden to high temperatures and a strong anomalous divergence (which scales as the singular contribution to the heat capacity) proximate the Hidden Order transition. Understood within a Ginzburg-Landau framework for coupled order parameters, these measurements imply that the Hidden the transition temperature over a wide range of dopings. However, the magnetic states of these dopings have not been well characterized, with only a small number of studies on polycrystalline samples reported in the literature. In this work, we present an investigation of the magnetic properties of single crystal samples of URu$_2$Fe$_x$Si$_2$ and URu$_2$Os$_x$Si$_2$. Our μSR results demonstrate that both of these dopings show an antiferromagnetic ground state between $x = 0.1$ and $x = 0.4$ that evolves with increasing temperature into the paramagnetic state by a second order transition.

3:06PM J22.00004 Optical conductivity of URu$_2$Si$_2$: gaps and electron phonon coupling. R.P.S.M LOBO, ESPCI, CNRS, UPMC — We measured the in-plane and out-of-plane optical conductivity of URu$_2$Si$_2$. The hidden order transition at 17 K shows the opening of a gap in both polarizations, with a sharp decrease in the optical scattering rate. Above the hidden order we find a redistribution of spectral weight that isoelectronic substitution of Ru with Fe acts as “chemical pressure” that evolves with increasing temperature into the paramagnetic state by a second order transition.

3:18PM J22.00005 Antiferromagnetism in Fe and Os doped URu$_2$Si$_2$ studied by μSR. M.N. WILSON, A.M. HALLAS, T. MEDINA, T.J. MUNISIE, G.M. LÜKE, Department of Physics & Astronomy, McMaster University, 1280 Main St., West Hamilton, Ontario L8P 4M1, Canada, T.J. WILLIAMS, Quantum Condensed Matter Division, Neutron Sciences Directorate, Oak Ridge National Lab, Oak Ridge, TN, 37831, USA, S.C. CHEUNG, B.A. FRANSEN, L. LIU, Y.J. UEMURA, Department of Physics, Columbia University, New York, New York 10027, USA — URu$_2$Si$_2$ is a material that has been studied extensively for almost three decades in an effort to characterize its unusual “hidden order” state. One common method used to study this compound is to perturb the ground state by doping with various metals. Such doping usually causes the transition temperature to drop, and the hidden order state to transition into an antiferromagnetic state. In contrast to this common behavior, the isoelectronic dopings Fe and Os cause a substantial increase in the transition temperature over a wide range of dopings. However, the magnetic states of these dopings have not been well characterized.

3:30PM J22.00006 Chemical pressure tuning of URu2Si2 via isoelectronic substitution of Ru with Fe. MARC JANOSCHEK, Los Alamos Natl Lab, PINAKI DAS, Ames Laboratory, NORAVEE KANCHANAVATTE, University of California San Diego, JOEL S. HELTON, National Institute of Standards and Technology, KEVIN HUANG, University of California San Diego, RYAN E. BAUJBACH, National High Magnetic Field Laboratory, Florida State University, ERIC D. BAUER, Los Alamos Natl Lab, YANIC ZHAO, WILLIAM RATCLIFF, National Institute of Standards and Technology, BEN D. WHITE, M. BRIAN MAPLE, University of California San Diego, JEFF W. LYNN, National Institute of Standards and Technology — We have used specific heat and neutron diffraction measurements on single crystals of URu$_2$Fe$_x$Si$_2$ for Fe concentrations $x \leq 0.7$ to establish that isoelectronic substitution of Ru with Fe acts as “chemical pressure” $P_{ch}$. Neutron diffraction reveals a sharp increase of the uranium magnetic moment at $x = 0.1$, reminiscent of the “hidden order” (HO) to large moment antiferromagnetic (LMAFM) phase transition in URu$_2$Si$_2$. Using the unit cell volume, and the isothermal compressibility $\kappa_T$ for URu$_2$Si$_2$, we determine $P_{ch}$ as function of $x$. The resulting temperature $T$-chemical pressure $P_{ch}$ phase diagram for URu$_2$Fe$_x$Si$_2$ is in good agreement with the established temperature $T$-external pressure $P$ phase diagram of URu$_2$Si$_2$. Thus, URu$_2$Fe$_x$Si$_2$ provides a new opportunity to study the close relationship between the HO and LMAFM phases with methods that cannot be used under pressure, and may shed some new light on the elusive order parameter of the HO.

3:42PM J22.00007 Elastoresistivity in the “Hidden Order” compound URu$_2$Si$_2$-$x$P$_x$. CAMILLA MOIR, Florida State University, National High Magnetic Field Laboratory, RYAN BAUJBACH, National High Magnetic Field Laboratory, ANDREW GALLAGHER, KUAN-WEN CHEN, Florida State University, National High Magnetic Field Laboratory, ARKADY SHEKHTER, GREG BOEBINGER, SCOTT RIGGS, National High Magnetic Field Laboratory — The intermetallic compound URu$_2$Si$_2$ undergoes a phase transition near 17.5 K, with clear thermodynamic and transport signatures. However, despite nearly 30 years of research, the nature of the order parameter remains unknown. This “hidden order” phase, and its relationship to the superconductivity that appears below 1.4 K, remains a central puzzle in the physics of correlated electron materials. In order to unfold the phenomena that are nascent in pure URu$_2$Si$_2$, we recently developed a flux growth technique that allows us to grow dopings through Si→P. This technique is unique because it enables the use of high vapor pressure elements. We find that phosphorous substitution suppresses the hidden order transition temperature until, at roughly 1.5% doping, a quantum phase transition is reached. We measure the doping evolution of the temperature dependent elastoresistivity focusing on the behavior of the nematic component ($b_{2g}$) as the Hidden Order transition is approached.

3:54PM J22.00008 Unfolding the physics of URu$_2$Si$_2$ through chemical substitution (Si → P). RYAN BAUJBACH, ANDREW GALLAGHER, KUAN-WEN CHEN, NHMF, Florida State Univ., FUMITAKE KAMETANI, ASC, NHMF, Florida State Univ., NAOKI KIKUGAWA, Natl. Inst. Mat. Sci., Tsukuba, Japan, NHMF, Florida State Univ., SAMANTHA CARY, THOMAS ALBRECHT-SCHMITT, Dept. Chem. and Biochem., Florida State Univ. — URu$_2$Si$_2$ features all of the major phenomena that are at the focus of current research in correlated electron materials, including an exotic ordered state ("hidden order"), unconventional superconductivity, and anomalous metallic behavior. We recently undertook to study URu$_2$Si$_2$ using the novel tuning parameter Si → P substitution which, in a simple picture, simply adds electrons to the conduction band. Substitution of high vapor pressure elements in URu$_2$Si$_2$ is unprecedented, and is enabled by our new molten metal flux technique [1]. We find a rich phase diagram that includes two quantum phase transitions that are associated with hidden order and antiferromagnetism, respectively. In the hidden order region, the superconducting transition temperature is initially enhanced with P, after which it approaches zero before hidden order is destroyed, suggesting that URu$_2$Si$_2$ might be electronically displaced from the optimal doping. The high order and antiferromagnetic regions are distant from each other, indicating that their origins are quite different. We will discuss these results and implications for understanding hidden order, superconductivity, and quantum criticality.


4:06PM J22.00009 Ultrasound in a Metamagnet and the Single Energy Scale Model. B. SHIVARAM, University of Virginia, VERNON ULRICH, Grove City College, PRADEEP KUMAR, University of Florida, V. CELLI, University of Virginia — Ultrasound velocity measurements in the heavy electron compound UPt$_3$ for magnetic fields up to 33 T are reported. We show that the single energy scale model (B.S.Shivaram et al., Phys. Rev. B, 89, 241107(R), 2014) captures the observed key features of the field dependence in the sound velocity shift, $\Delta v_s$. The shift $\Delta v_s$ at $H_c$ is inversely dependent on temperature above a certain “Dingle Temperature” and assumes a fixed value at very low T. This “saturation” in $\Delta v_s$ is accounted for by level broadening in the single energy scale model.
4:18PM J22.00010 Thermal and Transport properties of $U_2Pt_{1-x}\text{Ir}_xC_2$, MIN GU KANG, CALDES, Institute of Basic Science, Pohang, Korea, Department of Physics, POSTECH, Pohang, Korea, NICK WAKEHAM, Los Alamos National Laboratory, Materials Physics and Applications Division, Los Alamos, New Mexico 87545, USA, NI NI, Department of Physics & Astronomy, UCLA, Los Angeles, California 90024-1769, USA, ERIC BAUER, Los Alamos National Laboratory, Materials Physics and Applications Division, Los Alamos, New Mexico 87545, USA, JEEHOON KIM, CALDES, Institute of Basic Science, Pohang, Korea, Department of Physics, POSTECH, Pohang, Korea, FILIP RONNING, Los Alamos National Laboratory, Materials Physics and Applications Division, Los Alamos, New Mexico 87545, USA — We report thermal and transport properties of $U_2Pt_{1-x}\text{Ir}_xC_2$ from which a magnetic phase diagram is obtained. Pure $U_2IrC_2$ is an antiferromagnet at 6.5 $K$, whose Neel temperature initially rises to 13.2 $K$ at $x=0.8$ and subsequently is suppressed to zero temperature with increasing Pt content near $x=0.4$. Heat capacity data at $x=0.4$ shows an upturn at low temperature, which is consistent with proximity to a quantum critical point and considered as non-Fermi liquid behavior. The entropy after the phonon contribution has been subtracted has a value of 0.18 $R\ln 2$ at the Neel temperature of $U_2IrC_2$, revealing an itinerant nature of the 5f electrons in this compound. On the Pt rich side of the phase diagram, superconductivity is suppressed by $x=0.15$. The residual resistivity increases by a factor of 10 from pure Pt ($x=0$) to $x=0.15$ where superconductivity is suppressed to zero. The phase diagram is compared to pressure tuned and Rh doped $U_2PtC_2$ demonstrating the role of electronic tuning in this system.

4:30PM J22.00011 Single crystal growth and study the physical properties of non-centrosymmetric $UIrSi_3$, SHANTA SAHA, JOHNPIERRE PAGLIONE, Center for Nano Physics and Advanced Materials, Dept. of Physics, University of Maryland, College Park, Maryland — Heavy-fermion superconductivity in the non-centrosymmetric crystal structure has drawn much attention [1]. It is theoretically argued that the order parameter contains not only a spin-singlet part, but also an admixture of a spin-triplet state. The compound $UIrSi_3$ crystallizes in the non-centrosymmetric BaNiSn$_2$ structure which is closely related to the well-known ThCr$_2$Si$_2$-type [2]. Preliminary study on polycrystalline $UIrSi_3$ shows antiferromagnetic order below Neel temperature $T_N = 42 K$ [2]. Its lanthanide analog CeIrSi$_3$ shows heavy-fermion superconductivity under pressure [1]. Therefore, further investigation on $UIrSi_3$ would be meaningful. We will present our attempt to grow single crystal of $UIrSi_3$ by Czochralski method in a tetra-arc-furnace and study of its physical properties.

4:42PM J22.00012 Tuning the ground state of the Kondo lattice in $UTBi_2$ ($T = Ag, Au$) single crystals, PRISCILA ROSA, University of California, Irvine, YONGKANG LUO, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, PASCOAL PAGLIUSO, University of Campinas, ERIC BAUER, JOE THOMPSON, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, ZACHARY FISK, University of California, Irvine — Motivated by the interesting magnetic anisotropy found in the Ce-based heavy fermion family CeTX$_2$ ($T = \text{transition metal}, X = \text{pnictogen}$), here we study the novel U-based parent compounds $UTBi_2$ ($T = Ag, Au$) by combining magnetization, electrical resistivity, and heat-capacity measurements. The single crystals, synthesized by the self-flux method, also crystallize in the tetragonal HfCuSi$_2$-type structure (space group P4/nmm). Interestingly, although $UAuBi_2$ is a low-$\gamma$ antiferromagnet below $T_N = 181 K$, $UAuBi_2$ is a moderately heavy uniaxial ferromagnet below $T_C = 22 K$. Nevertheless, both compounds display the easy-magnetization direction along the c-axis and a large magnetocrystalline anisotropy. Our results point out to an incoherent Kondo behaviour in the paramagnetic state and an intricate competition between crystal field effects and two anisotropic exchange interactions, which lead to the remarkable difference in the observed ground states.

4:54PM J22.00013 Direct Observation of a Superconducting Spin Resonance in the Heavy Fermion Antiferromagnetic Superconductor $UNi_2Al_3$, JERO D WAGMAN, JONATHAN GAUDENT, McMaster University, COLLIN BROHOLM, JOSE RODRIG\'EZ, National Institute of Standards and Technology, BARRY WINN, MELISSA GRAVES-BROOK, Oak Ridge National Laboratory, JIM GARRETT, Brockhouse Institute for Materials Research, BRUCE GAULIN, McMaster University — We present neutron scattering data identifying a superconducting spin resonance in the heavy fermion, antiferromagnetic superconductor $UNi_2Al_3$. This resolves a longstanding issue in the comparison of $UNi_2Al_3$ to its isostructural sister $UPd_2Al_3$. These material both undergo antiferromagnetic phase transitions at relatively high temperatures, $T_N = 4.6 K$ and 14.5 $K$ respectively, before respectively superconducting below 1.2 and 2 $K$(B. D. Gaulin, et al, PRB 66, 174520 (2002)). However, previous reports suggest that only the magnetic fluctuations in $UPd_2Al_3$ display sensitivity to superconductivity via a superconducting spin resonance - the build up in the superconducting ground state of excess scattered intensity at a well defined resonance energy centered on a magnetic wave-vector. We resolve this disparity by clearly identifying a superconducting spin resonance in $UNi_2Al_3$ at the incommensurate wavevector $Q = (\frac{1}{2} \pm 0.11 0 \frac{1}{2})$. This re-establishes the relationship between these sister compounds and further evidences the intimate correlation of magnetism and superconductivity. 

Tuesday, March 3, 2015 2:30PM - 5:30PM – Session J23 DCOMP: Theory and Simulation of Excited-State Phenomena in Semiconductors and Nanostuctures II

2:30PM J23.00001 Accurate effective masses from first principles, JONATHAN LAFLAMME JANSSEN, XAVIER GONZE, Université catholique de Louvain, Institute of Condensed Matter and Nanosciences, Nanoscopic Physics — The accurate ab initio description of effective masses is of key interest in the design of materials with high mobility. However, up to now, they have been calculated using finite-difference estimation of density functional theory (DFT) electronic band curvatures. To eliminate the numerical noise inherent to finite-difference and obtain an approach that is more suitable for material design using high throughput computing, we develop a method allowing to obtain the curvature of DFT bands using Density-Functional Perturbation Theory (DFPT), taking a change of wavevector as a perturbation. Also, the inclusion of $G_0W_0$ corrections to DFT bands in our method will be presented.
dependent density-functional theory (TDDFT) is more efficient, but standard functionals do not produce excitons in extended systems. We present a new, approach the nanosecond time scale, suggesting the possibility of engineering a phonon bottleneck through geometry modification.

to the ground state by an order of magnitude. GQDs with zigzag edges demonstrate a significantly longer hot carrier lifetime in low-lying excited states that using time-dependent density functional theory to calculate nonadiabatic coupling between excitations. Employing the reduced density matrix method geometry dependence in these systems. We examine hot carrier relaxation due to lattice vibrations in GQDs of varying size and edge type (armchair or zigzag),

We gratefully acknowledge support from DOE under Grant Nos. DE-FG02-05ER46203 and DE-FG02-05ER46204.

Electronic and optical properties of a metal-organic framework with ab initio many-body perturbation theory. KRISTIAN BERLAND, Univ. of Oslo, Dept. Physics, SMN, KYUHO LEE, Lawrence Berkeley National Lab., Molecular Foundry, SAHAR SHARIFZADEH, Dept. of Electrical and Computer Engineering, Boston University, JEFFREY B. NEATON, Dept. of Physics, UC Berkeley — With their unprecedented surface area, and their structural and chemical tunability, metal-organic frameworks (MOFs) are being thoroughly explored for applications related to gas storage. Less studied are their electronic, excited-state, and optical properties. Here we explored such properties of Mg-MOF-74 using a combination of density functional theory (DFT) and many-body perturbation theory (MBPT) within the GW approximation and the Bethe-Salpeter equation (BSE) approach. The near-gap electronic conduction states were found to fall into two distinct categories: molecular-like and 1d-dispersive. Further, using the BSE approach, we predict a strongly anisotropic absorption spectrum, which we link to the nature of its strongly-bound excitons. Our calculations are found to be in good agreement with experimental absorption spectra, validating our theoretical approach.

This work is supported by Chalmers Area of Advance: Materials, Vetenskapsradet, DOE, and computational resources provided by NERSC.

Polarization-dependent force driving the Eg mode in bismuth under optical excitation: comparison of first-principles theory with ultra-fast x-ray experiments. STEPHEN FAHY, EAMONN MURRAY. Tyndall National Institute, University College Cork — Using first principles electronic structure methods, we calculate the induced force on the Eg (zone centre transverse optical) phonon mode in bismuth immediately after absorption of a ultrafast pulse of polarized light. To compare the results with recent ultra-fast, time-resolved x-ray diffraction experiments, we include the decay of the force due to carrier scattering, as measured in optical Raman scattering experiments, and simulate the optical absorption process, depth-dependent atomic driving forces, and x-ray diffraction in the experimental geometry. We find excellent agreement between the theoretical predictions and the observed oscillations of the x-ray diffraction signal, indicating that first-principles theory of optical absorption is well suited to the calculation of initial atomic driving forces in photo-excited materials following ultrafast excitation.

This work is supported by Science Foundation Ireland (grant no. 12/IA/1601) and EU Commission under the Marie Curie Incoming International Fellowships (grant no. PiIF-GA-2012-329695).

Nonadiabatic coupling and hot carrier relaxation in graphene quantum dots. JONATHAN TRINASTIC, Quantum Theory Project, University of Florida, IEK-HENG CHU, University of California-San Diego, HAI-PING CHENG, Quantum Theory Project, University of Florida — Graphene quantum dots (GQDs) have many possible applications in a variety of research areas, including photovoltaics, catalysis, and sensors. Experimental research has suggested the existence of long hot carrier relaxation times on the order of 100-200 ps due to carrier-phonon interactions, however little theoretical work has examined phonon-induced relaxation and its size or geometry dependence in these systems. We examine hot carrier relaxation due to lattice vibrations in GQDs of varying size and edge type (armchair or zigzag), using time-dependent density functional theory (TDDFT) to calculate nonadiabatic coupling between excitations. Employing the reduced density matrix method to calculate relaxation rates, we find a 100 ps relaxation time constant for low-lying excited states in a GQD with 132 carbon atoms, matching experiment. We also find that carbon-chain ligands attached to the QD edges significantly change the nonadiabatic recombination rates to the ground state by an order of magnitude. GQDs with zigzag edges demonstrate a significantly longer hot carrier lifetime in low-lying excited states that approach the nanosecond time scale, suggesting the possibility of engineering a phonon bottleneck through geometry modification.

This work is supported by DOE/BES DE-FG02-02ER45995.

Excitons in solids with non-empirical hybrid time-dependent density-functional theory. CARSTEN ULLRICH, University of Missouri, ZENG-HUI YANG, Temple University, FRANCESCO SOTTILE, ETSF, Ecole Polytechnique, Palaiseau — The Bethe-Salpeter equation (BSE) accurately describes the optical properties of solids, but is computationally expensive. Time-dependent density-functional theory (TDDFT) is more efficient, but standard functionals do not produce excitons in extended systems. We present a new, non-empirical hybrid TDDFT approach whose computational cost is much less than BSE, while the accuracy for both bound excitons and the continuum spectra is comparable to that of the BSE. Good performance is observed for both small-gap semiconductors and large-gap insulators.

This work supported by NSF grant DMR-1408904.

Electron Excitation Dynamics of Molecules Induced by Optical Near-Field. KATSUYUKI NOBUSADA, MASASHI NODA, Institute for Molecular Science — Optical response of molecules is undoubtedly essential for understanding their physicochemical properties. In conventional theoretical approaches to the optical response, far-field light and matter interaction has been discussed. However, recent advanced nano fabrication allows us to produce very precise nanostructures and optical response in a nanometer region plays a crucial role in developing functional materials. To understand the nano-optical response, we must explicitly treat the light-matter interaction, i.e., optical near field and matter interaction, occurred in a nanometer region. Very recently, we have developed an original TDDFT computational method with the aim of understanding optical-near-field excitation dynamics in nanostructures. Our computed results clearly show interesting phenomena that are completely absent in the conventional optical response under a dipole approximation. We will discuss some computed results of unusual electron excitation dynamics such as two-photon excitation and dissociation of molecules by an optical near field.

This research was supported by Grants-in-Aid (No. 25288012) and the K computer project (Nos. hp120035 and hp140054).
We further combine the electron dynamics calculation in the TDDFT with the Maxwell’s equation for electromagnetic fields so as to achieve simultaneous
time-dependent Kohn-Sham equation in real-time, it is possible to describe nonperturbative nonlinear electron dynamics induced by intense laser fields.

We have been developing a theoretical and computational method to describe electron dynamics in crystalline solids irradiated by laser pulses. Our method is based on the time-dependent density functional theory (TDDFT), which enables us to treat quantum electron dynamics in the first principles level. By solving the time-dependent Kohn-Sham equation in real-time, it is possible to describe nonperturbative nonlinear electron dynamics induced by intense laser fields. We further combine the electron dynamics calculation in the TDDFT with the Maxwell’s equation for electromagnetic fields so as to achieve simultaneous
descriptions of both micro-meter-scale laser-field propagation and nanometer-scale electron dynamics induced by the fields. We call it “Maxwell + TDDFT multiscale simulation.” As an application of the method, we show calculated transferred energy distribution from a laser pulse to a bulk SiO2 sample. We evaluated the laser damage threshold and the ablation depth from the distribution. We found that the calculation nicely reproduced measured results of both threshold and depth.

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MIN LEE, Center for Relativistic Laser Science, TOMOHITO OTOBE, Japan Atomic Energy Agency, GEORGE F. BERTSCH, University of Washington — intense laser pulses

Innsbruck, HEIKO APPEL, Fritz-Haber-Institut, Berlin, ILYA TOKATLY, Universidad del Pais Vasco, San Sebastian, ANGEL RUBIO

Institut, Berlin, CAMILLA PELLEGRINI, Universidad del Pais Vasco, San Sebastian, MICHAEL RUGENTHALER, Institut fur Theoretische Physik, Universitat

Bolton, UK, FRANCOISE REMACLE, Département de Chimie, Université de Liège, Belgium, MATTHIEU VERSTRAETE, Département de Physique, Université de Liège, Belgium — The advent of attosecond optical pulses, by allowing to control the breaking and rearrangement of chemical bonds, opens the door to many new applications, like novel catalysis mechanisms, photosensitive reactions, the preparation of states for quantum computing, etc. This control of the chemistry is made possible by the time scale of the attosecond pulses, which are effectively instantaneous with respect to the movement of the atomic nuclei, thus allowing the generation of a population of electronic states which is strongly out of equilibrium. In this work we investigate the electron dynamics of several molecular systems under the influence of attosecond pulses using the real-time formulation of time-dependent density functional theory (TD-DFT). We show a comparison of the performance of several exchange-correlation functionals by comparing TD-DFT calculations with equation of motion CCSD and CAS-SCF quantum chemistry methods, as well as applications of the method to the simulation of transient absorption spectroscopy.

4:06PM J23.00009 Study of attosecond dynamics of small and medium sized molecules induced by ultra-short optical pulses using TD-DFT , MICAEL OLIVEIRA, GABRIELE D’AVINO, Département de Physique, Université de Liège, Belgium, TOMASZ KUS, BENOIT MIGNOLE, Département de Chimie, Université de Liège, Belgium, THEODOROS PAPADOPOULOS, Institute of Renewable Energy and Environmental Technologies (IREET), Department of Engineering, Bolton, UK, FRANCOISE REMACLE, Département de Chimie, Université de Liège, Belgium, MATTHIEU VERSTRAETE, Département de Physique, Université de Liège, Belgium — The advent of attosecond optical pulses, by allowing to control the breaking and rearrangement of chemical bonds, opens the door to many new applications, like novel catalysis mechanisms, photosensitive reactions, the preparation of states for quantum computing, etc. This control of the chemistry is made possible by the time scale of the attosecond pulses, which are effectively instantaneous with respect to the movement of the atomic nuclei, thus allowing the generation of a population of electronic states which is strongly out of equilibrium. In this work we investigate the electron dynamics of several molecular systems under the influence of attosecond pulses using the real-time formulation of time-dependent density functional theory (TD-DFT). We show a comparison of the performance of several exchange-correlation functionals by comparing TD-DFT calculations with equation of motion CCSD and CAS-SCF quantum chemistry methods, as well as applications of the method to the simulation of transient absorption spectroscopy.

4:18PM J23.00010 Optical properties of alkali halide crystals from all-electron hybrid-exchange TD-DFT calculations , ROSS WEBSTER, Imperial College, LEONARDO BERNASCONI, STFC Rutherford Appleton Laboratory, NICHOLAS HARRISON, Imperial College — I will present a study of the electronic and optical properties of a series of alkali halide crystals, based on a recent implementation of hybrid TD-DFT in the all-electron Gaussian basis set code CRYSTAL [1]. This TD-DFT implementation includes on-site correlation and long range electron-hole interactions by including non-local Fock exchange in the functional. I will examine in particular, the impact of the Gaussian basis set size and quality on the prediction of the band gap, optical gap, and exciton binding energy of these systems, expanding on our previous work [2]. I will show that the polarisability criterion proposed by Rappoport and Furche for molecular systems [3], can be used to converge calculated excited-state properties with the basis set size for periodic systems. I will compare results from CRYSTAL calculations with GW+BSE calculations, previous plane-wave pseudopotential estimates and with experimental data. Finally, I will explore the potential for development of this method, including choice of exchange-correlation kernel, and our current work on a wide range of systems.


4:30PM J23.00011 A fast real time time-dependent density functional theory simulation method , LIN-WANG WANG, Lawrence Berkeley National Laboratory, ZHI WANG, Lawrence Berkeley National Laboratory, Berkeley; Institute of Semiconductors, Chinese Academy of Sciences, SHU-SHENG LI, Institute of Semiconductors, Chinese Academy of Sciences — We have developed an efficient real time, time-dependent density functional theory (TD-DFT) method that can increase the effective time step from 1 attosecond to 10 femtosecond, or 0.1. 0.5 femtosecond. Our algorithm, which carries out the non-adiabatic molecular dynamics TDFT simulations, can have comparable speed to the Born-Oppenheimer (BO) ab initio molecular dynamics (MD). As an application, we simulated the process of an energetic CI particle colliding onto a monolayer of MoSe2. Our simulations show a significant energy transfer from the kinetic energy of the CI particle to the electronic energy of MoSe2, and the result of TDFT is very different from that of BO MD simulations. This new algorithm will enable the use of real-time TD-DFT for many new simulations involving carrier dynamics and electron-phonon couplings.

This work is supported by the Director, Office of Science, BES/MSED, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, through the Material Theory program in LBNL. Zhi Wang is supported by the China Scholarship Council.

4:42PM J23.00012 Correlated Light-Matter Interactions in Cavity QED , JOHANNES FLICK, Fritz-Haber-Institut, Berlin, CAMILLA PELLEGRINI, Universidad del Pais Vasco, San Sebastian, MICHAEL RUGENTHALER, Institut fur Theoretische Physik, Universitat Innsbruck, HEIKO APPEL, Fritz-Haber-Institut, Berlin, ILYA TOKATLY, Universidad del Pais Vasco, San Sebastian, ANGEL RUBIO, Universidad del Pais Vasco San Sebastian — In the last decade, time-dependent density functional theory (TDDFT) has been successfully applied to a large variety of problems, such as calculations of absorption spectra, excitation energies, or dynamics in strong laser fields. Recently, we have generalized TDDFT to also describe electron-photon systems (QED-TDDFT) [1,2]. Here, matter and light are treated on an equal quantized footing. In this work, we present the first numerical calculations in the framework of QED-TDDFT. We show exact solutions for fully quantized prototype systems consisting of atoms or molecules placed in optical high-Q cavities and coupled to quantized electromagnetic modes. We focus on the electron-photon exchange-correlation (xc) contribution by calculating exact Kohn-Sham potentials using fixed-point inversions and present the performance of the first approximated xc-potential based on an optimized effective potential (OEP) approach.


3:54PM J23.00008 First-principles calculation for electron dynamics in dielectrics induced by intense laser pulses , SHUNSUKE A. SATO, KAZUHIRO YABANA, University of Tsukuba, YASUSHI SHINOHARA, Max Planck Institute, KYUNG-MIN LEE, Center for Relativistic Laser Science, TOMOHITO OTOBE, Japan Atomic Energy Agency, GEORGE F. BERTSCH, University of Washington — We have been developing a theoretical and computational method to describe electron dynamics in crystalline solids irradiated by laser pulses. Our method is based on the time-dependent density functional theory (TDDFT), which enables us to treat quantum electron dynamics in the first principles level. By solving the time-dependent Kohn-Sham equation in real-time, it is possible to describe nonperturbative nonlinear electron dynamics induced by intense laser fields. We further combine the electron dynamics calculation in the TDDFT with the Maxwell’s equation for electromagnetic fields so as to achieve simultaneous
descriptions of both micro-meter-scale laser-field propagation and nanometer-scale electron dynamics induced by the fields. We call it “Maxwell + TDDFT multiscale simulation.” As an application of the method, we show calculated transferred energy distribution from a laser pulse to a bulk SiO2 sample. We evaluated the laser damage threshold and the ablation depth from the distribution. We found that the calculation nicely reproduced measured results of both threshold and depth.
4:54PM J23.00113 Fast Integral method for the calculation of Hartree and Exchange terms in DFT and TDDFT$^1$, MICHAEL ZUZOFSKI, AMIR BOAG, AMIR NATAN, Dept. of Physical Electronics, Tel-Aviv University, Israel — The Hartree and Exchange terms can become a computational intensive task in DFT and TDDFT calculations of large structures. Existing methods use either iterative solvers such as conjugate gradient or multi-grid methods or use FFT for the calculation of those terms via the solution of the Poisson equation. With iterative solvers, the problem of setting the boundary conditions is often time consuming by itself as approximations such as the multipole expansion might not converge easily for structures with high aspect ratio. With FFT one needs to use a larger box for the calculation of finite systems. We present an alternative integral method to calculate the Hartree and Exchange terms in DFT and TDDFT. We first describe the algorithm and show that this has $O(N)$ scaling for elongated structures. We then show some examples of long 1D chains ground state and time dependent calculations that use this algorithm. Finally we discuss some possible applications for more advanced functionalities that include the Fock exchange or screened exchange.

$^1$A.N. wishes to acknowledge support from ISF grant 1722/13, AN and AB wish to acknowledge support from the bi-national Israel-France research grant.

5:06PM J23.00114 Band Gap Studies in Density Functional Theory$^1$, THOMAS E. BAKER, Department of Physics & Astronomy, University of California, Irvine, California 92697 USA, LUCAS WAGNER, Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling.FEW, Vrije Universiteit, De Boelelaan 1083, 1081HV Amsterdam, The, MILES STOUDENMIRE, Perimeter Institute for Theoretical Physics, Waterloo, Ontario, N2L 2Y5 Canada, KIERON BURKE, Department of Chemistry and of Physics, University of California, Irvine, California 92697 USA, STEVEN WHITE, Department of Physics & Astronomy, University of California, Irvine, California 92697 USA — We examine the exact properties of Density Functional Theory (DFT) in one dimension and compare it with the numerically exact answer provided by Density Matrix Renormalization Group. Using the exact answers, we can compare exact Density Functional Theory quantities against commonly used approximations. Approximations tend to underestimate the band gap of the material. We compare the exact DFT quantities with the approximations to explore the band gap problem and provide numerical proofs of principle.

$^1$We gratefully acknowledge support from the Department of Energy (DE-SC0008696). T.E.B. acknowledges support from the Achievement Rewards for College Scientists Fellowship.

5:18PM J23.00115 Real-time quantum electron-phonon dynamics$^1$, VALERIO RIZZI, TCHAVDAR TODOROV, JORGE KOHANOFF, Queen’s University Belfast, ALFREDO CORREA, Lawrence Livermore National Laboratory — Electrons and atomic motion out of equilibrium exchange energy and momentum. Physical processes that involve this exchange include Joule heating, inelastic electron tunneling, and thermalization of hot electrons in an irradiated material. An explicit dynamical treatment of both subsystems is essential to model such non-adiabatic phenomena and requires the ability to describe the interaction of the coupled electrons and nuclei without enforcing equilibration a priori. Therefore, being able to describe an electronic system in real time together with the underlying ionic system is a key feature for first-principles electron-phonon methods. We have developed an approach for real-time phonon-assisted electron transfer in nanowires, explicitly tracking out-of-equilibrium systems that exchange energy. Our model is fully quantum mechanical: it overcomes the limitations of the Ehrenfest (quantum-classical) approximation and doesn’t require thermostats, or the treatment of either subsystem as a bath. We can probe a range of timescales: from attoseconds (electronic timescale) to picoseconds (typical of atomic vibrations). The comparison with exact simulations of systems with a single phonon and a single electron has proved an invaluable validation tool for our method. We are able to describe the population inversion of an excited electronic system coupled to phonons and phonon-assisted conduction in systems with Anderson localization.

$^1$Leverhulme Trust

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Tuesday, March 3, 2015 2:30PM - 5:30PM —
Session J24 Quantum Monte Carlo Simulations of Fermion and Boson Systems I 203AB - Juana Moreno, Louisiana State University

2:30PM J24.00001 Quantum phases of dipolar bosons in multi-layered optical lattice geometries, BARBARA CAPOGROSSO-SANSONE, Homer L. Dodge Dept. of Physics and Astronomy, University of Oklahoma — Dipolar interactions are responsible for stabilizing novel quantum many-body states in ultracold systems. In this talk we consider dipolar bosons trapped in $N \geq 2$ optical lattice layers. These configurations provide an ideal setup to explore novel physics resulting from the long range and anisotropic character of the dipolar interaction. We present results based on Path Integral Quantum Monte Carlo by the two-worm and a novel N-worm algorithm for dipolar hard-core bosons whose dipole moments are aligned perpendicularly to the optical lattice layers. Several non-trivial phases are stabilized. For two-dimensional bi-layer geometries these phases include pair-superfluidity, pair-supersolidity, and solid phases. For stacks of one-dimensional layers (tubes) superfluidity of multimers, solids, countersuperfluids are stabilized and they have a threshold-less nature with respect to the dipolar interaction.

3:06PM J24.00002 Detecting Goldstone Modes Using Entanglement Entropy in Quantum Monte Carlo, BOHDAN KULCHYTSKYY, CHRIS HERDMAN, University of Waterloo, STEPHEN INGLIS, Ludwig Maximilian University of Munich, ROGER MELKOV, University of Waterloo, Perimeter Institute — Bipartite entanglement entropy has emerged as a multifunctional tool in the study of condensed matter systems. In the context of systems with a spontaneously broken continuous symmetry, the scaling of this quantity has been predicted by Metlitski and Grover to have logarithmic subleading universal contribution to the boundary [1]. To test this, we conduct large-scale Quantum Monte Carlo simulations for a two-dimensional spin-1/2 XY-model at temperatures below the finite-system energy gap. Based on the predicted Renyi entropy scaling form, we are able to extract the number of Goldstone modes through the coefficient of the subleading logarithm. Further, we confirm that an additional subleading geometrical constant is present, which can be expressed in terms of a quantity in a free scalar field theory. This work illustrates the striking quantitative agreement that can be achieved between analytical continuum theory and lattice numerics, through calculations of Renyi entanglement entropies. [1] M. Metlitski and T. Grover arXiv:1112.5166 (2011)

3:18PM J24.00003 ABSTRACT WITHDRAWN —

3:30PM J24.00004 Solving fermion sign problem in quantum Monte Carlo by Majorana representation, HONG YAO, ZI-XIANG LI, YI-FAN JIANG, Institute for Advanced Study, Tsinghua University — We discover a new quantum Monte Carlo (QMC) method to solve the fermion sign problem in interacting fermion models by employing Majorana representation of complex fermions. We call it Majorana QMC (MQMC). Especially, MQMC is fermion sign free in simulating a class of spinless fermion models on bipartite lattices at half filling and with arbitrary range of (unfrustrated) interactions. To the best of our knowledge, MQMC is the first auxiliary field QMC method to solve fermion sign problem in spinless (more generally, odd number of species) fermion models. MQMC simulations can be performed efficiently both at finite and zero temperatures. We believe that MQMC could pave a new avenue to solve fermion sign problem in more generic fermionic models. (Zi-Xiang Li, Yi-Fan Jiang, and Hong Yao, arXiv:1408.2269).
3:42PM J24.00005 Quantum Monte Carlo simulations of bosons with complex interactions

VALERY ROUSSEAU, Louisiana State University — Many of the most exciting materials and phenomena being studied today, from oxide heterostructures to topological insulators or iron-based superconductors, are the ones in which an understanding of how quantum particles interact with each other is essential. In the last decade, the development and the improvement of quantum Monte Carlo algorithms combined with the increased power of computers has opened the way to the exact simulation of Hamiltonians that include various types of interactions, such as inter-species conversion terms or ring-exchange terms. Simultaneously, developments made in the field of optical lattices, laser cooling and magneto/optical trapping techniques have led to ideal realizations of such Hamiltonians. A wide variety of phases can be present, including Mott insulators and superfluids, as well as more exotic phases such as Haldane insulators, supersolids, counter-superfluids, or the recently proposed Feshbach insulator. These experimental realizations of the various forms of the Hubbard model can have interesting applications, in particular they provide a possible way of performing quantum computing, and have also given rise to a new field known as Atomtronics, the equivalent of Electronics where the carriers are replaced by atoms. I will illustrate these ideas with examples of Hamiltonians that have been studied and some results. In order to study these systems, it is crucial to identify the various phases that are present, which can be characterized by a set of order parameters. Of particular importance in this task is the superfluid density. It is well known that the superfluid density can be related to the response of the free energy to a boundary phase twist, or to the fluctuations of the winding number. However, these relationships break down when complex interactions are involved. To address this problem, I will propose a general expression of the superfluid density, derived from real and thought experiments. I will discuss two interesting applications of my method to the SF transition of softcore bosons with 2nd neighbor hopping and to atom-molecule mixtures.


1This work is supported by NSF OISE-0952300.
We study charge- and spin-ordered states in the two-dimensional extended Hubbard model on a triangular lattice with a triangular lattice filling of 1/3 filling. While the nearest-neighbor Coulomb repulsion $V$ induces charge-ordered states, the competition between on-site $U$ and nearest-neighbor $V$ interactions lead to quantum phase transitions to an antiferromagnetic spin-ordered phase with honeycomb charge order. In order to avoid the fermion sign problem and handle frustrations here we use quantum Monte Carlo methods with the string-bond tensor network ansatz for fermionic systems in two dimensions. We determine the phase boundaries of the several spin- and charge-ordered states and show a phase diagram in the on-site $U$ and the nearest-neighbor $V$ plane. The numerical accuracy of the method is compared with exact diagonalization results in terms of the size of matrices $D$. We also test the use of lattice symmetries to improve the string-bond ansatz.

1Work at Mississippi State University was supported by the US Department of Energy grant DE-FG02-06ER46315.

Viable mouse liver. We use an SJL mouse model to study liver inflammation in vivo using the spatially and spectrally resolved nIR signature of the localized d(AAAT). An advancement in biosensor development is the use of near infrared fluorescent carbon nanotube sensors for in-vivo detection [2]. Here, we show that PEG-ligated SWNT sensors.

Another area of phase that exhibits highly selective recognition for specific molecules. To prove the generality of this phenomenon, we report three examples of heteropolymers—MoRe or corona phase molecular recognition [1] as a method of discovering synthetic antibodies, or nanotube-templated recognition sites from a heteropolymer 2D electronic structures of carbon nanotubes and graphene respectively can be utilized to advance new concepts in molecular detection. We introduce CoPh-Nanosensor Interfaces

Wang, University of Maryland

Cornell University — Graphene channel field-effect biosensors are demonstrated for detecting the binding of double-stranded DNA and poly-l-lysine. Sensors based on CVD graphene transferred using a clean, etchant-free transfer method. The presence of DNA and poly-l-lysine are detected by the change in the Dirac mobility, such as the ternary alloy CuAlNi, are metals that have the fascinating ability to “remember” their original shape: Once deformed, the simple act of heating can thermomechanically return them to their original configuration. At the heart of this process is a martensitic phase transition, a solid-solid transition that can be induced by either a temperature change or by external stress. Cycling between phases of SMAs reveals hysteresis in their stress-strain relationships and transformation temperatures. Moreover, these characteristics evolve over many transformation cycles. We report on in-situ X-ray Photon Correlation Spectroscopy (XPCS) measurements of the microstructural evolution of a CuAlNi alloy that underlies these hysteresis effects. By simultaneously monitoring changes in X-ray speckle patterns from the two solid phases as the alloy was thermally cycled through both partial and full transformations, we have seen reversible microstructural hysteresis loops and irreversible loops that reveal mesoscopic plastic deformation in the material.

Tuesday, March 1, 2015 2:30PM - 5:30PM —
Session J26 DCP: Focus Session: At the Interface of Molecules and Materials II

Wang, University of Maryland

2:30PM J26.00001 Corona Phase Molecular Recognition (CoPhMoRe) or corona phase molecular recognition [1] as a method of discovering synthetic antibodies, or nanotube-templated recognition sites from a heteropolymer library. We show that certain synthetic heteropolymers, once constrained onto a single-walled carbon nanotube by chemical adsorption, also form a new corona phase that exhibits highly selective recognition for specific molecules. To prove the generality of this phenomenon, we report three examples of heteropolymers—nanotube recognition complexes for riboflavin, L-thyroxine and estradiol. The platform opens new opportunities to create synthetic recognition sites for molecular detection. We have also extended this molecular recognition technique to neurotransmitters, producing the first fluorescent sensor for dopamine. Another area of advancement in biosensor development is the use of near infrared fluorescent carbon nanotube sensors for in-vivo detection [2]. Here, we show that PEG-ligated d(AAAT)_{n} DNA wrapped SWNT are selective for nitric oxide, a vasodilator of blood vessels, and can be tail vein injected into mice and localized within the viable mouse liver. We use an SJL mouse model to study liver inflammation in vivo using the spatially and spectrally resolved nIR signature of the localized SWNT sensors.


3:06PM J25.00007 ABSTRACT WITHDRAWN —

4:18PM J25.00008 Strength and Dislocation Structure Evolution of Small Metals under Vibrations . ALFONSO NGAN, University of Hong Kong — It is well-known that ultrasonic vibration can soften metals, and this phenomenon has been widely exploited in industrial applications concerning metal forming and bonding. In this work, we explore the effects of a superimposed small oscillatory load on metal plasticity, from the nano- to macro-size range, and from audible to ultrasonic frequency ranges. Macroscopic and nano-indentation were performed on aluminum, copper and molybdenum, and the results show that the simultaneous application of oscillatory stresses can lower the hardness of these samples. Moreover, in situ TEM and EELS observations show that subgrain formation and reduction in dislocation density generally occurred when stress oscillations were applied. These findings point to an important knowledge gap in metal plasticity — the existing understanding of ultrasound softening in terms of the vibrations either imposing additional stress waves to augment the quasi-static applied load, or heating up the metal, whereas the metal’s intrinsic deformation resistance or dislocation interaction processes are assumed unaltered by the ultrasound, is proven wrong by the present results. Furthermore, in the case of nonindentation, the continuous stress-deformation measurement technique for nanoindentation measurement assumes that the imposed signal-carrier oscillations do not intrinsically alter the material properties of the specimen, and again, the present results prove that this can be wrong. To understand the enhanced subgrain formation and dislocation annihilation, Discrete Dislocation Dynamics (DDD) simulations were carried out and these show that when an oscillatory stress is superimposed on a quasi-static applied stress, reversals of motion of dislocations may occur, and these allow the dislocations to revisit repeatedly suitable configurations for annihilation. DDD, however, was unable to predict the observed subgrain formation presumably because the number of dislocations that can be handled is not large enough. Subgrain formation was directly predicted by a new simulation method of dislocation plasticity based on the dynamics of dislocation density functions.

4:54PM J25.00009 To Slip or Snap: Finite Length Chains and Yield Mechanisms in Polyethylene Fibers1 . THOMAS O’CONNOR, MARK ROBBINS, Johns Hopkins University, Physics and Astronomy — Understanding the microscopic mechanisms of yield in oriented polymer fibers is a long-standing problem. Advances in polymer processing have produced highly ordered polyethylene (PE) fibers with tensile strengths between 4-7 GPa, but these values are far less than the theoretical limiting strength of 25 Gpa due to C-C bond scission. This reduction in strength is caused by the presence of defects within the fiber. The simplest type of defect is chain ends which reflect the finite length of polymer chains. The presence of chain ends allows a polymer fiber to yield by chain slip without scission of covalent bonds. Here we present extensive united atom (UA) and all atom (AA) molecular dynamics simulations of crystalline PE fibers subjected to uniaxial tension. The fibers are fully aligned crystals constructed from chains of finite length N, with N spanning 3 orders of magnitude (10^2 – 10^4 monomers). We explore the yield behavior of these systems and relate it to the dynamics of the underlying chain end defects. UA tensile strengths are systematically smaller than AA by a factor of about 3. Both show a saturation in tensile strength as N rises above 500 monomers. This reflects a saturation in the stress for chain ends to slip and implies a maximum tensile strength of 6 Gpa.

3Financial Support from: NSF IGERT-0801471; US Army Research Laboratory W911NF-12-2-0022.

5:06PM J25.00010 X-Ray Speckle Measurements of Hysteresis in a Shape Memory Alloy . MICHAEL ROGERS, Department of Physics, University of Ottawa, MARK SUTTON, Department of Physics, McGill University — Shape memory alloys (SMAs), such as the ternary alloy CuAlNi, are metals that have the fascinating ability to “remember” their original shape: Once deformed, the simple act of heating can thermomechanically return them to their original configuration. At the heart of this process is a martensitic phase transition, a solid-solid transition that can be induced by either a temperature change or by external stress. Cycling between phases of SMAs reveals hysteresis in their stress-strain relationships and transformation temperatures. Moreover, these characteristics evolve over many transformation cycles. We report on in-situ X-ray Photon Correlation Spectroscopy (XPCS) measurements of the microstructural evolution of a CuAlNi alloy that underlies these hysteresis effects. By simultaneously monitoring changes in X-ray speckle patterns from the two solid phases as the alloy was thermally cycled through both partial and full transformations, we have seen reversible microstructural hysteresis loops and irreversible loops that reveal mesoscopic plastic deformation in the material.

5:18PM J25.00008 Strength and Dislocation Structure Evolution of Small Metals under Vibrations . ALFONSO NGAN, University of Hong Kong — It is well-known that ultrasonic vibration can soften metals, and this phenomenon has been widely exploited in industrial applications concerning metal forming and bonding. In this work, we explore the effects of a superimposed small oscillatory load on metal plasticity, from the nano- to macro-size range, and from audible to ultrasonic frequency ranges. Macroscopic and nano-indentation were performed on aluminum, copper and molybdenum, and the results show that the simultaneous application of oscillatory stresses can lower the hardness of these samples. Moreover, in situ TEM and EELS observations show that subgrain formation and reduction in dislocation density generally occurred when stress oscillations were applied. These findings point to an important knowledge gap in metal plasticity — the existing understanding of ultrasound softening in terms of the vibrations either imposing additional stress waves to augment the quasi-static applied load, or heating up the metal, whereas the metal’s intrinsic deformation resistance or dislocation interaction processes are assumed unaltered by the ultrasound, is proven wrong by the present results. Furthermore, in the case of nonindentation, the continuous stress-deformation measurement technique for nanoindentation measurement assumes that the imposed signal-carrier oscillations do not intrinsically alter the material properties of the specimen, and again, the present results prove that this can be wrong. To understand the enhanced subgrain formation and dislocation annihilation, Discrete Dislocation Dynamics (DDD) simulations were carried out and these show that when an oscillatory stress is superimposed on a quasi-static applied stress, reversals of motion of dislocations may occur, and these allow the dislocations to revisit repeatedly suitable configurations for annihilation. DDD, however, was unable to predict the observed subgrain formation presumably because the number of dislocations that can be handled is not large enough. Subgrain formation was directly predicted by a new simulation method of dislocation plasticity based on the dynamics of dislocation density functions.

3:06PM J25.00006 Detection of DNA and Protein using CVD Graphene-channel FET Biosensors . ABHILASH SEBSTIAN, ANIKET KAKATKAR, ROBERTO DE ALBA, HAROLD CRAIGHEAD, JEEVAK PARPIA, Centre for Materials Research, Cornell University — Graphene channel field-effect biosensors are demonstrated for detecting the binding of double-stranded DNA and poly-l-lysine. Sensors consist of CVD graphene transferred using a clean, etchant-free transfer method. The presence of DNA and poly-l-lysine are detected by the change in the Dirac Voltage (the voltage at which the graphene’s resistance peaks) of the graphene transistor. Sensors show large shifts in the Dirac voltage ~ 17 V after exposure to ~ 580 pM of poly-l-lysine and ~ 14 V upon exposure to 300 pM of DNA. The polarity of the response changes to positive direction with poly-l-lysine and negative direction with DNA. Sensors show detection limits of 8 pM for 48.5 kbp DNA and 11 pM for poly-l-lysine. The biosensors are easy to fabricate, reusable and are promising as sensors of a wide variety of charged biomolecules.
of how the molecular orbital is renormalized is addressed. Photosynthesis. In this work we report density functional theory (DFT) and many-body GW calculations to investigate CO2 adsorption on III-nitride semiconductor surfaces.

YING-CHIN CHEN, HONG GUO, McGill Univ — Photon-induced chemical transformation of CO2 is a very interesting direction of green-house gas reduction. LAY-SENG CHONG, PHILIPPE GUYOT-SIONNEST, UNIL Geneva — While much research on colloidal quantum dots is focused on their potential as visible emitter or light harvester, this talk will cover our investigations of the mercury chalcogenide colloidal quantum dots in the thermal mid-infrared ranges of 3-5 microns and 8-12 microns where the atmosphere is transparent. HgTe is a zero-gap semiconductor. As a result, colloidal quantum dots (QD) of sizes between 10 and 20 nm readily lead to infrared gaps tuning between 3 and 12 microns respectively. It is also very promising that infrared photodetection using dried films of these QDs has now been demonstrated up to 12 microns. Further improvement through chemistry are likely and will be required to raise the detectivity to the level required to transform thermal infrared detection technology. In contrast to HgTe QDQDs which tend to be intrinsic, beta-HgS and HgSe QDQDs are naturally n-doped, in the first such instance with QDQDs. Furthermore, the doping is modulated by modifying the surface composition, and this effect is attributed to the tuning of the energy level with respect to the environment, via the surface electrostatics. With controlled doping, both HgSe and HgS QDQDs have now led to the first operation of mid-infrared QD photodetector based on the intraband absorption. This is a breakthrough in the field of colloidal quantum dots where interband transitions had been exclusively used for the past 30 years. One challenge with both interband and intraband infrared QDQDs will be to reduce the nonradiative recombination, which will improve the detectivity as well as allow to use their infrared luminescence.

3:30PM J26.00004 Infrared detection with colloidal quantum dots based on interband and intraband transitions , PHILIPPE GUYOT-SIONNEST, University of Chicago — While much research on colloidal quantum dots is focused on their potential as visible emitter or light harvester, this talk will cover our investigations of the mercury chalcogenide colloidal quantum dots in the thermal mid-infrared ranges of 3-5 microns and 8-12 microns where the atmosphere is transparent. HgTe is a zero-gap semiconductor. As a result, colloidal quantum dots (QD) of sizes between 10 and 20 nm readily lead to infrared gaps tuning between 3 and 12 microns respectively. It is also very promising that infrared photodetection using dried films of these QDs has now been demonstrated up to 12 microns. Further improvement through chemistry are likely and will be required to raise the detectivity to the level required to transform thermal infrared detection technology. In contrast to HgTe QDQDs which tend to be intrinsic, beta-HgS and HgSe QDQDs are naturally n-doped, in the first such instance with QDQDs. Furthermore, the doping is modulated by modifying the surface composition, and this effect is attributed to the tuning of the energy level with respect to the environment, via the surface electrostatics. With controlled doping, both HgSe and HgS QDQDs have now led to the first operation of mid-infrared QD photodetector based on the intraband absorption. This is a breakthrough in the field of colloidal quantum dots where interband transitions had been exclusively used for the past 30 years. One challenge with both interband and intraband infrared QDQDs will be to reduce the nonradiative recombination, which will improve the detectivity as well as allow to use their infrared luminescence.

4:06PM J26.00005 Unraveling Molecular Structure in Stern Layer at Charged Water Interface using sum-frequency vibrational spectroscopy , YU-CHIEH WEN, Institute of Physics, Academia Sinica, SHUAI ZHA, SHANSHAN YANG, CHUANSHAN TIAN, Department of Physics, Fudan University, Y. RON SHEN, Department of Physics, University of California, Berkeley, California — Charged aqueous interfaces, such as membrane/water and electrochemical interfaces, are essential in many chemical, biological, and environmental processes. Interactions between heterogeneous interfacial molecules and the consequent molecular network dictate properties and functions of the interfaces; however, the microscopic-level picture of the charged water interfaces remains substantially unclear. Here we demonstrate probing of the molecular structure in Stern layer at aqueous interfaces using sum-frequency vibrational spectroscopy. We show that at anionic surfactant/water interfaces, the hydrogen-(H)-bonding strength and network in the Stern layer depend sensitively on conformation and ionization of the surfactants, suggesting a relevant influence of the surfactant-water charge transfer. In addition, ion adsorption to the interface is shown to distort the interfacial water structure. Our study offers exciting opportunities to acquire microscopic insights into interfaces for catalytic and electrochemical applications.

4:18PM J26.00006 Mind the Entropy: Electronic and Thermal Fluctuations of Large Molecules on Metals , REINHARD MAURER, Yale University, WEI LIU, IGOR POLTAVSKYI, Fritz-Haber Institute of the Max-Planck Society, HARALD OBERHOFER, THOMAS STECHER, Technische Universitaet Muenchen, ALEXANDRE TKATCHENKO, Fritz-Haber Institute of the Max-Planck Society, KARSTEN REUTER, Technische Universitaet Muenchen — The prevailing working hypothesis in vacuum surface science is that equilibrium properties of adsorbed molecules are largely altered by finite temperature effects. In this work we illustrate that this is not the case for the adsorption geometry, energetics, and desorption temperature of the molecular switch Azobenzene adsorbed to Ag(111). Comparing with X-ray standing wave measurements and temperature programmed desorption experiments we find strong discrepancies to static Density-Functional Theory calculations. Anharmonic corrections and ab-initio molecular dynamics simulation of the free energy of desorption account for the thermal fluctuations and inclusion of many-body dispersion effects accounts for the electronic fluctuations. In addition, we demonstrate that finite temperature effects lead to an incorrect prediction of the correct desorption temperature. This implies that an accurate description of adsorbate interactions and entropies of adsorption in most realistic functional hybrid metallic organic systems necessitates a full account of the inherent anharmonicity of adsorbate and substrate in addition to an accurate description of dispersion interactions.

4:30PM J26.00007 Stressed and Compressed Polymersomes , ROBERT HAYES, CHANGQIAN YU, STEVE GRANICK, Univ of Illinois - Urbana — Polymersomes are well-defined vesicular structures that have been studied extensively for encapsulation, controlled release and as cell mimics, inter alia. While polymersomes at ambient conditions are reasonably well-understood, comparatively little is known about how structure and properties change when subject to variations in their local environment. In this talk, atomic force microscopy is used to probe PEO-PBD polymersomes adsorbed at a solid liquid interface under osmotic pressure. We reveal interesting changes in shape and solvation not captured by classical theory.

4:42PM J26.00008 Effect of CO2 on a polystyrene adsorbed nanolayer1 , DEBORAH BARKLEY, NAISHENG JIANG, LEVENT SENDOGLUAR, XIAOYU DI, MANI SEN, MAYA K. ENDOH, TADANORI KOGA, Stony Brook University, Stony Brook, NY, BULENT AKGUN, Center for Neutron Research, National Institute of Standards and Technology and Bogazici University, Bebek, Istanbul, Turkey, MICHAEL DIMITRIOU, SUSIL SATIJA, Center for Neutron Research, National Institute of Standards and Technology — We report the role of compressed carbon dioxide (CO2) in a mobility gradient of polymer chains near a planar solid substrate. A series of bilayers of bottom hydrogenated polystyrene and top deuterated polystyrene layers were prepared on Si substrates, and high pressure neutron reflectivity (NR) was used to study diffuse motion at the polymer/polymer interface. The interdiffusion is hindered when the distance is less than 3Rg (Rg, radius of polymer gyration). This reduced chain diffusivity is attributed to CO2-induced polymer adsorption on the substrate, transforming the 0.6Rg thick region from the substrate interface into an irreversibly adsorbed polymer layer. The cohesion strength is attributed to loops in the adsorbed chains with which the neighboring chains can entangle.

1T. K. acknowledges the partial financial support from NSF Grants (CMMI-084826 and CMMI-1332499).

4:54PM J26.00009 First-principles investigation of CO2 absorption on III-nitride surfaces , YING-CHIN CHEN, HONG GUO, McGill Univ — Photon-induced chemical transformation of CO2 is a very interesting direction of green-house gas reduction. An accurate description of electronic structure at the interface between CO2 and the photocatalysts is important for understanding the process of artificial photosynthesis. In this work, we present density functional theory (DFT) and many-body GW calculations to investigate CO2 adsorption on III-nitride semiconductor surface. The adsorption geometry is determined at the DFT level and the electronic structure is investigated at both DFT and GW levels. A detailed illustration of how the molecular orbital is renormalized is addressed.
5:06PM J26.00010 Ab initio molecular-dynamics study of EC decomposition process on Li$_2$O$_2$ surfaces, YASUNOBU ANDO$^1$, Department of Materials Engineering, The University of Tokyo, TAMIO IKESHOJI, MINORU OTANI$^2$, Nanosystem Research Institute, AIST — We have simulated electrochemical reactions of the EC molecule decomposition on Li$_2$O$_2$ substrate by ab initio molecular dynamics combined with the effective screening medium method. EC molecules adsorb onto the peroxide spontaneously. We find through the analysis of density of states that the adsorption state is stabilized by hybridization of the sp$^2$ orbital and the surface states of the Li$_2$O$_2$. After adsorption, EC ring opens, which leads to the decomposition of the peroxide and the formation of a carboxy group. This kind of alkyl carbonate formed on the Li$_2$O$_2$ substrate was found in experiments actually

$^1$Nanosystem Research Institute, AIST; ESICB, Kyoto University

$^2$ESICB, Kyoto University

5:18PM J26.00011 Understanding 3C-SiC/SiO$_2$ interfaces in SiC-nanofiber based solar cells from ab initio theory$^1$, TAUFIK ADI NUGRAHA, STEFAN WIPPERMANN, Max-Planck-Institute for Iron Research — Nanostructured materials — such as e. g. hybrid nanocomposites consisting of inorganic semiconductor nanofibers and organic surfactants — provide genuinely novel pathways to exceed the Shockley-Queisser limit for solar energy conversion. The synthesis of such functionalized nanofibers can be performed completely using only inexpensive wet chemical solution processing. However, the synthesis conditions often lead to complex interfacial structures involving thin oxide layers between the nanofiber and surfactants, whose atomic details are poorly understood at best. Here we present a combined density functional theory and tight binding investigation of interfaces between 3C-SiC nanofiber surfaces and SiO$_2$. Considering a wide variety of possible interfacial structures we utilize a grand canonical approach to generate a phase diagram and predict the structural details of the interface as a function of the chemical potentials of Si, O and H. This study provides directions about how the synthesis conditions lead to specific types of interfacial structures and their impact on the electronic properties of the interface.

$^1$The authors wish to thank U. Gerstmann, S. Greulich-Weber and W. G. Schmidt for helpful discussions. S. W. acknowledges BMBF NanomatFutur Grant No. 13N12972.

Tuesday, March 3, 2015 2:30PM - 4:54PM —

Session J27 DCP: Focus Session: Chemical Physics of Clusters: Bridging from Angstrom-scale Clusters to Micron-scale Aerosol Particles III

2:30PM J27.00001 Solvation Effects on Structure and Charge Distribution in Anionic Clusters$^3$, J. MATHIAS WEBER, JILA and Department of Chemistry & Biochemistry, University of Colorado at Boulder — The interaction of ions with solvent molecules modifies the properties of both solvent and solute. Solvation generally stabilizes compact charge distributions compared to more diffuse ones. In the most extreme cases, solvation will alter the very composition of the ion itself. We use infrared photodissociation spectroscopy of mass-selected ions to probe how solvation affects the structures and charge distributions of metal-CO$_2$ cluster anions.

$^3$We gratefully acknowledge the National Science Foundation for funding through Grant CHE-0845618 (for graduate student support) and for instrumentation funding through Grant PHY-1125844.

2:30PM J27.00002 Proton transfer in acetaldehyde and acetaldehyde-water clusters: Vacuum ultraviolet photoionization experiment and theoretical calculations, OLEG KOSTKO, TYLER P. TROY, BISWAJIT BANDYOPADHYAY, MUSAHID AHMED, Lawrence Berkeley National Lab — Acetaldehyde, a probable human carcinogen and of environmental importance, upon solvation provides a test bed for understanding proton transfer pathways and catalytic mechanisms. In this study, we report on single photon vacuum ultraviolet photoionization of acetaldehyde and acetaldehyde-water clusters. Appearance energies of protonated clusters are extracted from the experimental photoionization efficiency curves and compared to electronic structure calculations. The comparison of experimental data to computational results provides mechanistic insight into the fragmentation mechanisms of the observed mass spectra. Using deuterated water for isotopic tagging, we observe that proton transfer is mediated via acetaldehyde and not water in protonated acetaldehyde-water clusters.

3:18PM J27.00003 Does the 18-Electron Rule Apply to CrSi$_{12}$?$^1$, MARISSA BADDICK ABREU,VIKAS CHAUHAN, ARTHUR REBER, SHIV KHANNA, Virginia Commonwealth University — Understanding the bonding between silicon and transition metals is valuable for devising strategies for incorporating magnetic species into silicon. CrSi$_{12}$ is the standard example of a cluster whose apparent high stability has been explained by the 18-electron rule. We critically examine the bonding and nature of stability of CrSi$_{12}$ and show that its electronic structure does not conform to the 18-electron rule. Through theoretical studies we find that CrSi$_{12}$ has 16 effective valence electrons assigned to the Cr atom and an unoccupied 3d$^3$ orbital. We demonstrate that the cluster’s apparent stability is rooted in a crystal field-like splitting of the 3d orbitals analogous to that of square planar complexes. CrSi$_{12}$ is shown to follow the 18-electron rule and exhibits all the conventional markers characteristic of a magic cluster. We will also present results on the stability and electronic structure of FeSi$_{12}$ clusters and in particular examine the valence configuration of FeSi$_{12}$ since Fe has two additional valence electrons compared to Cr.

$^1$We acknowledge support from the Department of Energy (DOE) under Award Number DE-SC0006420.

3:30PM J27.00004 Effect of N- and P-Type Doping on the Oxygen-Binding Energy and Oxygen Spillover of Supported Palladium Clusters$^3$, ARTHUR C. REBER, SHIV N. KHANNA, Virginia Commonwealth University — The oxygen-binding energy is one of the primary factors determining catalytic activity in oxidation reactions. One strategy for controlling the binding of a reactant to a surface is to dope the surface to create complementary donor–acceptor pairs. As oxygen is an acceptor, we have investigated the effect of doping on the oxygen-binding energy on Pd atoms and clusters supported on a rutile TiO$_2$(110) surface. We find that the P-type doping of the TiO$_2$ surface dramatically reduces the O-binding energy to Pd. When extended to Pd$_2$-supported clusters, we find that the P-type dopant decreases the energy for the oxygen to bind at spillover sites directly to the TiO$_2$ surface. In Pd$_2$O$_2$, the oxygen-binding energy is reduced with P-type doping, suggesting that this strategy may be used to control the oxygen-binding energy to supported catalysts.

$^3$This work was supported by the Air Force Office of Scientific Research (AFOSR) Basic Research Initiative Grant FA9550-12-1-0481.
3:42PM J27.00005 Cluster Study of Anion Specificity in Solutions: From Molecular-Like Species to Nano-Sized Droplets1, XUE-BIN WANG, Pacific Northwest National Lab — In this talk, I will present our cluster approach using size-selected, low-temperature photoelectron spectroscopy and ab inito calculations to study a variety of complex anion solvation across the Hofmeister series. Pronounced anion specific effects and rich solute-solvent interactions have been discovered en-route to solvation evolution from molecular species to nano-sized droplets. We found significant solute anisotropy effects in preferably selecting solvent network to align solute permanent dipole with the solvent electric field in hydrated neutral clusters. Thermodynamic advantage of organic acids in facilitating formation of bisulfate ion clusters, an important issue related to atmospheric chemistry and aerosol particle formation will also be discussed. 

1This work was supported by the US Department of Energy, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences & Biosciences.

4:18PM J27.00006 Ligand-modulated interactions between charged monolayer-protected Au144(SR)60 gold nanoparticles in physiological saline1, OSCAR VILLARREAL, LIAO CHEN, ROBERT WHETTEN, MIGUEL YACAMAN, Univ of Texas, San Antonio — We studied the interactions of functionalized Au144 nanoparticles (NPs) in a near-physiological environment through all-atom molecular dynamics simulations. The AuNPs were coated with a homogeneous selection of 60 thiolates: 11-mercapto-1-undecanesulfonate, 5-mercapto-1-pentanesulfonate, 5-mercapto-1-pentane-amine, 4-mercapto-benzoate or 4-mercapto-benzamide. These ligands were selected to elucidate how the aggregation behavior depends on the ligands’ sign of charge, length, and flexibility. Simulating the dynamics of a pair of identical AuNPs in a cell of saline of 150 mM NaCl in addition to 120 Na+/Cl- counter-ions, we computed the aggregation affinities from the potential of mean force as a function of the pair separation. We found that NPs coated with negatively charged, short ligands have the strongest affinities mediated by multiple Na+ counter-ions residing on a plane in-between the pair and forming “salt bridges” to both NPs. Positively charged NPs have weaker affinities, as Cl counter-ions form fewer and weaker salt bridges. The longer ligands’ large fluctuations disfavor the forming of salt bridges, enable hydrophobic contact between the exposed hydrocarbon chains and interact at greater separations due to the fact that the screening effect is rather incomplete.

1Supported by the CONACYT, NIH, NSF and TACC.

4:30PM J27.00007 Structural and charge inhomogeneity in supported Pt clusters1, F.D. VILA, J.J. REHR, U. of Washington, A.I. FRENKEL, Yeshiva U. — Nanoparticle materials are ubiquitous in heterogeneous catalytic processes and there is broad interest in their physical and chemical properties. However, global probes such as XAS and XPS reveal their ensemble properties, missing details of their local electronic and structural changes upon desorption. For example, upon single CO adsorption, the Pt-Pt bonds formed by coordinated Pt atoms are locally expanded by 5%, with little change in the rest of the particle. Coordination also has a large effect on the net charge of the Pt atoms, with a net loss of charge upon adsorption. Finally, we show how high coverage inverts the charge distribution in the clusters.

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

4:42PM J27.00008 New Insights into the Structure of Multimetallic Nanoparticles and their Advanced Characterization, SUBARNA KHANAL, NABRAJ BHATTARAI, JESUS VELÁZQUEZ-SALAZAR, GREGORY GUISBIERS, MIGUEL JOSE-YACAMAN, University of Texas at San Antonio — Noble multimetallic nanoparticles have led to exciting progress in a versatile array of applications. For the purpose of better tailoring of nanoparticles activities and understanding the correlation between their structures and properties, control over the composition, shape, size and architecture of bimetallic and multimetallic nanomaterials plays an important role on revealing their new or enhanced functions for potential applications. Advance electron microscopy techniques were used to provide atomic scale insights into the structure-properties of different materials: Pt-Pd, Au-Au, Cu-Cu, Pt-AgPd-Pt, and AuCu/Pt nanoparticles. These multimetallic nanoparticles have raised interest for their various applications in fuel cells, ethanol and methanol oxidation reactions, hydrogen storage, and so on. The nanostructures were analyzed by transmission electron microscopy (TEM) and aberration-corrected scanning transmission electron microscopy (Cs-corrected STEM), in combination with high angle annular dark field (HAADF), bright field (BF), energy dispersive X-ray spectroscopy (EDS), and electron energy loss spectroscopy (EELS) detectors. These techniques allowed us to probe the structure at the atomic level of the nanoparticles revealing new structural information and elemental composition of the nanoparticles.

Tuesday, March 3, 2015 2:30PM - 5:30PM – Session J28 GMAG DMP FIAP: Focus Session: Spin-Hall Effect I 205 - Ken-Ichi Uchida, Tohoku University

2:30PM J28.00001 The Spin Hall Effect in Rare Earth Thin Films, NEAL REYNOLDS, JONATHAN GIBBONS, JOHN HERON, Cornell University Physics Department, DARRELL SCHLOM, Cornell University Materials Science and Engineering, DANIEL RALPH, Cornell University Physics Department — The spin Hall effect results in a spin current which flows transverse to an applied electric field in heavy metals, and which can be used to apply an efficient spin transfer torque to the ferromagnetic layer in heavy metal/ferromagnet bilayer structures. We report experimental investigations of the strength of the spin Hall effect in lanthanide rare earth materials. To ensure trustworthy results, we compare the results of several complementary measurement techniques: off-resonant second harmonic detection of current-induced magnetic tilting, spin-torque ferromagnetic resonance, and spin pumping. We report on both the anti-damping and effective-field components of the spin torque generated by the spin Hall effect.

2:42PM J28.00002 Nonequilibrium spin polarization induced charge Hall effect, DAZHI HOU, Z. QIU, WPI Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan, R. IGUCHI, Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan. K. SATO, WPI Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan, K. UCHIDA, G. W. BAUER, EIJII SAITO, Tohoku University, Sendai 980-8577, Japan — The nonequilibrium spin polarization lies at the heart of information processing in spin-based devices. The generation and manipulation of the spin polarization have been realized by various approaches, however, the spin polarization is usually considered to have negligible effect on the electric transport property, especially for systems of high electron concentration like metals (e_F ~ eV). Here we show that the nonequilibrium spin polarization can cause a novel Hall voltage in a conventional metallic alloy at room temperature, which is due to a new mechanism and closely related to the spin Nernst effect.
2:54PM J28.00003 Spin Hall effect by surface roughness1. LINGJUN ZHOU, VAHRAM GRIGORYAN, Fudan University, China. SADAMICHI MAEKAWA, Japan Atomic Energy Agency, Japan. XUHUI WANG, King Abdullah University of Science and Technology, Saudi Arabia. JIANG XIAO, Fudan University, China — spin Hall effect and its inverse effect, caused by the spin orbit interaction, provide the interconversion between spin current and charge current. Since the effects make it possible to and manipulate spin current electrically, how to realize the large effects is an important in both physics and applications. To do so, materials with heavy elements, which have strong spin orbit interaction, have been examined so far. Here, we propose a new mechanism to enhance the spin Hall effect without heavy elements, i.e. surface roughness in metallic thin films. We examine Cu and Al thin films with surface roughness and find that they give the spin Hall effect comparable to that in bulk Au. We demonstrate that the spin Hall effect induced by surface roughness has the side jump direction but not skew scattering.

1This work was supported by the special funds for the Major State Basic Research Project of China (2014CB921600, 2011CB925601) and the National Natural Science Foundation of China (91121002).

3:06PM J28.00004 Optical detection of spin Hall effect in metals1. OLAF VAN T ERVE, AUBREY HANBICKI, KATHY MCCREARY, CONNIE LI, BERRY JONKER, Naval Research Lab — Here we present room temperature measurements of the spin Hall effect in non-magnetic metals such as Pt and β-W using a standard bench top magneto-optic Kerr effect (MOKE) system2. With this system, one can readily determine the angular dependence of the induced polarization on the bias current direction, the orientation of the spin Hall induced polarization, and the sign of the spin Hall angle. When a bias current is applied, the spin Hall effect causes electrons of opposite spin to be scattered in orthogonal directions, resulting in a spin accumulation at the surface of the film. The MOKE signal tracks the applied square wave bias current with an amplitude and phase directly related to the spin Hall angle. Using this technique, we show that the spin Hall angle of β-W is opposite in sign and significantly larger than that of Pt, and follow the structural phase transition from β-W to α-W as the film is annealed through the dependence of the spin Hall angle on crystal structure. We also use this technique to detect spin diffusion from β-W into Al thin films.

2This work was supported by internal programs at NRL and the NRL Nanoscience Institute.

3:18PM J28.00005 Extremely large, gate tunable spin Hall angle in 3D Topological Insulator pn junction1, 2. K M MASMUS HABIB, REDWAN SAJJAD, AVIK GHOSH, Univ of Virginia — The band structure of the surface states of a three dimensional Topological Insulator (3D TI) is similar to that of graphene featuring massless Dirac Fermions. We show that due to this similarity, the chiral tunneling of electron in a graphene pn junction also appears in 3D TI. Electrons with very small incident angle (modes) are allowed to transmit through a TI pn junction (TIPNJ) due to the chiral tunneling. The rest of the electrons are reflected. As a result, the charge current in a TIPNJ is suppressed. Due to the spin momentum locking, all the small angle modes are spin-down states. Therefore, the transmitted end of the TIPNJ becomes highly spin polarized. On the other hand, the spin of the reflected electron is flipped due to spin momentum locking. This enhances the spin current at the injection end. Thus, the interplay between the chiral tunneling and spin momentum locking reduces the charge current but enhances the spin current at the same time, leading to an extremely large (~20) spin Hall angle. Since the chiral tunneling can be controlled by an external electric field, the spin Hall angle is gate tunable. The spin current generated by a TIPNJ can be used for energy-efficient switching of nanoscale ferromagnets, which is an essential part of spintronic devices.

2This work is supported by the NRI INDEX center.

3:30PM J28.00006 Growth of β-Tungsten Films Towards a Giant Spin Hall Effect Logic Device, AVAYA JAYANTHINARASIMHAM, MANASA MEDIKONDA, AKITOMO MATSUBAYASHI, State University of New York, Albany, PRASANNA KHARE, HYUNCHER CHONG, RICHARD MATYI, ALAIN DIEBOLD, VINCENT LABELLA, SUNY, Polytechnic Institute — Spin-orbit coupling in metastable β-W generates spin transfer torques strong enough to flip magnetic moment of an adjacent magnetic layer. In a MTJ stack these torques can be used to switch between high and low resistive states. This technique can be used in designing efficient magnetic memory and non-volatile spin logic devices. Deposition conditions selective to β-W need to be understood for the large scale fabrication of such devices. The transition from β to α phase of Tungsten is strongly governed by thickness of W layer, base pressure and oxygen availability for example, above 5 nm β film relaxes and forms an α phase. Resistivity measurements as well as x-ray photoelectron spectroscopy and x-ray diffraction and reflectivity analysis are performed to determine the phase and thickness of tungsten films. We show that β phase is influenced by ultrathin thermal oxide of Si layer and the amount of oxygen flow during the growth. These results demonstrate a reliable technique to fabricate β-W film up to 20 nm on bare Si and silicon dioxide, while providing insight to growing it anywhere in the device stack.

3:42PM J28.00007 Spin polarized tunneling study on spin Hall effect metals and topological insulators1. LUQIAO LIU, IBM TJ Watson Research Center — Spin orbit interactions give rise to interesting physics phenomena in solid state materials such as the spin Hall effect (SH) and topological insulator surface states. Those effects have been extensively studied using electrical detection techniques so far. However, to date most experiments focus only on characterizing electrons near Fermi surface, while the spin-orbit interaction is expected to be dependent on electrons’ energies. Here we develop a tunneling spectroscopy technique to measure spin Hall materials and topological insulators under finite bias voltages. By electrically injecting spin polarized current into spin Hall metals or topological insulators through nonmagnetic material/oxide/ferromagnet (FM) junctions and measuring the induced transverse voltage, we are able to quantify the magnitude of the SHE in typical 5d transition metals and the spin momentum locking in topological insulators. The obtained spin Hall angles in Ta, Pt, W and Ir at zero bias are consistent with the results from spin torque experiments, and measuring the induced transverse voltage, we are able to quantify the magnitude of the SHE in typical 5d transition metals and the spin momentum locking in topological insulators. The obtained spin Hall angles in Ta, Pt, W and Ir at zero bias are consistent with the results from spin torque experiments, and measuring the induced transverse voltage, we are able to quantify the magnitude of the SHE in typical 5d transition metals and the spin momentum locking in topological insulators. The obtained spin Hall angles in Ta, Pt, W and Ir at zero bias are consistent with the results from spin torque experiments. Using this technique, we show that the spin-Hall angle of α-W into Al thin films.

1This work is supported by the DARPA MESO program (N00014-11-1-1110).

Role of transparency of platinum-ferromagnet interface in determining intrinsic magnitude of spin Hall effect

Weifeng Zhang, Stanford Univ, Wei Han, International Center for Quantum Materials, Peking University, Xin Jiang, Western Digital, See-Hyun Yang, Stuart Parkin, IBM Research - Almaden — The spin Hall effect (SHE) converts charge current to pure spin currents in orthogonal directions in materials that have significant spin-orbit coupling. The efficiency of the conversion is described by the spin Hall angle (SHA). The SHA can most readily be inferred by using the generated spin currents to excite or rotate the magnetization of ferromagnetic films or nano-elements via spin-transfer torques. Some of the largest spin torque derived spin Hall angles (ST-SHA) have been reported in platinum. By using spin torque ferromagnetic resonance (ST-FMR) measurements, we show that the transparency of the Pt-ferromagnet interface to the spin current plays a central role in determining the magnitude of the ST-SHA. We measure a much higher ST-SHA in Pt/cobalt (0.11) compared to Pt/permalloy (0.05) bilayers when the interfaces are assumed to be completely transparent. Taking into account the transparency of these interfaces, as derived from spin-mixing conductivities, we find that the intrinsic SHA in platinum has a much higher value of 0.19 as compared to the ST-SHA. The importance of the interface transparency is further exemplified by the insertion of atomically thin magnetic layers at the Pt/permalloy interface that we show strongly modulates the magnitude of the ST-SHA.

Spin Hall effects from mesoscopic Pt films with high resistivity

Chuan Qin, Department of Physics and Astronomy, University of Delaware, Yongming Luo, Chao Zhou, Department of Physics, Fudan University, YunJiao Cai, Shuhuan Chen, Department of Physics and Astronomy, University of Delaware, Yizheng Wu, Department of Physics, Fudan University, Yi Ji, Department of Physics and Astronomy, University of Delaware — The spin Hall effect (SHE) and inverse spin Hall effect (ISHE) are explored in mesoscopic lateral structures. Each structure consists of a Pt stripe, a Cu channel and a Py spin injector/detector. Low-resistance AlOx layers are placed at all interfaces. Two groups of structures are made with different sizes of the Pt/AlOx/Cu interfaces. The average resistance values of interfaces are 80 ohm in one group and 4 ohm in the other. Despite the resistance difference by a factor of 20, the average SHE signals only differ by a factor of 1.8 with the low-resistance structures showing higher signals. For a low-resistance interface, the ISHE signal is enhanced due to a more efficient absorption of the pure spin current but at the same time the signal reduction due to current shunting is also more severe. We are able to estimate the effect of shunting and the rate of spin absorption and obtain the product of spin Hall angle and the Pt spin diffusion length. It is noteworthy that the resistivity of the Pt stripe is substantially larger than that of an extended film. The large Pt resistivity contributes positively to the size of the signals but also implies short Pt spin diffusion length (<2nm). A sizable Pt spin Hall angle of >0.09 is estimated.

The Enhancement of spin Hall torque efficiency and Reduction of Gilbert damping in spin Hall metal/normal metal/ferromagnetic trilayers

Minh-Hai Nguyen, Chi-Feng Pai, Daniel C. Ralph, Robert A. Buhrman, Cornell Univ — The spin Hall effect (SHE) in ferromagnet/heavy metal bilayer structures has been demonstrated to be a powerful means for producing pure spin currents and for exerting spin-orbit damping-like and field-like torques on the ferromagnetic layer. Large spin Hall (SH) angles have been reported for Pt, beta-Ta and beta-W films and have been utilized to achieve magnetic switching of in-plane and out-of-plane magnetized nanomagnets, spin torque auto-oscillators, and the control of high velocity domain wall motion. For many of the proposed applications of the SHE it is also important to achieve an effective Gilbert damping parameter that is as low as possible. In general the spin orbit torques and the effective damping are predicted to depend directly on the spin-mixing conductance of the SH metal/ferromagnet interface. This opens up the possibility of tuning these properties with the insertion of a very thin layer of another metal between the SH metal and the ferromagnet. Here we will report on experiments with such trilayer structures in which we have observed both a large enhancement of the spin Hall torque efficiency and a significant reduction in the effective Gilbert damping. Our results indicate that there is considerable opportunity to optimize the effectiveness and energy efficiency of the damping-like torque through engineering of such trilayer structures.

Phase diagram and optimal switching induced by spin Hall effect

Shu Yan, Ya. B. Bazaliy, Department of Physics and Astronomy, University of South Carolina — In a ferromagnet/heavy-metal bilayer device with strong spin Hall effect, an in-plane current excites magnetic dynamics through spin-torque transfer. We analyze bilayers with a perpendicularly magnetized ferromagnet and calculate three-dimensional phase diagrams describing switching due to application of external magnetic field at a fixed current. For fields applied in the plane formed by the film normal vector and the current direction, we find the location of the additional equilibria created by the spin torque and give analytic expressions for two different destabilization boundaries. We further discuss the nature of switching at each boundary and qualitatively describe the magnetic state evolution. By analyzing the phase portraits of the system we give the condition at which switching from “up” to “down” state proceeds through this intermediate state. Using numeric simulations we analyze the switching time and compare it to that of a spin valve with a perpendicular polarizer.

Enhanced anti-damping torque in double-Spin-Hall trilayers

Satoru Emori, Tianxiang Nan, Carl Boone, Trevor Oxholm, David Budil, Northeastern University, John Jones, Brandon Howe, Gail Brown, Air Force Research Laboratory, Nian Sun, Northeastern University — In magnetic thin-film heterostructures, current-induced anti-damping torque can switch magnetization [1], drive domain walls [2], and induce precessional dynamics [3]. The spin Hall effect in ferromagnet/normal-metal bilayers is an especially promising mechanism for generating a robust anti-damping torque. We report on enhanced tuning of resonant magnetization dynamics in in-plane magnetized Ta/CoFeB/Pt trilayers, where both the Ta and Pt layers serve as spin-Hall sources. The change in resonant linewidth induced by in-plane DC current is measured using spin-torque ferromagnetic resonance (FMR) [4] and cavity-based FMR [5]. With optimized Ta and Pt layer thicknesses, we observe in 4-nm thick CoFeB a damping modification of >3 x 10^-3 per 10^{11} A/m^2 of DC current, effectively more than doubling the anti-damping torque compared to conventional spin-Hall bilayers. This finding provides a new possibility for increasing the efficiency of spin-Hall driven devices.


Tuesday, March 3, 2015 2:30PM - 4:54PM — Session J29 GMAG DMP FIAP: Focus Session: Ultrafast Spin-Dynamics 206A - Charlie Karis, University of Uppsala
2:30PM J29.00001 All-Optical Control of Magnetization in various Ferromagnetic Structures

RAJASEKHAR MEDAPALLI, University of California San Diego, VINCENT JOLY, Universite de Lorraine, YUKIKO TAKAHASHI, NIMS, Japan, STEPHANE MANGIN, Institut Jean Lamour, Universite de Lorraine, YESHAIHUA FAINMAN, ERIC FULLERTON, University of California San Diego — Until recently, the only class of material that demonstrated all-optical switching (AOS) is a narrow range of rare-earth (RE) and transition-metal (TM) alloy compositions. However, recent experimental investigations have broadened the choice of materials for AOS and showed that optical control of magnetization is a much more general phenomenon. These materials include wide variety of ferrimagnetic RE-TM alloys, RE-free synthetic ferrimagnets and, moreover, ferromagnetic thin films, multi-layers and even their granular films. By employing a magnetization sensitive microscopy technique we investigated the AOS in various ferromagnetic materials like Co/Pt multi-layers as a function of material composition, structure, laser pulse fluence, and multi-layer thickness and also in FePt granular thin films, as a function of grain sizes. Our results show the optimal material conditions in ferromagnets and highlight pathways for reducing possible energy consumption for the AOS in these materials. Moreover, our time-resolved pump-probe measurements on CoPt thin films and their multi-layers reveal the ultrafast magnetization response to the 100 fs laser pulses and its role in AOS.

1Work at UCSD supported by the ONR MURI program

2:42PM J29.00002 Ultrafast Dynamics near the M-edge in Chromium

GERARD SALVATELLA, RAFAEL GORT, THOMAS MICHLMAYR, ANDREAS VATERLAUS, YVES ACREMANN, None — Upon excitation by a femtosecond laser pulse a ferromagnet can be demagnetized on a sub-picosecond timescale. During the demagnetization both energy and angular momentum are exchanged between the electron gas and the lattice. However, the mechanisms and the characteristic times through which such exchanges occur are still controversial. A strong debate remains on whether bulk spin-flips or spin-currents are the primary cause of momentum transfer. To shed light on this topic two types of experiments are undertaken. First, demagnetization is studied in a pump-probe experiment in Ni for different pump-pulse durations. It is observed that shorter laser pulses demagnetize nickel more efficiently than longer pulses. The experiment reveals two processes: a fast process demagnetizes the sample within less than a picosecond and causes a remagnetization on the same timescale. Simultaneously, a slower process causes a magnetization loss that lasts tens of picoseconds. For long pulses only the slow remagnetization process is relevant. Second, a delayed double pulse experiment is performed in which the induced heat from the first pump pulse influences the demagnetization caused by the second through the increase of either the lattice or the electron temperatures.

3:06PM J29.00004 Ultrafast demagnetization: A transport effect?

GERARD SALVATELLA, RAFAEL GORT, THOMAS MICHLMAYR, ANDREAS VATERLAUS, Laboratory for Solid State Physic, ETH Zurich — The ultrafast loss of magnetization caused by a femtosecond laser pulse is still not well understood. One of the important contributions is spin flip scattering in the bulk of the magnetic material, mediated by the presence of phonons. The second contribution is the creation of spin currents, which transport spin angular momentum from the magnetic film into the substrate, where spin slips can take place outside of the view of the observer. Spin currents have been predicted by Battiato et al., PRL p.105, 027203 (2010). Here, we discuss a simple thermodynamic model describing laser induced spin currents as a cause of the temperature dependent shift of the chemical potentials. Experiments are discussed, which may be able to separate the effect of the lattice temperature from spin transport effects.

3:18PM J29.00005 Ultrafast spin switching in a canted antiferromagnetic YFeO3 driven by pulsed THz radiations

KIM TAEHEON, HAN SUN YOUNG, HAN JEONG WOO, HAN Gwangju Institute of Science and Technology (GIST), CHUL KANG, CHUL-SIK KEE, Advanced Photonics Research Institute, Gwangju Institute of Science and Technology, SEOHONG JUNG, JAEHUN PARK, Pohang Accelerator Laboratory, POSTECH, YUSUKE TOKUNAGA, RIKEN Center for Emergent Matter Science (CEMS), YOSHINORI TOKURA, University of Tokyo, LEE JONG SEOK, Gwangju Institute of Science and Technology (GIST) — We investigate the precessional motion of the magnetic moment in the canted antiferromagnetic YFeO3 which is excited by a linearly polarized terahertz (THz) pulse at room temperature. By tuning the spectral component of the input THz pulse around the quasi-ferromagnetic mode located near 0.3 THz, we have experimentally clarified the resonance effect of the magnetic moment in the canted antiferromagnet. Furthermore, we demonstrate that the spin state can be switched all-optically on a picosecond time-scale using THz spectral component of the input THz pulse around the quasi-ferromagnetic mode located near 0.3 THz, we have experimentally clarified the resonance effect.

3:30PM J29.00013 Ultrafast magnetization dynamics in heterogeneous granular FePt media

GRAF PIERRE, GRANITZKA PATRICK, ALEXANDER REID, SIMES/SLAC, WILLIAM SCHLOTTER, GEORGI DAKOVSKII, ANKUSH MITRA, LCLS/SLAC, PADRAIC SHAFFER, LBNL, MEHTA VIRAT, OLAV HELLWIG, HGST, ANDREAS SCHERZ, XFEL, JOACHIM STÖHR, HERMANN DÜRR, NIMS, Japan, STEPHANE MANGIN, Institut Jean Lamour, Universite de Lorraine, YESHAIHUA FAINMAN, ERIC FULLERTON, University of California San Diego — Ultrafast magnetization dynamics in heterogeneous granular FePt media have recently been studied with fs laser pump-probe techniques[Becker, et al APL 104, 152412 (2014)]. Large 400 GHz eigenfrequencies are observed due to the huge FePt magnetic anisotropy. However, such optical techniques only measure the collective spin precession of all grains without spatial resolution. Here we investigate the nanoscale magnetization dynamics in FePt with fs pump-probe pulses from the Linac Coherent Light Source at Stanford. We show that optical excitation leads to distinctly different magnetic responses due to the size distribution of FePt grains. While part of the laser-excited magnetic grains demagnetize nickel more efficiently than longer pulses. The experiment reveals two processes: a fast process demagnetizes the sample within less than a picosecond and causes a remagnetization on the same timescale. Simultaneously, a slower process causes a magnetization loss that lasts tens of picoseconds. For long pulses only the slow remagnetization process is relevant. Second, a delayed double pulse experiment is performed in which the induced heat from the first pump pulse influences the demagnetization caused by the second through the increase of either the lattice or the electron temperatures.
3:42PM J29.00007 Laser-induced ultrafast spin dynamics in di-, tri- and tetranuclear nickel clusters, and the M process, DEBAPRIYA CHAUDHURI, Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Germany, HONGPING XIANG, Department of Physics and Astronomy, California State University Northridge, California, USA, GEORGIOS LEFKIDIS, WOLFGANG HÜBNER, Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Germany — We present a theoretical investigation of the ultrafast magneto-optical dynamics in clusters with 2, 3 and 4 Ni atoms. We study cooperative effects by increasing both the number of active centers and the multiplicities (up to quintets) in our Hilbert space. In the dinuclear cluster Ni2 a novel spin-flip scenario based on the M process is established. This process is highly operative in case the standard M process fails. In the trinuclear cluster Ni3Na2 simultaneous spin-flip and spin-transfer is observed. Local spin-switch is also achieved via a non-linear M process which involves two off-resonant transitions. Finally, in the tetranuclear cluster (Ni4)2 the use of quintets provides an insight into an irreversible demagnetization scenario. We believe that our systematic investigation allows us to establish a relation between the magnetic centers and the multiplicities. Our research represents an important step towards the miniaturization of spintronic devices and functionalization of various logic elements based on molecular structure.

3:54PM J29.00008 A look at the Dynamics of Ultrafast Magnetization Reversal1, CHRIS RODGERS, GUOPING ZHANG, Indiana State University — There is an ever pressing need to figure out ways to store more data at a faster rate. The implementation of All Optical Magnetization Reversals is a potential step in this direction. There is a strong experimental understanding of the phenomenon. However, a clear theoretical model doesn’t exist. The theoretical model presented here is a potential step towards an understanding of this phenomenon. Through a computer simulation, we show that magnetization reversal could potentially occur through the interaction of the circular polarization of an ultrafast laser pulse, and the orbital angular momentum of a bound spin particle.

4:06PM J29.00009 Optimal Control of Magnetization Dynamics in Ferromagnetic Materials using TDDFT1, PETER ELLIOTT, KEVIN KRIEGER, E.K.U GROSS, Max Planck Institute of Microstructure Physics — Recently [1] intense laser-field induced ultrafast demagnetization was observed in ab-initio simulations using Time-Dependent Density Functional Theory (TDDFT) for various ferromagnetic materials (Fe,Co,Ni). From a practical and technological viewpoint, it is useful if the induced dynamics (e.g. of the total magnetic moment) are controllable. In this talk we apply optimal control theory together with TDDFT calculations to tailor the intense laser pulses so as to achieve a particular outcome (e.g. maximize the total moment lost) while also including any required constraints (e.g. pulse duration, pulse frequencies, maximum fluence, etc).

1Supported by U.S. Department of Energy and Indiana State University

4:18PM J29.00010 Thermal spin torque driven by ultrafast heat current in metallic spin-valve structures, GYUNG-MIN CHOI, University of Illinois, BYOUNG-CHUL MIN, Korea Institute of Science and Technology, KYUNG-JIN LEE, Korea University, DAVID CAHILL, University of Illinois — Spin transfer torque (STT), coupling of the angular momentum of the spin of electrons and the magnetization of a ferromagnet, enables the manipulation of nanomagnets with spin currents rather than magnetic fields. STT has been most often realized by passing electrical currents through magnetic layers. Generation of STT by passing a heat current through magnetic layers has been theoretically predicted. This so-called “thermal STT” relies on the transport of thermal energy, as opposed to the transport of electrical charge, and provides new functionality for device applications. Here, we provide direct evidence of thermal STT generated by ps time-scale heat currents on the order of 100 GW m⁻². In metallic spin valve structures, the physical mechanism for thermal STT is the spin-dependent Seebeck effect (SDSE). We create ultrafast heat currents using ps duration pulses of laser light in the NM1/FM1/NM2/FM2 structure: FM1 acts as a spin generation layer by SDSE and FM2 acts as a spin detection layer by STT; NM1 acts as a heat absorbing layer and NM2 acts as a heat sink layer. The magnetization dynamics of FM2 are probed by time-resolved magneto-optic Kerr effect with a time resolution of 1 ps. By incorporating different ferromagnetic layers, which have different signs for SDSE, and varying the thickness of the heat sink layer, we are able to control the sign and magnitude of thermal spin torque.

4:30PM J29.00011 Spin accumulation in out of equilibrium mesoscopic superconductors, DENIS CHEVALLIER, Univ de Leiden, CLEMENT DUTREIX, Univ Paris-Sud 11, MARINE GUICOU, IPHT Saclay, CHARIS QUIAY, MARCO APRILI, Univ Paris-Sud 11, CRISTINA BENA, IPHT Saclay — We study the spin accumulation in a junction between a superconductor and a ferromagnet or a normal metal in presence of a Zeeman magnetic field applied to the superconductor, and when the junction is taken out of equilibrium by applying a voltage bias. We first apply a DC voltage on the junction and show that the spin relaxation time (ns) is larger than the charge relaxation time (ps) inducing a spin-charge separation in the superconductor. Then we calculate the time-dependence of the spin accumulation for an applied AC voltage. We find that the measured spin accumulation depends on the frequency of the applied bias. This dependence allows one to extract directly the spin relaxation time in the superconductor which is in complete agreement with the experimental result.

4:42PM J29.00012 Spin-dependent Otto quantum heat engine based on a molecular substance, WOLFGANG HÜBNER, GEORGIOS LEFKIDIS, CHUANDING DONG, DEBAPRIYA CHAUDHURI, University of Kaiserslautern and Research Center OPTIMAS, LEVAN CHOTORLISHVILI, JAMAL CHATORLISHVILI, J. BERAKDAR, Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany — We explore the potential of single molecules for thermodynamic cycle[2]. To this end we propose two molecular heat engines based on the realistic Ni₄ dimer: a quantum Otto engine and a modified quantum Otto engine for which laser-induced optical excitations substitute for one of the heat-exchange points. For reliable predictions and to inspect the role of spin and electronic correlations we perform fully correlated ab initio calculations of the electronic states and the excited states. We analyze the efficiency and the word output of the derived engines and find an enhancement when the spin degree of freedom is included. We also use the von Neumann entropy to describe correlations and entanglement of the engines during the cycles. Furthermore, we link our results to previous results regarding an isobaric stroke[3] and a magnetic quantum Diesel engine on the same substance[4].


Tuesday, March 3, 2015 2:30PM - 5:30PM – Session J30 GMAG DMP: Focus Session: Magnetic Imaging and Characterization 206B - Yves Idzerda, Montana State University
2:30PM J30.00001 Moment Mapping of bcc Fe$_{1-x}$Mn$_x$ Alloy Films on MgO(001) YVES IDZERDA, HARSH BHATIKAR, Montana State Univ, ELIKE ARENHOLZ, Advanced Light Source — The magnetic moments of ~20 nm single crystal films of compositionally graded Fe$_{1-x}$Mn$_x$ films (0.1 ≤ x ≤ 0.2) grown on MgO(001) are determined by spatially resolved moment mapping using X-ray absorption spectroscopy (XAS) and magnetic circular dichroism (MCD). RHEED measurements confirmed that the growth of Fe$_{1-x}$Mn$_x$ films remained epitaxial and in the bcc phase up to x=0.35 but, like Fe growth, is rotated 45 degrees with respect to the MgO(001) surface net. This is beyond the bulk bcc stability limit of x=0.12. Both magnetometry and XMC measurements show that the net magnetic moment of these alloy films behave similarly to the bulk behavior, with a gradual moment reduction at low Mn concentrations followed by an abrupt departure from the Slater-Pauling curve and disappearance of the moment at x=0.15. By generating a compositional dependence of the reflection total electron yield cross section, we show that the spin polarization is present in the 5nm thick alloy film. In conclusion, we are able to map the Fe spin moment using linear and circular polarized soft X-rays, the local composition and elemental moments can be simultaneously mapped across the surface of the sample. The Fe moment is found to gradually reduce with increasing Mn content with a very abrupt decline at x=0.15. Surprisingly, the Mn moment shows a very small net moment (<0.1 m$_{B}$) at all compositions, suggesting a complicated Mn spin structure.

2:42PM J30.00002 Spectroscopically Resolved Imaging of Spin Dynamics in Ferromagnets Using Nitrogen-Vacancy Centers in Diamond JASON LIU, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, MA SAKI NAGATA, Institute for Chemical Research, Kyoto University, R.D. MCMICHAEL, Center for Nanoscale Science and Technology, National Institute of Standards and Technology — During the past decade, research into nitrogen-vacancy (NV) centers, a known defect in diamonds, has increased in popularity. This popularity is due to the ability to optically prepare and measure the magnetic state of the spin triplet associated with the NV center. Optically, the ground state electrons can be excited by a 532 nm wavelength laser and the fluorescence results in the emission of red photons. Optically detected magnetic resonance (ODMR) is possible because the $m_s = ± 1$ states create weaker fluorescence. Magnetometers with detectivity on the order of 10$^3$ nT/Hz$^{1/2}$ have been demonstrated. In this talk, the design and performance of a scanning diamond NV center magnetometer for magnetization dynamics in ferromagnetic samples will be presented. In this instrument, a microwave magnetic field is used to excite precession in magnetic nanostructures and resulting shifts in the stray field are detected by changes in the ODMR of the diamond NV centers.

2:54PM J30.00003 A nitrogen-vacancy center magnetometer for measuring magnetization dynamics in ferromagnetic nanostructures JASON LIU, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, MA SAKI NAGATA, Institute for Chemical Research, Kyoto University, R.D. MCMICHAEL, Center for Nanoscale Science and Technology, National Institute of Standards and Technology — During the past decade, research into nitrogen-vacancy (NV) centers, a known defect in diamonds, has increased in popularity. This popularity is due to the ability to optically prepare and measure the magnetic state of the spin triplet associated with the NV center. Optically, the ground state electrons can be excited by a 532 nm wavelength laser and the fluorescence results in the emission of red photons. Optically detected magnetic resonance (ODMR) is possible because the $m_s = ± 1$ states create weaker fluorescence. Magnetometers with detectivity on the order of 10$^3$ nT/Hz$^{1/2}$ have been demonstrated. In this talk, the design and performance of a scanning diamond NV center magnetometer for magnetization dynamics in ferromagnetic samples will be presented. In this instrument, a microwave magnetic field is used to excite precession in magnetic nanostructures and resulting shifts in the stray field are detected by changes in the ODMR of the diamond NV centers.

3:06PM J30.00004 Imaging Magnetic Vortices Dynamics Using Lorentz Electron Microscopy with GHz Excitations JYING WANG, CHUNHUI DU, TING TANG, JASON LIU, Center for Nanoscale Science and Technology, National Institute of Standards and Technology — Magnetic vortices in thin films are naturally formed spiral spin configurations with a core polarization pointing out of the film plane. They typically represent ground states with high structural and thermal stability as well as four different chirality-polarity combinations, offering great promise in the development of spin-based devices. For applications to spin oscillators, non-volatile memory and logic devices, the fundamental understanding and precise control of vortex excitations and dynamic switching behavior are essential. The compact dimensionality and fast spin dynamics set grand challenges for direct imaging technologies. Recently, we have developed a unique method to directly visualize the dynamic magnetic vortex motion using advanced Lorentz electron microscopy combined with GHz electronic excitations. It enables us to map the orbit of a magnetic vortex core in a perpendicular square with <5nm resolution and to reveal subtle changes of the gyrotropic motion as the vortex is driven through resonance. Further, in multilayer spin-valve disks, we probed the strongly coupled coaxial vortex motion in the dipolar- and indirect exchange-coupled regimes and unraveled the underlying coherence and modulation. Our approach is complementary to X-ray magnetic circular dichroism and is of general interest to the magnetism community as it paves a way to study fundamental spin phenomena with unprecedented resolution and accuracy. Collaborations with S.D. Pollard, J.F. Pulecio, D.A. Arena and K.S. Buchanan are acknowledged.

3:18PM J30.00005 Direct imaging of interacting vortex orbits and deformations with Lorentz transmission electron microscopy SHAWN POLLARD, State Univ of NY- Stony Brook, Department of Physics and Astronomy, JAVIER PULECIO, YIMEI ZHU, Brookhaven National Laboratory, Condensed Matter Physics and Materials Science Department — Understanding the interactions between confined, interacting magnetic quasiparticles, such as magnetic vortices, is essential towards developing both an understanding of their mutual coupling, as well as limitations for a variety of spintronic devices. However, due to a lack of spatial resolution afforded by traditional techniques, direct observation of the changes of vortex orbits in real space has been lacking. Utilizing high resolution Lorentz TEM, we image the time averaged vortex trajectories in multi-vortex permalloy rectangular and elliptical planes while applying an oscillating in-plane field tuned to the vortex gyrotropic mode. Using an additional in-plane DC field, we observe a transition of the vortex orbits from circular to heavily distorted as the vortices are driven together, a result of increased interaction strength in laterally coupled vortex pairs. Furthermore, in closely spaced vortex pairs, the strong coupling results in a single resonance frequency. As the vortices are moved apart, pinning effects begin to dominate, and the peak frequency is no longer singular. Micromagnetic simulations are utilized to further elucidate the coupled behavior and obtain time-resolved information of the dynamic process.

1Work supported by DOE-BES, Materials Sciences and Engineering Division, under Contract No. DE-AC02-98CH10886.

1Work supported by DOE-BES, Materials Sciences and Engineering Division, under Contract No. DE-AC02-98CH10886.
Using the tip of a low temperature scanning tunneling microscope (STM), we position Fe atoms on a Cu surface. This allows for the study of magnetic lattices built on surfaces, exploring the transition from individual quantum spins to classical magnetism. We report the first three-dimensional mapping of charge-density wave domains in bulk polycrystalline chromium samples using differential-aperture x-ray microdiffraction at the Advanced Photon Source.

NRMFM probe uses a magnet-on-cantilever geometry and is equipped with dual x-y-z piezoelectric motion stages, for micron-step coarse positioning and sub-nanometer fine positioning of both the laser interferometer and the sample with respect to the cantilever, permitting three-dimensional scanning-mode detection of nuclear magnetism. The probe keeps the cantilever detector in high vacuum, maintaining a high Q-factor, while the local NMR properties of nearby aqueous samples in glass microtubes are measured. The entire probe head fits in either a 3.5-cm bore magnet or in an electromagnet with a similarly small gap.

This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357

5:06PM J30.00012 Nucleation and Control of Magnetic Quasi-particles via Extrinsic and Intrinsic Energies1, JAVIER PULECIO, Dept. CMPMS, Brookhaven National Laboratory, PETER WARNICKE, SLS, Paul Scherrer Institute, DARIO ARENA, NSLS, Brookhaven National Laboratory, MI-YOUNG IM, CXRO, LBNL and Dept. Emerging Mater. Science, DGIST, SHAWN POLLARD, Dept. of Phys. and Astro., Stony Brook University, PETER FISCHER, CXRO, LBNL and Dept. Phys., UC Santa Cruz, YIMEI ZHU, Dept. CMPMS, Brookhaven National Laboratory — Magnetic quasi-particles present an excellent opportunity to study fundamental magnetic properties and dynamics. The fine balance of energies including demagnetization, direct exchange, external perturbations, crystalline anisotropy, indirect exchange, and DMI, allows for the nucleation of a diverse ensemble of spin textures such as vortices, merons, and skyrmions, all of which demonstrate unique behavior. We present our investigations of single vortex symmetry breaking under external perturbations and demonstrate a method to determine the core polarity using Lorentz Transmission Electron Microscopy [1]. We also discuss how to tailor the high-frequency dynamics of coupled coaxial vortices using indirect exchange interactions [2]. We conclude by discussing the nucleation of unconventional chiral spin textures in nano-disc heterostructures using a complementary multi-technique approach, i.e. micromagnetic modeling, FMR, MFM, MTXM, and LTEM.

1DOE BES #DE-AC02-98CH10886, DOE BES #DE-AC02-05-CH1231, NRF Korea MEST #2012K1A4A3053565.

5:18PM J30.00013 Single spin relaxometry of spin noise from a ferromagnet, FRANCESCO CASOLA, 1) Harvard-Smithsonian Center for Astrophysics, 60 Garden St., Cambridge, MA 02138, USA, 2) Department of Physics, Harvard University, TOEND DER SAR, Department of Physics, Harvard University, 17 Oxford St., Cambridge, MA 02138, USA, RONALD WALSWORTH, 1) Harvard-Smithsonian Center for Astrophysics, 60 Garden St., Cambridge, MA 02138, USA, 2) Department of Physics, Harvard University, AMIR YACOBY, Department of Physics, Harvard University, 17 Oxford St., Cambridge, MA 02138, USA — The introduction of new schemes for the measurement of spatially resolved dynamic magnetic properties of strongly correlated electrons is essential for the study of condensed matter magnetism and the development of novel spintronic devices. Here we show the possibility to detect the magnetic spin noise produced by a thin (~30 nm) layer of a patterned micro-sized ferromagnet (Ni81Fe19) by optical initialization and read-out of the single spin state of a nearby nitrogen vacancy center (NV) in diamond. For the interpretation of our results, we develop a general framework describing single-spin stray field detection in terms of a filter function sensitive mostly to spin fluctuations with wavevector \( \sim 1/d \), where \( d \) is the NV-ferromagnet distance. Our results pave the way towards quantitative and non-perturbative detection of spectral properties in nanomagnets, establishing NV center magnetometry as an emergent probe of collective spin dynamics in condensed matter [1].


Tuesday, March 3, 2015 2:30PM - 5:30PM —
Session J31 GMAG DMP FIAP: Focus Session: Spin-Dependent Phenomena in Semiconductors: Probing Spins in 2D Materials and Semiconductors 207A - Aubrey Hanbicki, Naval Research Laboratory

2:30PM J31.00001 Tightly bound excitons in monolayer transition metal dichalcogenides, JIE SHAN, Penn State University — Atomically thin transition metal dichalcogenides (TMDs) MX2 (M = Mo, W, X = S, Se, Te) have emerged as a new class of two-dimensional (2D) semiconductors. Monolayer TMDs possess a honeycomb lattice structure with broken inversion symmetry that permits interesting valley dependent optical selection rules and Berry curvature effects. Yet, another very distinctive feature of electrons in 2D semiconductors is the significantly reduced dielectric screening of Coulomb interactions. An important consequence of strong Coulomb interactions is the formation of tightly bound excitons. They significantly modify the optical response of the material and play a defining role in the optoelectronic processes. In this talk, I will discuss our recent experiments on the binding energy of excitons and trions and their spin-valley properties in TMDs.

3:06PM J31.00002 Direct observation of spin-to-charge conversion in MoS2 monolayer with spin pumping, CHENG CHENG, VIKTORIA IVANOVS’KAJA, JUAN-CARLOS ROJAS SANCHEZ, BRUNO DLUBAK, PIERRE SENEOR, Unité Mixte de Physique CNRS/Thales and Université Paris Sud, YOUNG HEE LEE, GANZHEN HAN, CINAP Institute for Basic Science; Department of Energy Science, Sungkyunkwan University, HYUN KIM, CINAP Institute for Basic Science, Sungkyunkwan University, HEEJUN YANG, CINAP Institute for Basic Science; Department of Energy Science, Sungkyunkwan University, ABDELMAJID ANANE, Unité Mixte de Physique CNRS/Thales and Université Paris Sud — Unlike graphene, layered transition-metal dichalcogenides are 2D wide bandgap semiconductors with large intrinsic spin-orbit coupling (SOC) and valley-spin coupling, which makes them a unique playground for spintronics. We present here the first demonstration of spin injection into monolayer MoS2 with spin pumping from a 3D ferromagnetic (FM) film, circumventing the impedance mismatch at the metal-semiconductor interface. We measured the transverse voltage generated by spin-to-chARGE current conversion in MoS2 with broadband (3 GHz-9 GHz) ferromagnetic resonance (FMR) setup. The observed symmetric Lorentzian signals are in \( \mu \)V range under small rf excitations well below 1 Oe. This voltage magnitude is unexpected for inverse spin Hall effect and is interpreted in the frame of inverse Rashba-Edelstein effect (iREE) due to strong SOC in MoS2. By applying a moderate gate voltage (up to 10 V) on the MoS2/FM multilayer, we observe clear modulation (up to 30%) of the linewidth and amplitude of the iREE signal, indicating electrical tuning of the spin mixing conductance.

3:18PM J31.00003 Proximity Induced Exchange Splitting in Graphene1, SHANSHAN SU, Department of Electrical and Computer Engineering, University of California, Riverside, YAPIS BARLAS, Department of Physics and Astronomy, University of California, Riverside, ROGER LAKE, Department of Electrical and Computer Engineering, University of California, Riverside — We perform an ab-initio study of the proximity effect in a two-dimensional (2D) heterostructure composed of graphene and a thin film ferromagnetic insulator (europium oxide, EuO). Two different structures are considered i) graphene on a EuO layer and ii) graphene sandwiched between two EuO layers. Both structures show two-fold degenerate low-energy bands at the \( \Gamma \) point in the Brillouin zone, however, the former heterostructure shows a clear energy gap in the spectrum whereas the latter exhibits degenerate band crossings. The two different spectra result from a competition of proximity induced exchange splitting on the graphene sheet and sub-lattice mass induced due to the crystal field effect. Addition of spin-orbit coupling in the sandwiched structure indicates lifting of this two-fold degeneracy leading to band anti-crossings if the inversion symmetry perpendicular to the graphene plane is broken.

1This work was supported as part of the Spins and Heat in Nanoscale Electronic Systems (Spins) an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award #DE-SC0012670.
3:30PM J31.00004 Gate-voltage controlled spin pumping effects: spin injection from YIG and Co into metal and graphene based 2D materials. ALAN KALITSY, MINT Center, University of Alabama, Tuscaloosa, AL, USA. MAIRBEK CHSHIEV, SPINTEC, UMR (8191) CEA/CNRS/UJF/Grenoble INP, INAC, 17 rue des Martyrs, 38054 Grenoble Cedex, France. OLEG MRYASOV, MINT Center, University of Alabama, Tuscaloosa, AL, USA. — Spin current injection into nonmagnetic semiconductors and oxides is crucial component of spintronics. The spin pumping mechanism free from the impedance mismatch is a promising way to inject spin current into nonmagnetic materials [1]. Here we present theory of spin current injected into non-magnetic films which arises from magnetization precession. We apply this theory to two cases: (i) insulating yttrium iron garnet ferromagnet/nonmagnetic metal interfaces and (ii) hcp-Co/single layer graphene interface. The electron transport calculations are based on the non-equilibrium Green Function formalism within the tight binding Hamiltonian model [2]. We show that magnitude of the pumped spin current can be efficiently controlled by the gate voltage.


3:42PM J31.00005 Cross-correlation spin noise spectroscopy of interacting multi-component spin systems. LUI YANG, DIBYENDU ROY, SCOTT CROOKER, NIKOLAI SINITSYN, Los Alamos National Laboratory — Interacting multi-component spin systems are ubiquitous in semiconductor spintronics; e.g. carrier-mediated ferromagnetism in magnetic semiconductors, or electronic spin coupling to nuclear spin baths. Traditionally, inter-species spin interactions are studied by experimental methods that are necessarily perturbative; e.g. by intentionally polarizing or depolarizing one spin species and detecting the response of the other. Here, we show that multi-probe spin noise spectroscopy can reveal interspecies spin-spin interactions — under conditions of strict thermal equilibrium — by cross-correlating the stochastic fluctuation signals exhibited by each of the constituent spin species. We develop a theory for such noise cross-correlations in thermal equilibrium. As a proof of principle, we compare the results with an experimental study of a well-understood interacting spin system — a mixture of warm Rb and Cs vapors — by applying a new type of two-color spin noise spectroscopy [1,2]. Noise correlations directly reveal the presence of inter-species spin-spin interactions. Such non-invasive and noise-based techniques should be generally applicable to any multi-component spin system in which the fluctuations of the constituent components are detectable.


3:54PM J31.00006 A method for wide-bandwidth spin noise measurements without a large background1, BRENNAN C. PURSLEY, XINLIN SONG, Applied Physics Program, University of Michigan, Ann Arbor, MI, USA, VANESSA SIH, Department of Physics, University of Michigan, Ann Arbor, MI, USA — Spin noise measurements have rapidly evolved over the last few decades to become a class of highly sensitive characteristic tools [1,2]. Presently used methods, though quite sensitive, suffer from large backgrounds. We report on an experiment that yields signal proportional to the spin noise, without further processing. Our demonstration utilizes ultrafast optical techniques, but the signal processing could also be applied to pulsed electrical measurements. We will discuss the experiment, necessary equipment, and data sets from a GaAs sample.


4:06PM J31.00007 Detection of quantum entanglement using cross-correlation spin noise spectroscopy. DIBYENDU ROY, Max Planck Institute for the Physics of Complex Systems, NIKOLAI A. SINITSYN, Theoretical Division, Los Alamos National Laboratory — Nature of spin-spin correlations between two interacting spin subsystems in thermal equilibrium can be probed using cross-correlation spin noise spectroscopy [1] with two linearly polarized off-resonant laser beams of different wavelength. Here we propose to use such cross-correlator of spins to detect and quantify quantum correlations such as quantum entanglement between the spin subsystems. We demonstrate our proposal for interacting quantum dots.


4:18PM J31.00008 Effects of Strain and Quantum Confinement in Optically Pumped Nuclear Magnetic Resonance in GaAs: Interpretation Guided by Spin-Dependent Band Structure Calculations, CLIFFORD BOWERS, RYAN WOOD, SAHA DIPTA, JOHN TOKARSKI, LAUREN MCCARTHY, GARY SANDERS, CHRISTOPHER STANTON, Univ of Florida - Gainesville, STEPHEN MCGILL, ARNEIL REYES, PHIL KUHNS, National High Magnetic Field Laboratory FSU, JOHN RENO, Sandia National Laboratories. — Magnetic Resonance in GaAs: Interpretation Guided by Spin-Dependent Band Structure Calculations — A combined experimental-theoretical study of optically pumped NMR (OPNMR) has been performed in a GaAs/AlGaAs quantum well film bonded to a Si substrate with thermally induced biaxial strain. The photon energy dependence of the Ga OPNMR signal was recorded at magnetic fields of 4.9 and 9.4 T at a temperature of 4.8-5.4 K. The data were compared to the nuclear spin polarization calculated from the differential absorption to spin-up and spin-down states of the electron conduction band using a modified Pidgeon Brown model. Comparison of theory with experiment facilitated the assignment of features in the OPNMR energy dependence to specific interband Landau level transitions. The results provide insight into how effects of strain and quantum confinement are manifested in optical nuclear polarization in semiconductors.

4:30PM J31.00009 Orbital Angular Momentum Imprints Studied Using Optical Vortex Pumpprobe Spectroscopy1, M. A. NOYAN, A. L. EXARHOS, J. M. KIKKAWA, Department of Physics and Astronomy, University of Pennsylvania — We introduce a second generation magneto-optical spectroscopy based on orbital angular momentum of light. Our technique is analogous to methods such as time resolved Faraday/Kerr rotation, but instead of utilizing photon spin, we use holographic gratings to pump and probe materials using photons carrying orbital angular momentum (OAM). We will discuss our first time resolved experiments studying pump-induced OAM dichroism in bulk semiconductors. 100 fs pump pulses with alternating orbital angular momentum ±h create OAM imprints whose momentum distributions resemble right- or left-handed “whirlpools” or vortices. The OAM memory of the sample is then measured using a probe beam whose ±h OAM components are detected in a balanced photodiode bridge. We find that in n-GaAs, the dynamical OAM signal shows a unique timescale when compared to population and spin dynamics and, surprisingly, lasts considerably longer than the momentum scattering time. This method should be of further interest for studying non-equilibrium dynamics in a variety of orbitally coherent systems.

1 We gratefully acknowledge support from NSF DMR-1206270.
4:42PM J31.00010 Room-Temperature Magneto-Optical Phenomena in Organo-Metal Halide Perovskites. — TING WU, YU-CHE HSIAO, MINGXING LI, Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee, 37996, USA, NAM-GOO KANG, JIMMY MAYS, Department of Chemistry, University of Tennessee, Knoxville, Tennessee, 37996, USA, BIN HU, Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee, 37996, USA — Organo-metal halide perovskites have become extremely interesting light-emitting, photovoltaic and lasing materials. The first magneto-optical phenomena, namely magneto-absorption effects, were reported in 1994 for very low temperature and high field (20 Tesla). Here, we report room-temperature magneto-optical phenomena at low field (<200 mT) from such perovskites. We find that room-temperature magneto-optical effects require high excitation intensity. At high excitation intensities we can observe magnetic field effects on photoluminescence, photocurrent, and electroeluminescence. The magneto-optical phenomena indicate that both light-emitting and photovoltaic responses undergo a spin-dependent process. Furthermore, at low excitation intensities organo-metal halide perovskites exhibit negligible magnetic field effects. Therefore, we can conclude that the magneto-optical phenomena are from spin-dependent charge recombination in light-emitting and photovoltaic processes. This presents a new mechanism to control the light-emitting and photovoltaic functions in organo-metal halide perovskites by using spins. This presentation will discuss the key parameters in controlling magneto-optical phenomena in organo-metal halide perovskites.

4:54PM J31.00011 Laser-induced ultrafast spin dynamics and ERASE functionality on quasi-linear molecular ions. — GEORGIOS LEFKIDIS, University of Kaiserslautern and Research Center OPTIMAS, CHUN LI, SHAOBIN ZHANG, Northwestern polytechnical University, Xi’an, China, WOLFGANG HÜBNER, University of Kaiserslautern and Research Center OPTIMAS — We present an ab initio investigation of the A-process-based ultrafast spin manipulation on positively charged two-magnetic-center molecular ions bridged by non-magnetic oxygen [1]. Multiple derived spin-switching and spin-transfer scenarios on the quasi-linear structure [Fe-O-Co]⁺ are used to build two closed, reversible spin-dynamics cycles with respect to the spin localization and orientation. A mechanism addressing the “ERASE” functionality is proposed by properly exploiting the irreversibility of some laser-induced spin-manipulation scenarios, and the resulting Shannon entropy change is analyzed. We compare with a previously suggested mechanism based on chirped laser pulses [2]. Such controllable spin-dynamics cycles and logic functionality demonstrate promising applications in the design of spintronic devices on isolated magnetic molecule [3].

3:06PM J32.00002 Influence of structural asymmetries on LaNiO$_3$-LaMnO$_3$ interfaces, MARTA GIBERT, University of Geneva, MICHEL VIRET, CEA Saclay, PAULO ZUBKOF, UCL London, SARA CATALANO, University of Geneva, CINTHIA PIAMON-TEZE, SLS-PSI, NICOLAS JAOUEN, SOLEIL, JEAN-MARC TONNERRE, CNRS, Instiut Neel, ALMUDENA TORRES-PARDO, Complutense University of Madrid, ALEX GLOTER, ODILE STEPHAN, University of Paris-Sud, JEAN-MARC TRISCONE, University of Geneva — Complex electronic reconstruction at interfaces between transition metal oxides play a key role on the emergence of novel functionalities in these materials. In this context, we reported on the observation of exchange bias in superlattices composed of nominally paramagnetic metallic LaNiO$_3$ and semiconducting ferromagnetic LaMnO$_3$ ultrathin layers [1], which exemplifies how interface engineering can induce a magnetic structure in LaNiO$_3$. Here, we investigate the properties of LaNiO$_3$-LaMnO$_3$ bilayers, i.e. SrTiO$_3$/LaNiO$_3$/LaMnO$_3$. TEM images have shown that the interface LaNiO$_3$/LaMnO$_3$ is sharper than the LaMnO$_3$/LaNiO$_3$ one, which displays two monolayers intermixing. This structural asymmetry results in very distinct properties: enhanced conductivity and extremely reduced magnetization is observed for the "sharp interface" samples in contrast to the rough ones. State-of-the-art synchrotron techniques reveal differences in interfacial charge transfer and induced magnetic moments in the Ni atoms, and allow us to reproduce the magnetic profile of each LMO layer. The role of orbital occupation will also be explored.


3:18PM J32.00003 ABSTRACT WITHDRAWN

3:30PM J32.00004 Charge and Strain Control of Interface Magnetism, M.R. FITZSIMMONS, LANL, K. DUMESNIL, Institut Jean Lamour, N. JAOUEN, Synchrotron SOLEIL, T. MAROUTIAN, G. AGNUS, Université Paris-Sud, J.-M. TONNERRE, Université Grenoble Alpes, B. KIRBY, NIST, E. FOHTUNG, NMSU, B. HOLLADAY, E.E. FULLERTON, O. SHPYRKO, S.K. SINHA, UCSD, Q. WANG, A. CHEN, Q.X. JIA, LANL — We studied the influence of an electric field applied to an La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO) layer in a LSMO/Pb$_{2/3}$Sr$_{1/3}$TiO$_3$ (PZT)/Nb-doped SrTiO$_3$ (STO) heterostructure by measuring its magnetization depth profile using resonant x-ray magnetic reflectivity. The saturation magnetization of the ferromagnetically-ordered LSMO was not affected by the direction of the polarization of the PZT. However, the ferromagnetic thickness and magnetization of the LSMO film at remanence were reduced for hole-charge accumulation at the LSMO/PZT interface. To understand the independent roles of strain and hole-doping, we performed neutron scattering experiments of La$_{1-x}$Sr$_x$MnO$_3$ films grown on Nb-doped STO in which bending strain (via 4-point bending jig) or electric field (via parallel plate capacitor) was applied to the films. We observed that bending strain affects the saturation magnetization of the LSMO film, whereas electric field affects the remnant magnetization of the film. These observations suggest strain may be a more effective means to control magnetism than charge.

3:42PM J32.00005 Mapping magnetism with atomic resolution using aberrated electron probes, JUAN IDROBO, Oak Ridge National Laboratory, JAN RUSZ, Uppsala University, MICHAEL A. MCGUIRE, CHRISTOPHER T. SYMONS, RANGA RAJU VATSAVAI, ANDREW R. LUPINI, Oak Ridge National Laboratory — In this talk, we report a direct experimental real-space mapping of magnetic circular dichroism with atomic resolution in aberration-corrected scanning transmission electron microscopy (STEM). Using an aberrated electron probe with customized phase distribution, we reveal with electron energy-loss (EEL) spectroscopy the checkerboard antiferromagnetic ordering of Mn moments in La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO)/La$_{0.7}$Sr$_{0.3}$FeO$_3$ (LSFO) heterostructures. The results in a magnetic circular dichroic signal with intrinsically larger signal-to-noise ratios than those obtained via nanodiffraction techniques (where most of the transmitted electrons are discarded). The novel experimental setup presented here, which can easily be implemented in aberration-corrected STEM, opens new paths for probing dichroic signals in materials with unprecedented spatial resolution.

3:54PM J32.00006 Insight into spin transport in oxide heterostructures from interface-resolved magnetic mapping, M.N. GRISOLIA, F.Y. BRUNO, C. VISANI, Unite Mixte de Physique CNRS/Thales, 91767 Palaiseau (FRANCE) and Université Paris-Sud, 91405 Orsay (FRANCE), S. VALENCIA, R. ABRUDAN, A.A. UNAL, Helmholtz-Zentrum Berlin, 12489 Berlin (GERMANY), M. VARELA, J. TORNOS, A. RIVERA-CAZALDA, Z. SFEIRIOUI, C. LEON, J. SANTAMARIA, U. Complutense 28040 Madrid (SPAIN), S. J. PENNYCOOK, The University of Tennessee, TN 37996 (USA), J.E. VILLEGES, A. BARTHELEMY, M. BIBES, Unite Mixte de Physique CNRS/Thales, 91767 Palaiseau (FRANCE) and Université Paris-Sud, 91405 Orsay (FRANCE) — At interfaces between complex oxide materials, orbital and magnetic reconstructions may produce states of matter absent from the materials involved, offering novel possibilities for electronic and spintronic devices. Here we show that magnetic reconstruction has a strong influence on spin transport. In epitaxial heterostructures combining layers of antiferromagnetic LaFeO$_3$ (LFO) and ferromagnetic La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO), we find that a net magnetic moment is induced in the first few unit planes of LFO near the interface with LSMO. Using X-ray photoemission electron microscopy, we show that the ferromagnetic domain structure of the LMO electrodes is imprinted into the antiferromagnetic tunnel barrier, endowing it with spin selectivity. Finally, we find that coexisting ferromagnetic and antiferromagnetic interactions strongly influence the tunnel magnetoresistance of LSMO/LFO/LSMO junctions through competing spin polarization and spin filtering effects.

4:06PM J32.00007 Exchange coupling in (111)-oriented La$_{0.7}$Sr$_{0.3}$MnO$_3$/La$_{0.7}$Sr$_{0.3}$FeO$_3$ superlattices, YUE JIA, RAJESH CHOPDEKAR, Department of Chemical Engineering and Materials Science, Univ. of California, Davis, ELKE ARENHOLZ, ANTHONY YOUNG, MATTHEW MARCUS, ANDREAS SCHOLL, Advanced Light Source, Lawrence Berkeley National Laboratory, YAYOI TAKAMURA, Department of Chemical Engineering and Materials Science, Univ. of California, Davis — Epitaxial La$_{0.7}$Sr$_{0.3}$MnO$_3$/La$_{0.7}$Sr$_{0.3}$FeO$_3$ (LSFO) superlattices serve as ideal systems to explore the magnetic structure and exchange coupling in (111)-oriented perovskite oxides. The (111) orientation offers a buckled honeycomb structure resembling that of graphite with the stacking of highly polar layers. Furthermore, the bulk LSFO magnetic structure predicts that the (111) interface should have fully uncompensated antiferromagnetic (AF) moments leading to exchange bias interactions. Detailed soft x-ray magnetic spectroscopy and microscopy reveal that interfacial effects and the ultrathin nature of the sublayers of the superlattices can stabilize orientations of the LSFO AF spin axis which differ from that of LSFO films and LSMO/LSFO bilayers. A portion of the interfacial AF moments can be reoriented to an arbitrary direction by a moderate external magnetic field through spin-flop coupling with the ferromagnetic LSMO sublayers with low magnetocrystalline anisotropy in the (111) plane.

4:18PM J32.00008 ABSTRACT WITHDRAWN

4:30PM J32.00009 ABSTRACT WITHDRAWN
4:42PM J32.00010 Signatures of a Two-Dimensional Ferromagnetic Electron Gas at the La$_{0.5}$Sr$_{0.5}$MnO$_3$/SrTiO$_3$ Interface Arising From Orbital Reconstruction$^3$, MARIA J. CALDERON, IMCM-CSIC, NORBERT NEMES, JUAN IGNACIO BELTRAN, FLAVIO BRUNO, JAVIER GARCIA-BARRIOCANAL, ZOHAIR SEFRIOU, CARLOS LEON, Universidad Complutense de Madrid, MAR GARCIA-HERNANDEZ, CARMEN MURGZ, LUIS BREY, IMCM-CSIC, JACOBO SANTAMARIA, Universidad Complutense de Madrid — The interface between two different oxides has properties different from the ones corresponding to the constituent layers in bulk. Different orders can arise due to the complexity of these materials in which the orbital degree of freedom, magnetism and lattice are strongly interdependent. Here we present a joint theoretical-experimental effort to understand the properties of a multilayer formed by a metallic ferromagnetic manganese oxide (La$_{0.5}$Sr$_{0.5}$MnO$_3$) and the insulating SrTiO$_3$. Magnetoresistance measurements as a function of the relative angle between the magnetic field and the interface plane have shown an unexpected in-plane peak. Calculations of resistivity in a model system including spin-orbit coupling reveal that the unexpected in-plane maximum is due to transport through a two-dimensional ferromagnetic electron gas formed by orbital reconstruction at the manganite interface. These orbital and magnetic reconstructions are supported by X-ray linear dichroism and ab-initio calculations. Advanced Materials DOI:10.1002/adma.201402829.


5:06PM J32.00012 Observation of a Three-Dimensional Quasi-Long-Range Charge Order in YBa$_2$Cu$_{3-x}$O$_7-/La$_{0.7}$Ca$_{0.3}$MnO$_3$ Heterostructures, THOMAS MION, JUNFENG HE, Boston College, PADRAIC SHAFER, Lawrence Berkeley National Laboratory, VU THANH TRA, National Chiao Tung University, QING HE, JIUNN-YUAN LIN, Lawrence Berkeley National Laboratory, YING-HAO CHU, Academia Sinica, ELKE ARENHOLZ, Lawrence Berkeley National Laboratory, RUIHUA HE, Boston College — Heterostructures with strong interfacial effects can exhibit novel physical properties non-existent in either of the constituent materials alone. In particular, striking phenomena are observed when materials with mutually incompatible order parameters are put together by interface control on the atomic level. YBa$_2$Cu$_{3-x}$O$_7-/La$_{0.7}$Ca$_{0.3}$MnO$_3$ (YBCO/LCMO) heterostructures, which are high temperature superconducting and a ferromagnet, respectively, have been observed to exhibit novel phenomena not present in either material alone. The proximity effect between superconductivity and ferromagnetism is a three-dimensional quasi-long-range charge order that is generated exclusively at the interface. Here, we report on a new electronic order in this system which competes with superconductivity. It is a three-dimensional quasi-long-range charge order, distinct from the recently observed two-dimensional charge order in bulk YBCO. Our finding contributes to establishing YBCO/LCMO heterostructures as a unique material platform in which superconductivity, charge order and ferromagnetism coexist and interact with each other.

4:54PM J32.00011 Emergent ferromagnetism in NdMnO$_3$/SrMnO$_3$ superlattices, ARTUR GLAVIC, STUART CALDER, Quantum Condensed Matter Division; Oak Ridge National Laboratory, VALENTINO COOPER, HEMANT DIXIT, Materials Science and Technology Division; Oak Ridge National Laboratory — The phenomenon of ferromagnetism evolving in digital superlattices of two antiferromagnets LaMnO$_3[n]$/SrMnO$_3[n]$ has been well established [1-2]. We show that this interface effect can be observed in systems with different rare earth manganites as well, exemplified in the Nd system grown on LSAT and TBsO$_3$ substrates. With polarized neutron reflectometry we prove that not only 2/1 unit cell samples become ferromagnetic but that interface ferromagnetism can be induced whenever a single layer of SrMnO$_3$ is introduced in the NdMnO$_3$ system. These results show that the strain state of the superlattice system is of much less importance for the induced magnetization then the Mn$^{3+}$/Mn$^{4+}$ electronic state.


5:18PM J32.00013 The Electrophoretic-like Mechanism of Huge Current effect in Electronically Phase Separated Manganite Wires, LIFENG YIN, WENGANG WEL, JIAN SHEN, State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai 200433, China — Electronically phase separated (La, Pr)CaMnO$_3$ manganite wires are found to exhibit huge current effect. As the current density increase, the resistivity of wires decreases dramatically, and the metal-insulator transition temperatures get enhanced. However, the superconducting Quantum Interference Device measurements show that the magnetizations with current on and off are almost identical. It is further confirmed by magnetic force microscope measurements, i.e. the current only changes the shape of ferromagnetic domain, while not the volume of ferromagnetic domain. The results conform to a phenomenological model in which the inherent nanoscale insulating and metallic domains are rearranged through electrophoretic-like processes to open and close percolation channels.
2:54PM J33.00003 Input spike trains suppress chaos in balanced neural circuits, RAINER ENGELKEN, MICHAEL MONTEFORTE, FRED WOLF, Max Planck Institute for Dynamics and Self-Organization — A longstanding hypothesis claims that structured input in neural circuits enhances reliability of spiking responses. While studies in single neurons well support this hypothesis [Mainen, Sejnowski 1995] the impact of input structure on the dynamics of recurrent networks is not well understood. Earlier studies of the dynamic stability of the balanced state used a constant external input [van Vreeswijk, Sompolinsky 1996, Monteforte, Wolf 2010] or white noise [Lajoie et al. 2014]. We generalize the analysis of dynamical stability for balanced networks driven by input spike trains. An analytical expression for the Jacobian enables us to calculate the full Lyapunov spectrum. We solved the dynamic equations using the fixed point attractor method to extract the production rate and attractor dimension. We examined the transition from constant to stochastic input in various scenarios. We find a suppression of chaos by input spike trains. We also find that both independent bursty input spike trains and common input more strongly reduces chaos in spiking networks. Our study extends studies of chaotic rate models [Molgedey et al. 1992] to spiking neuron models and opens a novel avenue to study the role of sensory streams in shaping the dynamics of large networks.

3:06PM J33.00004 Low-dimensional stochastic dynamics underlie the emergence of spontaneous movement in electric fish1, ALEXANDRE MELANSON, Univ of Ottawa, JAMES J. JUN, Janelia Farm, JORGE F. MEJIAS, New York University, LEONARD MALER, ANDRE LONGTIN, Univ of Ottawa — Observing unconstrained animals can lead to simple descriptions of complex behaviours. We apply this principle here to infer the neural basis of spontaneous movements in electric fish. Long-term monitoring of fish in freely swimming, stimuli-free conditions has revealed a sequence of behavioural states that alternate randomly between periods of activity, movement, high active sensing rate) and inactivity (no movement, low active sensing). We show that key features of this sequence are well captured by a 1-D diffusion process in a double well energy landscape, where we assume the existence of a slow variable that modulates the relative depth of the wells. Model validation is two-fold: i) state duration distributions are well fitted by exponential mixtures, indicating non-stationary transition rates in the switching process. ii) Monte Carlo simulations with progressive tilting of the double well is consistent with the observed transition triggered average. We interpret the stochastic variable of this dynamical model as a decision-like variable that, upon reaching a threshold, triggers the transition between states. Thus we identify threshold crossing as a possible mechanism for spontaneous movement initiation and offer a dynamical explanation for slower behavioural changes.

3:18PM J33.00005 Millisecond-Scale Motor Encoding in a Cortical Vocal Area1, ILYA NEMENMAN, Emory University, CLAIRE TANG, University of California, San Francisco, DIALA CHEHAYEB, Emory University, KYLE SRIVASTAVA, Georgia Institute of Technology and Emory University, SAMUEL SOBER, Emory University — Studies of motor control have almost universally examined firing rates to investigate how the brain shapes behavior. In principle, however, neurons could encode information through the precise temporal patterning of their spike trains as well as (or instead of) through their firing rates. Although the importance of spike timing has been demonstrated in sensory systems, it is largely unknown whether timing differences in motor areas could affect behavior. We tested the hypothesis that significant information about trial-by-trial variations in behavior is represented by spike timing in the songbird vocal motor system. We found that neurons in motor cortex convey information via spike timing far more often than via spike rate and that the amount of information conveyed at the millisecond timescale greatly exceeds the information available from spike counts. These results demonstrate that information can be represented by spike timing in motor circuits and suggest that timing variations evoke differences in behavior.

3:30PM J33.00006 Mechanical Surface Waves Accompany Action Potential Propagation, BERNAMIN MACHTA, Lewis Sigler Institute, Princeton University, AHMED EL HADY, Princeton Neuroscience Institute, Princeton University — The action potential (AP) is the basic mechanism by which information is transmitted along neuronal axons. Although the excitability nature of axons is understood to be primarily electrical, many experimental studies have shown that a mechanical displacement of the axonal membrane co-propagates with the electrical signal. While the experimental evidence for co-propagating mechanical waves is diverse and compelling, there is no consensus for their physical underpinnings. We present a model in which these mechanical displacements arise from the driving of mechanical surface waves, in which potential energy is stored in elastic deformations of the neuronal membrane and cytoskeleton while kinetic energy is stored in the movement of the axoplasmic fluid. In our model these surface waves are driven by the traveling wave of electrical depolarization that characterizes the AP, altering the electrostatic forces across the membrane as it passes. Our model allows us to predict the shape of the displacement that should accompany any traveling wave of voltage, including the well-characterized AP. We expect our model to serve as a framework for understanding the physical origins and possible functional roles of these AWs in neurobiology. See Arxiv/1407.7600

3:42PM J33.00007 Stimulation reveals structural drivers of dynamic brain reorganization, SARAH MULDOON, Univ of Pennsylvania and US Army Research Laboratory, JEAN VETTEL, US Army Research Laboratory, DANIELLE BASSETT, Univ of Pennsylvania — Understanding the brain as a complex network of interacting components can provide insight into cognitive function. From this perspective, one can study two types of networks: the anatomical network composed of physical connections between neurons or brain regions, and the functional networks constructed from coherent neurophysiological activity. However, the relationship between these two types of networks is far from understood. Do underlying anatomical networks drive functional networks and if so how? Theoretical predictions from linear models suggest that stimulation of certain brain regions can more easily move the brain into different states, forming a type of “control.” Yet, the brain is far from a linear system. Using a nonlinear model of brain activity derived from diffusion spectrum imaging of white matter connectivity and Wilson-Cowan dynamics, we test the relationship between regional connectivity patterns and the ability of regional stimulation to impart change in functional network configurations. We find that local regional connectivity relates to network controllability and that the system is sensitive to perturbations in the underlying network structure.

3:54PM J33.00008 Cell fate variation of neural stem cells treated with carbon nanotubes1, MASSOOMA GIRBHAI, SABRINA JEDLICKA, Lehigh University, MING ZHENG, National Institute of Standards and Technology, SLAVA V. ROTKIN, Lehigh University — Delivery of materials, such as drug compounds or imaging agents for treatment or diagnosis of disease still presents a biomedical challenge. Nanotechnological advances have presented biomedicine with a number of agents that possess the appropriate size and chemistry to pass through the blood brain barrier. Functionalized carbon nanotubes are one such agent, which can potentially aid in drug and gene delivery to the central nervous system. In addition, carbon nanotubes have already been applied in several areas of nerve tissue engineering to probe and augment cell behavior, and to track subcellular components, and to study the growth and organization of neural networks. Although the production of functionalized carbon nanotubes has escalated in recent years, knowledge of cellular changes associated with exposure to these materials remains unclear. In this study, cellular phenotypes such as proliferation, growth and differentiation in C17.2 neural stem cells have been tested when treated with single-walled carbon nanotubes functionalized with synthetic ssDNA and RNA. The research has shown irregular behavior in the cell fate which could be due to changes in the cytoskeletal filaments. These results would be worth considering when developing strategies to deliver components to the central nervous system.

1 Funded by NSERC

1 Funded by NSF ECCS-120239
4:06PM J33.00009 Chimera States in a Hodgkin-Huxley Model of Thermally Sensitive Neurons , TERA GLAZE, SCOTT LEWIS, University of Missouri at St. Louis, KENNETH SHOWALTER, West Virginia University, SONYA BAHAR, University of Missouri at St. Louis — Chimera states, in which identically coupled groups of nonlinear oscillators exhibit very different dynamics, with one group performing synchronized oscillations and the other group showing desynchronized behavior, have recently been studied in computational models. Chimera states have also been demonstrated experimentally in optical and chemical systems. The behavior is particularly relevant in the context of neural synchronization, given the phenomenon of unihemispheric sleep in many animal species, including some mammals, and the recent observation of asymmetric sleep in human patients with sleep apnea. Here, we characterize chimera states using the Huber-Braun neural model, a Hodgkin-Huxley-like model of thermally sensitive neurons. We identify parameter regimes which exhibit chimera behavior and phase cluster states, both in a system with Abrams-Strogatz (mean field) coupling and in a system with Kuramoto (distance-dependent) coupling.

4:18PM J33.00010 Coordinated encoding between cell types in the retina: insights from the theory of phase transitions1 , TATYANA SHARPEE, Salk Institute for Biological Studies — In this talk I will describe how the emergence of some types of neurons in the brain can be quantitatively described by the theory of transitions between different phases of matter. The two key parameters that control the separation of neurons into subclasses are the mean and standard deviation of noise levels among neurons in the population. The mean noise level plays the role of temperature in the classic theory of phase transitions, whereas the standard deviation is equivalent to pressure, in the case of liquid-gas transitions, or to magnetic field for magnetic transitions. Our results for the form of a fusion, two recent discoveries of new types of ON and OFF ganglion cells, as well as the absence of multiple types of ON cells. We further show that, across visual stimulus contrasts, retinal circuits continued to operate near the critical point whose quantitative characteristics matched those expected near a liquid-gas critical point and described by the nearest-neighbor Ising model in three dimensions. Because the retina needs to operate under changing stimulus conditions, the observed parameters of cell types corresponded to metastable states in the region between the spinodal line and the line describing maximally informative solutions. Such properties of neural circuits can maximize information transmission in a given environment while retaining the ability to quickly adapt to a new environment.

1 NSF CAREER award 1254123 and NIH R01EY019493

4:54PM J33.00011 Optogenetic stimulation of a meso-scale human cortical model , PRASHANTH SELVARAJ, ANDREW SZERI, UC Berkeley, JAMIE SLEIGH, Waikato Clinical School, HEIDI KIRCH, UC San Francisco — Neurological phenomena like sleep and seizures depend not only on the activity of individual neurons, but on the dynamics of neuron populations as well. Meso-scale models of cortical activity provide a means to study neural dynamics at the level of the population of neurons. Additionally, they offer a safe and economical way to test the effects and efficacy of stimulation techniques on the dynamics of the cortex. Here, we use a physiologically relevant meso-scale model of the cortex to study the hypersynchronous activity of neuron populations during epileptic seizures. The model consists of a set of stochastic, highly non-linear partial differential equations. Next, we use optogenetic stimulation to control seizures in a hyperexcited cortex, and to induce seizures in a normally functioning cortex. The high temporal resolution this method offers makes a strong case for the use of optogenetics in treating meso scale cortical disorders such as epileptic seizures. We use bifurcation analysis to investigate the effect of optogenetic stimulation in the meso scale model, and its efficacy in suppressing the non-linear dynamics of seizures.

5:06PM J33.00012 Pore opening dynamics in the exocytosis of serotonin1 , GUILLERMO RAMIREZ-SANTIAGO, Universidad Nacional Autonoma de Mexico, MONTSERRAT C. CERCON, Consejo Nacional de Ciencia y Tecnologia, ALEJANDRO MARTINEZ-VALENCIA, ISRAEL SALINAS HERNANDEZ, LEONARDO RODRIGUEZ-SOSA, FRANCISCO F. DE-MIGUEL, Universidad Nacional Autonoma de Mexico — The current view of the exocytosis of transmitter molecules is that it starts with the formation of a fusion pore, which is a transient channel that connects the intravesicular and the extravesicular spaces, and is completed by the release of the rest of the transmitter contained in the vesicle upon the full fusion and collapse of the vesicle with the plasma membrane. However, under certain circumstances, a rapid closure of the pore before the full vesicle fusion produces only a partial release of the transmitter. Here we show that whole release of the transmitter occurs through fusion pores that remain open for tens of milliseconds without vesicle collapse. This was demonstrated through amperometric measurements of serotonin release from electrodense vesicles in the axon of leech Retzius neurons and mathematical modelling. By modeling transmitter release with a diffusion equation subjected to boundary conditions that are defined by the experiment, we showed that those pores with a fast half time constant remained opened and allowed the full quantum release without vesicle collapse, whereas pores with a slow rise time constant closed rapidly, thus producing partial release. We conclude that a full transmitter release may occur through the fusion pore in the absence of vesicle collapse.

1 This work was founded by a DGAPA-UNAM grants IN200914 and IN118410 CONACYT GRANT 130031, and CONACyT doctoral fellowships.

5:18PM J33.00013 Synaptic connectivity and spatial memory: a topological approach , RUSSELL MILTON, UT Houston, ANDREY BABICHEV, Rice University, YURI DABAGHIAN, Rice University, Baylor College of Medicine — In the hippocampus, a network of place cells generates a cognitive map of space, in which each cell is responsive to a particular area of the environment — its place field. The peak response of each cell and the size of each place field have considerable variability. Experimental evidence suggests that place cells encode a topological map of space that serves as a basis of spatial memory and spatial awareness. Using a computational model based on Persistent Homology Theory we demonstrate that if the parameters of the place cells spiking activity fall inside of the physiological range, the network correctly encodes the topological features of the environment. We next introduce parameters of synaptic connectivity into the model and demonstrate that failures in synapses that detect coincident neuronal activity lead to spatial learning deficiencies similar to the ones that are observed in rodent models of neurodegenerative diseases. Moreover, we show that these learning deficiencies may be mitigated by increasing the number of active cells and/or by increasing their firing rate, suggesting the existence of a compensatory mechanism inherent to the cognitive map.

Tuesday, March 3, 2015 2:30PM - 5:30PM –

2:30PM J34.00001 Wetting on surfaces with tailored nano-scale defects , KRISTINA DAVITT, ROMAIN LHERMEROULT, ETIENNE ROLLEY, Laboratoire de Physique Statistique de l’ENS Paris — Surface heterogeneity is acknowledged as a cause of contact angle hysteresis. More recently, it has also been recognized as having an important effect on contact line dynamics [1]. However, it has proven difficult to design quantitative experiments [2]. There are two fundamental difficulties: (i) to control the heterogeneity and (ii) to fabricate a true reference surface. In many methods, additional well-controlled defects may be added to a surface, however, the untreated substrate itself already presents some chemical or topographical disorder (typically nano-scale). This is illustrated by the fact that even on a purportedly defect-free surface the hysteresis is non-negligible (>a few degrees).
We report on the use of adsorbed short-chain polymer surfaces as nearly ideal reference surfaces (H < 0.01°). Topographical defects of controlled size, shape and density are then added using nanosphere lithography with dilute colloidal suspensions, and the dependence of the hysteresis and low-velocity dynamics on the defect parameters are determined.

2:42PM J34.00002 Contact line dynamics on a pseudo-brush, Romain Lhermetout, Kristina Davitt, Etienne Rolley, Laboratoire de Physique Statistique de l’ENS, 24 rue Lhomond 75005 Paris, France. Hugo Perrin, Bruno Andreotti, Laboratoire de Physique et Mecanique des Milieux Heterogenes de l’ESPCI, 10 rue Vauquelin 75005 Paris, France — Polymer brushes are nanometric layers of polymers that are attached to a solid surface. They are well-known for strongly modifying the mechanical properties of the surface. Although friction and slippage experiments have been performed on such systems [1], the impact of brushes on wetting dynamics has not yet been investigated. We report measurements of contact line dynamics of simple liquids over so-called pseudo-brushes adsorbed on silicon. We will show that this system exhibits (i) a surprisingly low hysteresis, a feature of great utility when studying the impact of added defects on the contact angle, (ii) a specific contribution to the dissipation, which is localized at the contact line, in addition to the viscous dissipation in the liquid wedge. The pseudo-brush contribution can be isolated from the total dissipation [2] and a simple model is used to explain the role of the pseudo-brush.


2:54PM J34.00003 Deformation of Nanoscale Elastomeric Free-Standing Films by Sessile Liquid Droplets, Rafael Schulman, Kari Dalnoki-Veress, McMaster University — The study of liquid droplets on soft, deformable substrates has recently garnered a great deal of attention. In particular, it has been found that droplets deform elastic surfaces at the contact line, and that this deformation can yield contact angles that do not obey Young’s law. Rather, the microscopic contact line geometry is dictated by a force balance between the three surface stesses, akin to the Neumann construction for droplets on liquid substrates. In our experiment, we place liquid droplets atop elastomeric free-standing films with thicknesses of hundreds of nanometers. Using optical microscopy, as well as atomic force microscopy, we directly measure the contact line geometry and induced deformation of the free-standing film.

3:06PM J34.00004 A thermodynamic model for the wetting characteristics of hierarchical physically-patterned surfaces, Michael Bell, Department of Physics, Penn State University, University Park, PA 16802, Azar Shahraz, Kristen Fichthorn, Ali Borhan, Department of Chemical Engineering, Penn State University, University Park, PA 16802 — An understanding of wetting is important for many applications, including superhydrophobic self-cleaning and low-drag surfaces. Many natural examples of such surfaces exist, including insect legs, bird feathers, and plant leaves. The mechanism of superhydrophobicity on these surfaces is known to be related to their hierarchical roughness (i.e., roughness on micro and nano length scales), though the precise role of hierarchical roughness is not yet well understood. We present a two-dimensional thermodynamic model of the wetting of a hierarchically-grooved surface for droplets with variable Bond number. By investigating wetting phenomena on a roughened interface, we are able to isolate different effects that contribute to the contact angle hysteresis. We find that the presence of microgrooves can yield contact angles that do not obey Young’s law. Rather, the microscopic contact line geometry is dictated by a force balance between the three surface stesses, akin to the Neumann construction for droplets on liquid substrates. In our experiment, we place liquid droplets atop elastomeric free-standing films with thicknesses of hundreds of nanometers. Using optical microscopy, as well as atomic force microscopy, we directly measure the contact line geometry and induced deformation of the free-standing film.

3:18PM J34.00005 Wetting ridge growth and contact line pinning on viscoelastic solid, Su Ji Park, Pohang Univ of Sci & Tech, Joshua B. Bostwick, Northwestern Univ., Jung Ho Je, Pohang Univ of Sci & Tech — Dynamic wetting behaviors on soft viscoelastic solids are potentially important to interpret complex biological processes resulted from cell-substrate interactions. When a droplet sits on a soft surface, its surface tension deforms the contact line, creating a “wetting ridge,” which causes characteristic spreading behaviors. The key to understand the underlying mechanisms is to investigate wetting ridge dynamics during spreading. However, it is challenging to explore wetting ridge dynamics, mostly due to limitations in observation. Here, we directly visualize wetting ridges in real-time during spreading using x-ray microscopy with a high spatio-temporal resolution. We reveal that the growth of wetting ridges is dominated by their broadening in early stage and by their heightening in later stage. The two growth mechanisms control the ridge-geometry and determine the spreading behaviors. Most importantly, we find that the contact line pinning is enhanced by increased flexibility of the ridge crest. Finally, we clarify two different mechanisms of pinning/depinning transitions: “stick-slipping” and “stick-breaking.”

3:30PM J34.00006 Self-pinning of a Nanosuspension Drop: MD Simulations, Baiou Shii, Edmund Webb, Lehigh University — The behavior of nano-fluids, or fluid suspensions containing nano-particles, has garnered tremendous attention recently for applications in advanced manufacturing. Contact line pinning by the particles or self-pinning has been extensively considered during contact line retreat due to solvent evaporation. Here we will present our results from MD simulations on self-pinning of an advancing contact line. For a wetting system of identical low viscosity, highly wetting drops. We reveal that the growth of wetting ridges is dominated by their broadening in early stage and by their heightening in later stage. The two growth mechanisms control the ridge-geometry and determine the spreading behaviors. Most importantly, we find that the contact line pinning is enhanced by increased flexibility of the ridge crest. Finally, we clarify two different mechanisms of pinning/depinning transitions: “stick-slipping” and “stick-breaking.”

3:42PM J34.00007 Inertial Wetting Kinetics for Nanometer Scale Droplets, Edmund Webb III, Baiou Shii, Lehigh University — Inertial spreading occurs immediately following contact between a droplet and solid surface. For low viscosity liquids with high wettability, high contact line velocities are observed during this stage. A counterintuitive result from atomic scale simulations is that even nanometer sized metallic drops exhibit a regime of wetting that is governed by inertial effects. Using a Tolman length corrected surface tension to account for liquid/vapor interface curvature effects that manifest in small drops, inertial spreading data from molecular dynamics simulations for varying drop size (down to a few nm diameter) can be collapsed onto a single curve using otherwise continuum scale inertial capillary flow theory. In addition, for inertial spreading on a low advancing contact angle surface, a second nanoscale effect is observed, which is related to curvature gradients that manifest along a significant portion of the liquid/vapor interface in the smallest drops. This is caused by rapid advancement of a precursor wetting film. The duration of the inertial regime is computed and shown to scale with the inertial/capillary time scale. Evidence is presented that capillary waves play a role in determining the duration of the inertial wetting regime for low viscosity, highly wetting drops.

3:54PM J34.00008 Inertia-driven droplet depinning on textured surfaces, Sungyoon Lee, Department of Mechanical Engineering, Texas A&M University, Benjamin Wilcox, Department of Aerospace Engineering, Texas A&M University, Ali Reza Hooshanginejad, Department of Mechanical Engineering, Texas A&M University, Alex Berger, Department of Aerospace Engineering, Texas A&M University, Feng Xu, Department of Mechanical Engineering, Texas A&M University, Edward White, Department of Aerospace Engineering, Texas A&M University — The stability of drops on surfaces subject to forcing by wind and gravity is relevant to heat exchangers, fuel cells, and aircraft icing, and it lacks understanding in a high Reynolds number regime. To experimentally investigate this phenomenon, water drops are placed on the rough aluminum floor of a tiltable wind tunnel and brought to critical conditions for varying drop sizes, inclination angles, and flow speeds. In particular, the evolving 3D droplet shapes under flow are reconstructed based on a laser-speckle interface measurement tool, while the critical flow rates of droplet depinning are also noted. By accounting for the contact angle hysteresis and the pressure build-up in a nearly turbulent boundary layer, the critical depinning flow rate is theoretically predicted and is compared to the experimental results. We also observe and explain the transition of the drop depinning behavior from inertia-dominated to gravity-dominated regimes at non-zero inclination angles.

3:54PM J34.00008 Contact line dynamics on a pseudo-brush, Romain Lhermetout, Kristina Davitt, Etienne Rolley, Laboratoire de Physique Statistique de l’ENS, 24 rue Lhomond 75005 Paris, France. Hugo Perrin, Bruno Andreotti, Laboratoire de Physique et Mecanique des Milieux Heterogenes de l’ESPCI, 10 rue Vauquelin 75005 Paris, France — Polymer brushes are nanometric layers of polymers that are attached to a solid surface. They are well-known for strongly modifying the mechanical properties of the surface. Although friction and slippage experiments have been performed on such systems [1], the impact of brushes on wetting dynamics has not yet been investigated. We report measurements of contact line dynamics of simple liquids over so-called pseudo-brushes adsorbed on silicon. We will show that this system exhibits (i) a surprisingly low hysteresis, a feature of great utility when studying the impact of added defects on the contact angle, (ii) a specific contribution to the dissipation, which is localized at the contact line, in addition to the viscous dissipation in the liquid wedge. The pseudo-brush contribution can be isolated from the total dissipation [2] and a simple model is used to explain the role of the pseudo-brush.

4:06PM J34.00009 Electrowetting on Semiconductors, CESAR PALMA, ROBERT DEEGAN, University of Michigan — In traditional electrowetting-on-dielectric (EWOD) a sessile drop rests on a thin dielectric separating it from a conductor. A voltage applied between the droplet and the conductor causes an increase in the solid-liquid interface area and a concomitant reduction of the contact angle. The change in the contact angle is well modeled by the Young-Lippmann equation. Here we report experiments where the conductor is replaced by lightly-doped, single-crystal silicon. We observe contact angle changes that are polarity-dependent as well as a non-reversible light-induced wetting transition. As suggested previously we assume that the charge distributions in the system have a direct analogue with the charges states of a metal-oxide-semiconductor capacitor. We calculate the free energy of the system taking into account both capillary and electrostatic contributions. By minimizing this result we derive a modified form of the Young-Lippmann equation. We further enhance our model to include the effect of pinning and well known semiconductor surface effects including interface charges and work function differences. We find that this model works well with experimental results.

4:18PM J34.00010 How cats and dogs drink differently?, SUNGHWAN JUNG, SEAN GART, JAKE SOCHA, Virginia Tech, PAVLOS VLACHOS, Purdue University — Drinking is defined as the animal action of taking water into the mouth, but to fluid mechanists, it is simply one kind of fluid transport phenomena. Classical fluid mechanics show that fluid transport can be achieved by either pressure-driven or inertia-driven processes. In a similar fashion, animals drink water using pressure-driven or inertia-driven mechanisms. For example, domestic cats and dogs lap water by moving the tongue fast, thereby developing the inertia-driven mechanism. We will investigate how cats and dogs drink water differently and discuss the underlying fluid mechanics.

4:30PM J34.00011 How droplets nucleate and grow on liquids and liquid impregnated surfaces1, SUSHANT ANAND, Massachusetts Inst of Tech-MIT, KONRAD RYKACZEWSKI, Arizona State University, SRINIVAS PRASAD BENGALURU SUBRAMANIAM, Massachusetts Inst of Tech-MIT, DANIEL BEYSENS, ESPCI-PMM, KRIPA VARANASI, Massachusetts Inst of Tech-MIT — Condensation on liquids has been studied extensively in context of breath figure templating, materials synthesis and self-cleaning surfaces. However, the mechanics of nucleation and growth on liquids remains unclear, especially on liquids that spread on the condensate. By examining the energy barriers of nucleation, we provide a framework to choose liquids that can lead to enhanced nucleation. We show that due to limits of vapor sorption within a liquid, nucleation is most favoured at the liquid–air interface and demonstrate that on spreading liquids, droplet submergence within the liquid occurs thereafter. We provide a direct visualization of the thin liquid profile that cloaks the condensed droplet on a liquid impregnated surface and elucidate the vapour transport mechanism in the liquid films. Finally, we show that although the viscosity of the liquid does not affect droplet nucleation, it plays a crucial role in droplet growth.

4:42PM J34.00012 Phase-Field Modeling of the Buoyancy-Driven Detachment of a Wall-Bound Pendant Drop1, ANDREA LAMORGESE, ROBERTO MAURI, DICI/University of Pisa, LABORATORY OF MULTIPHASE REACTIVE FLOW TEAM — We investigate numerically the critical conditions for detachment of an isolated, wall-bound emulsion droplet acted upon by surface tension and wall-normal buoyancy forces alone using a simple extension of a diffuse interface model for partially miscible binary mixtures that was previously employed for simulating several two-phase flow phenomena far and near the critical point ["Phase-Field Approach to Multiphase Flow Modeling," Milan J. Math. 79, 597 (2011)] to allow for static contact angles other than 90°. We use the same formulation of the Cahn boundary condition as first proposed by Jacqmin ["Contact-line dynamics of a diffuse fluid interface," J. Fluid Mech. 402, 57 (2000)] which accommodates a cubic (Heitmeier) interpolation of surface tensions between the wall and each phase at equilibrium. We show that this model can be successfully employed for simulating three-phase contact line problems in stable emulsions with nearly immiscible components. We also show the first numerical determination of critical Bond numbers as a function of static contact angle by phase-field simulation.

4:54PM J34.00013 Asymptotic model for three-dimensional coating flow of nematic liquid crystal on an inclined substrate1, MICHAEL LAM, New Jersey Institute of Technology, LIN TE-SHENG, National Chiao Tung University, LINDA CUMMINGS, LOU KONDIC, New Jersey Institute of Technology — We consider a coating flow of nematic liquid crystal (NLC) film on an inclined substrate. Exploiting the large aspect ratio in the geometry of interest, an asymptotic approach is utilized to derive a fourth order nonlinear partial differential equation governing the evolution of the free surface. Previous results have shown that there exist two-dimensional traveling wave solutions that translate down the substrate. In contrast to the analogous Newtonian flow, such solutions may be unstable to streamwise perturbations. Extending well-known results for Newtonian flow, we analyze the stability of the front with respect to transverse perturbations. Particular attention is paid to the interplay between the bulk elasticity and the anchoring conditions at the substrate and free surface. Using full numerical simulations, we validate the linear stability theory and present examples of downslope flow of NLC in the presence of both transverse and streamwise instabilities.

5:06PM J34.00014 Contact Angle: Consequence of minimized Casimir Energy, SUDDARSON SHIVAKUMAR, Southern IL Univ-Carbondale — In 1805, T. Young, in his classic work, expressed the cosine of the angle subtended by the surface of a liquid droplet on a solid surface in terms of the surface energies of the respective mediums-solid, liquid and gas. More recently, London derived the van der Waals interaction energy using the then recent advent of quantum mechanics. Later, in 1937, H. C. Hamaker attempted to derive the interaction energies between two interacting mediums in contact. But, the van der Waals interaction energies for two bodies diverges as the bodies come in contact. To circumvent this undesired divergence, Hamaker introduced a cut-off distance parameter in his analysis, which typically is argued to be of atomic length. All future work on contact angles, since Hamaker, to our knowledge, has never been discussed without relying on this cut-off parameter. We here show that the contact angle is independent of the cut-off parameter, and free of divergence. Thus, contact angle is a measurable physical quantity.

5:18PM J34.00015 Sub-nanometric substrate structural changes enhance the solid/liquid slip boundary condition1, JOSHUA MCGRAW, ANTOINE BRIDET, SAMUEL GRANDTHYLL, KARIN JACOBS, Saarland University, Experimental Physics, 66041 Saarbrücken — Alkylsilane self-assembled monolayers (SAMs) have long been used as model substrates for their ease of preparation and hydrophobic properties. We have long observed that these monolayers also provide a slip boundary condition for dewetting polymer films, and that the slip condition is switchable if the alkyl chain length is changed (from 12 to 18 backbone carbons, for example). Typically, this change is affected in a quantized way, using one or the other chain length, thus obtaining one or the other slip condition. It has been suggested that the specific structure of the resulting SAM controls the slip condition. Here, we present results in which this structure is changed in two continuous ways. First, we prepare SAMs containing bimode mixtures of alkylsilanes, with the composition as a control parameter. Second, we thermally anneal the SAMs, resulting in an irreversible loss of carbon from the monolayer. In both cases, we find an enhanced slip condition which is tuneable over a certain range.

1NSERC (Canada) and DFG (Germany) are acknowledged for financial assistance.
2:30PM J35.00001 Self-energy of a Cold Atom Interacting with an Elastic Membrane

SANGHITA SENGUPTA, University of Vermont, WEI-SHIUANG XU, MIT, DENNIS CLOUGHERTY, University of Vermont — The interaction of an atom with an elastic membrane is studied using Feynman-Dyson perturbation theory. The self-energy $\Sigma(E)$ of an atom with incident energy $E$ is calculated analytically to second-order in the atom-membrane interaction. We explicitly show that while the first-order contribution to the self-energy is well-behaved, the second-order contribution is divergent in the limit of infinite membrane size, and we identify the various divergent contributions. These results are discussed in the context of the “quantum sticking” and scattering of cold atoms from two dimensional materials such as graphene and monolayer transition metal dichalcogenides.

3We gratefully acknowledge support by the National Science Foundation under DMR-1062966.

2:42PM J35.00002 Effects of quantum coherence and interference in atoms near nano-particle

SUMAN DHAYAL, YURI ROSTOVTSEV, University of North Texas — Optical properties of ensembles of realistic quantum emitters coupled to plasmonic systems are studied using a self-consistent model. In particular, the coherent effects such as forming “dark states,” optical pumping, coherent Raman scattering, and the stimulated Raman adiabatic passage (STIRAP) are revisited in the presence of metallic nanoparticles. It is shown that the “dark states” are still formed but have more complicated structure, the optical pumping and the STIRAP cannot be employed in the vicinity of plasmonic nanostructures. The STIRAP technique should be used carefully, because it may not work or has at least new features in the presence of nanoparticles. We have also found difference of the local atomic polarization and the atomic polarization averaged over ensemble of atoms homogeneously spread near nanoparticles. The averaged polarization is strongly related to the polarization of the external field, meanwhile the local polarization can be very different from the one induced by the external field. The obtained results are important for excitation of single molecules, e.g. new components of scattering from single molecules can be used for efficient detection of nanoparticles.

2:54PM J35.00003 Observations of parity-time symmetry in optical systems: microtoroid resonators and moving hot atoms

JIANNING WEN, LIANG JIANG, Department of Applied Physics, Yale University, USA, YANHONG XIAO, Department of Physics, Fudan University, China, XIAOSHUN JIANG, National Laboratory of Solid State Microstructures and College of Engineering and Applied Sciences, Nanjing University, China, MIN XIAO, College of Engineering and Applied Sciences, Nanjing University, China; Physics, Univ of Arkansas, USA — Compound-photonic systems with gain and loss provide a powerful platform for testing various theoretical proposals on non-Hermitian parity-time (PT)-symmetric quantum mechanics and initiate new possibilities for shaping optical beams and pulses beyond conservative structures. Such systems can be designed as optical analogues of complex PT-symmetric potentials with real spectra. However, the beam dynamics can exhibit unique features distinct from conservative systems due to non-trivial wave interference and phase-transition effects. Here, we report two of our recent experiments on the realizations of PT-symmetric optics in two different systems: one uses two directly coupled high-Q silica-microtoroid resonators with balanced effective gain and loss [1]; while the other is the first experimental implementation in an optical system using moving atoms, in which the coupling of two optical modes is realized by coherent diffusion of atomic coherence [2]. In both studies, our theories show excellent agreements with the experimental observations. [1] L. Chang, X. Jiang, S. Hua, C. Yang, J. Wen, L. Jiang, G. Li, G. Wang, and M. Xiao, Nature Photonics 8, 524 (2014). [2] P. Peng, W. Qu, W. Cao, L. Zheng, S. Shen, J. Wen, L. Jiang, and Y. Xiao (submitted).

3:06PM J35.00004 Thermodynamic considerations of mechanical oscillations

CHIAO-HSUAN WANG, JQI/UMD, JACOB TAYLOR, JQI/NIST/QuICS — Recent experimental efforts in large-scale optomechanical systems have been made to observe coherent superpositions of macroscopic oscillators. However, the quantum harmonic oscillator treatment of macroscopic optomechanics may need further verification due to the presence of enormous numbers of internal degrees of freedom. We examine models of a mechanical oscillator coupled to many degrees of freedom in thermal contact with a bath, and find that spring-like classical oscillations can occur even if there is no underlying quantum mechanical oscillator. We provide a microscopic description of this thermal oscillator mechanism, and consider methods for distinguishing between quantum harmonic oscillations and other oscillatory behaviors.

3:18PM J35.00005 Measurement and control of a mechanical oscillator at its thermal decoherence rate

DALZIEL WILSON, VIVISHEK SUDHIR, NICOLAS PIRO, RYAN SCHILLING, AMIR GHADIMI, TOBIAS KIPPNBERG, Swiss Federal Institute of Technology in Lausanne — In real-time (Markovian) quantum feedback protocols, the outcome of a continuous measurement is used to stabilize a desired quantum state. Extending such protocols to macroscopic systems is a significant challenge, as the measurement must in this case compete with rapid environmental decoherence. We report on the realization of an interferometric sensor that approaches the requirements of quantum feedback for a solid-state, 4.3 MHz nanomechanical oscillator: namely, the ability to resolve its zero-point motion in the timescale of its thermal decoherence. The sensor is based on near-field cavity-optomechanical coupling, and realizes a measurement of the oscillator’s displacement with an imprecision 40 dB below that at the standard quantum limit, while maintaining an imprecision-backaction product within a factor of 5 of the Heisenberg uncertainty limit. As a demonstration of its utility, we use the measurement to feedback cool the oscillator to an phonon occupation of 5.4±0.7 (i.e., a ground state probability of 16%). Our results establish a new benchmark for the performance of a linear position sensor, and signal the emergence of engineered mechanical oscillators as practical subjects for measurement-based quantum control.

3:30PM J35.00006 Non-equilibrium quantum heating effects in driven, strongly-interacting optomechanics

AASHISH CLERK, MARC-Antoine LEMONDE, Department of Physics, McGill University — We study the influence of weak, nonlinear single-photon optomechanical interactions in a strongly driven cavity, focusing on the regime where these interactions become resonant due to the formation of optomechanical polaritons. We extend the Keldysh field-theory approach to this problem formulated in our previous work[1] to now consider how zero-point fluctuations give rise to effective temperatures in this driven, interacting system. We show that this quantum heating has distinct signatures in the effective temperature of both the photonic and phononic degrees of freedom, and can in principle be detected by looking at the spectrum of the light leaving the cavity.

that the study of the pulsations leads to interesting observations of the optical, thermal, and mechanical properties of the device.

The precise waveform and frequency of these pulsations can be tuned by altering the laser detuning and input power, and we have found that the mechanical properties of the device can be altered by changing the laser parameters.

Our experiments probing the properties of ripplons and thermal vibrations of the helium are expected to have high quality factors [1]. Here we report on progress towards coupling microwave photons in a superconducting microwave cavity with ripplons on superfluid helium. [1] P. Roche et al., Phys. Rev. Lett. 75, 3316 (1995)

The coupling of our device on the order of 5 kHz per nm of ripplon wave amplitude. In this talk, we will discuss the study of the pulsatons leading to interesting observations of the optical, thermal, and mechanical properties of the device.

4:06PM J35.00009 Regenerative Pulsations in Optomechanical Devices , HUGH RAMP, MOHAMMAD BITARAFAN, BRAD HAUER, XAVIER ROJAS, RAY DECORBY, JOHN DAVIS, Univ of Alberta — In optomechanical devices, the presence of a strong cavity field is often desired to observe mechanical motion. In this case it becomes important to consider the effects of non-linear optical processes occurring in the device medium, which alter the effective refractive index and absorption coefficient of the device. We study the example of the buckled-dome Fabry-Perot microcavity, in which light is trapped in a spherical cap formed by two Si-SiO₂ Bragg mirrors of radius 125 µm. In the presence of strong optical fields the silicone in the device undergoes a combination of (3) non-linear processes resulting in periodic shifts of the cavity optical resonance known as regenerative pulsations. We have found that the precise waveform and frequency of these pulsations can be tuned by altering the laser detuning and input power, and found that the study of the pulsations leads to interesting observations of the optical, thermal, and mechanical properties of the device.

4:18PM J35.00010 Optomechanics with ripplons on superfluid helium , GERWIN Koolstra, David Mckay, Ge Yang, University of Chicago, David Czaplewski, Argonne National Laboratory, Center for Nanoscale Materials, David Schuster, University of Chicago — Superfluid helium has arisen as a promising candidate for optomechanics systems. Due to extremely low loss well below the lambda point, vibrations on the helium – ripplons – are expected to have high quality factors [1]. Here we report on progress towards coupling microwave photons in a superconducting LC resonator (riplon-traps in Si chip) can be manipulated and detected using superconducting resonators. We estimate the coupling of our device on the order of 5 kHz per nm of ripplon wave amplitude. In this talk, we will discuss our experiments probing the properties of ripplons and thermal vibrations, forming a gram-scale, sideband resolved, optomechanical system. We demonstrate the detection of a series of acoustic modes with high quality factors as high as 3 x 10⁷. The lowest dissipation modes are limited by an intrinsic three phonon process at higher temperatures, which leads to a 7° dependent attenuation. In isotopically purified samples at temperatures below 10 mK, acoustic quality factors over 10¹⁰ may be possible. A system of this type may be utilized to study macroscopic quantized motion and as a frequency tunable, ultra-sensitive sensor of extremely weak displacements and forces, such as continuous gravity wave sources.

4:42PM J35.00012 Strong single-photon nonlinearities in a multimode optomechanical system in the weak coupling regime , Kjetil Borkje, Department of Physics, University of Oslo, Stefán Walter, Department of Physics, University of Basel — We theoretically study the dynamics of two optomechanical cells, where each cell consists of an optical cavity mode whose resonance frequency is modulated by the position of a mechanical resonator. The two cells are furthermore coupled via photon and phonon tunneling, such that both the photon and the phonon modes hybridize to form symmetric and antisymmetric supermodes. This setup can for example be implemented in an optomechanical crystal. We show that by laser driving one of the optical supermodes with appropriately chosen power and frequency, the system can display strong single-photon effects already when the optomechanical single-photon cooperativity becomes larger than unity. This means that single-photon nonlinearities become important at significantly smaller coupling rates than in a single-mode system. We study how this system can be used to manipulate light at the single-photon level and to realize interactions between individual photons.

5:06PM J35.00014 Quantum synchronization of two dissipatively coupled Van der Pol oscillators , Stefan Walter, University of Basel, University of Erlangen-Nürnberg, Andreas Nunnennkamp, University of Basel, University of Cambridge, Christoph Bruder, University of Basel — Synchronization is a universal phenomenon that is important both in fundamental studies and in technical applications. Here we study synchronization of two dissipatively coupled Van der Pol oscillators in the subthreshold regime and analyze the transition in terms of frequency entrainment and frequency locking. Due to quantum noise strict frequency locking is absent and replaced by a crossover from weak to strong frequency entrainment. The differences to the behavior of one quantum Van der Pol oscillator subject to an external drive are discussed. Moreover, a possible experimental realization of two coupled quantum Van der Pol oscillators in an optomechanical setting is described.

3.42PM J35.00007 Simulating a Parametric Oscillator-Based Dynamical Casimir Effect , Enrique Guererro, Humboldt State University, Alessandro Castelli, Luis A. Martínez, Raymond Chiao, Jay E. Sharping, University of California, Merced — We present simulations of a cavity for use in demonstrating the dynamical Casimir effect (DCE). The successful demonstration of the DCE gives rise to interesting opportunities to study questions in Quantum Mechanics and General Relativity. Crucial to this experiment is attaining resonant cavities with a high Q, a measurement of how purely our system resonates. Necessary Q values can and have been achieved using superconducting cavities, and the low losses in these cavities allows above threshold amplification of vacuum fluctuations. Simulations of the system are crucial to optimize cavity design parameters. Using COMSOL Multiphysics, we simulate a set of three resonant cavities to create and amplify radio frequency (11 GHz) electromagnetic wave. Coupling between different cavities is achieved via a membrane which is driven into motion by electromagnetic radiation pressure. The simulation is being conducted concurrently with preliminary cavity experiments.

3:54PM J35.00008 Optomechanical cooling in a correlated emission laser , WenChao Ge, M. SuHail Zubairy, Argonne National Laboratory, Center for Nanoscale Materials, David Schuster, University of Chicago — In optomechanical devices, the presence of a strong cavity field is often desired to observe mechanical motion. In this case it becomes important to consider the effects of non-linear optical processes occurring in the device medium, which alter the effective refractive index and absorption coefficient of the device. We study the example of the buckled-dome Fabry-Perot microcavity, in which light is trapped in a spherical cap formed by two Si-SiO₂ Bragg mirrors of radius 125 µm. In the presence of strong optical fields the silicone in the device undergoes a combination of (3) non-linear processes resulting in periodic shifts of the cavity optical resonance known as regenerative pulsations. We have found that the precise waveform and frequency of these pulsations can be tuned by altering the laser detuning and input power, and found that the study of the pulsations leads to interesting observations of the optical, thermal, and mechanical properties of the device.

4:30PM J35.00011 Superfluid Helium-4 as an Ultra-low Loss Optomechanical Element , Laura de Lorenzo, Keith Schwab, Caltech — We investigate the low loss acoustic motion of superfluid He-4 parametrically coupled to a high Q, superconducting niobium Te₁₀₁₁ microwave resonator, forming a gram-scale, sideband resolved, optomechanical system. We demonstrate the detection of a series of acoustic modes with high quality factors as high as 3 x 10⁷. The lowest dissipation modes are limited by an intrinsic three phonon process at higher temperatures, which leads to a 7° dependent attenuation. In isotopically purified samples at temperatures below 10 mK, acoustic quality factors over 10¹⁰ may be possible. A system of this type may be utilized to study macroscopic quantized motion and as a frequency tunable, ultra-sensitive sensor of extremely weak displacements and forces, such as continuous gravity wave sources.

5:06PM J35.00014 Quantum synchronization of two dissipatively coupled Van der Pol oscillators , Stefan Walter, University of Basel, University of Erlangen-Nürnberg, Andreas Nunnennkamp, University of Basel, University of Cambridge, Christoph Bruder, University of Basel — Synchronization is a universal phenomenon that is important both in fundamental studies and in technical applications. Here we study synchronization of two dissipatively coupled Van der Pol oscillators in the subthreshold regime and analyze the transition in terms of frequency entrainment and frequency locking. Due to quantum noise strict frequency locking is absent and replaced by a crossover from weak to strong frequency entrainment. The differences to the behavior of one quantum Van der Pol oscillator subject to an external drive are discussed. Moreover, a possible experimental realization of two coupled quantum Van der Pol oscillators in an optomechanical setting is described.
density turns out to be anisotropic which reveals its tensorial property. Counterintuitively, the bias of the anisotropy is alternating between $x$- and $y$-directions due to the nature of anisotropic interactions.

Simulating the loading of a bosonic quantum gas into a one-dimensional optical lattice with and without a trap, we find that the redistribution of atomic density non-adiabatically during lattice loading are one of the limiting factors that prevent the same low temperatures to be reached as in experiments without lattice.

Theoretical Physik, ETH Zurich, 8093 Zurich, Switzerland — In the quest to reach lower temperatures of ultra-cold gases in optical lattice experiments, we derive an extended mean-field formalism to study the thermodynamical properties of the Bose-Hubbard model. The framework can be viewed as the zero-frequency limit of bosonic dynamical mean-field theory (B-DMFT), but equally well and less accurately than in B-DMFT.

Department of Physics, Virginia Tech, Blacksburg, Virginia 24061, USA — Optical lattices can be tailored to realized a variety of different geometries. We model bosons confined to a bilayer configuration to allow a pseudospin degree of freedom in the layer index. Specifically, we model the Bose-Hubbard model on a bilayer square lattice with variable inter-layer hopping. Without the presence of interlayer hopping, the phase diagram only presents well known superfluid or Mott insulating phases. But interlayer hopping allows coupling of these two states. We find that an interesting incompressible phase emerges at half filling as we increase the interlayer hopping strength. We study the low temperature physics of the new phase and address the nature of pseudospin correlations in observables. We pair our effective theory with a quantum Monte Carlo study.

Department of Applied Science and Technology, Politecnico di Torino, I-10129 Torino, Italy, BARBARA CAPOGROSSO SANSONE, H. L. Dodge Department of Physics and Astronomy, The University of Oklahoma, Norman, Oklahoma, USA, VITTORIO PENNA, MARCO FEDELE DI LIBERTO, Utrecht University — The control of transport properties is a key tool at the basis of many technologically relevant effects in condensed matter. The clean and precisely controlled environment of ultracold atoms in optical lattices allows one to prepare simplified but instructive models, which can help to better understand the underlying physical mechanisms. Here we show that by tuning a structural deformation of the unit cell in a bipartite optical lattice, one can induce a phase transition from a superfluid into various Mott insulating phases forming a shell structure in the superimposed harmonic trap. The Mott shells are identified via characteristic features in the visibility of Bragg maxima in momentum spectra. The experimental findings are explained by Gutzwiller mean-field and quantum Monte Carlo calculations. Our system bears similarities with the loss of coherence in cuprate superconductors, known to be associated with the doping induced buckling of the oxygen octahedra surrounding the copper sites.

Theor. Physik, ETH Zurich, 8093 Zurich, Switzerland, ADRIAN KANTIAN, DPMC-MaNEP, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Geneva, Switzerland, BELA BAUER, Microsoft Research, Station Q, University of California, Santa Barbara, CA 93106, USA, MATTHIAS TROYER, DIETER JOSWICK, DARIO HUEGEL, Ludwig Maximilian University Munich, LODE POLLET, Department of Physics, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-University Munich — We derive an extended mean-field formalism to study the thermodynamical properties of the Bose-Hubbard model. The framework can be viewed as the zero-frequency limit of bosonic dynamical mean-field theory (B-DMFT), but equally well and less accurately than in B-DMFT.

Single-photon optomechanics in the strong coupling regime is promising to play a key role in the realization of superpositions of macroscopic objects (for testing the foundations of quantum theory) and enhancing the nonlinear optomechanical interactions (for possible applications in quantum information processing). The stationary/time-independent spectrum of a single-photon interacting with a tiny movable mirror (in the context of cavity quantum optomechanics) can exhibit the signatures of optomechanical interaction as the appearance of multiple side bands in the spectrum. Strong optomechanical coupling and the good cavity limit are the two main conditions that need to be satisfied in order to observe all resonances in the spectrum [J.-Q. Liao et. al., Phys. Rev. A, 85,025803 (2012)]. We investigate the time-dependent (TD) version of the spectrum in the weak mechanical damping limit [Single-photon time-dependent spectrum in quantum optomechanics, I. M. Mirza, S. van Enk, to appear in Phys. Rev. A (2014)], which reveals some novel effects that are not possible to observe otherwise. For instance, the TD spectrum indicates that a sufficient amount of time has to pass before one can observe the fully resolved spectrum, even if the strong coupling and good cavity conditions are respected. Moreover, the TD spectrum also exhibits the order (in time) in which different side bands appear, thus further explaining the different photon-phonon interactions responsible for the distinct resonances.

Optical lattices can be tailored to realized a variety of different geometries. We model bosons confined to a bilayer configuration to allow a pseudospin degree of freedom in the layer index. Specifically, we model the Bose-Hubbard model on a bilayer square lattice with variable inter-layer hopping. Without the presence of interlayer hopping, the phase diagram only presents well known superfluid or Mott insulating phases. But interlayer hopping allows coupling of these two states. We find that an interesting incompressible phase emerges at half filling as we increase the interlayer hopping strength. We study the low temperature physics of the new phase and address the nature of pseudospin correlations in observables. We pair our effective theory with a quantum Monte Carlo study.

5:18PM J35.00015 Single-photon time-dependent spectrum in quantum optomechanics, IMran M. MIRZA, STEVEN J. VAN ENK, Oregon Center for Optics, Department of Physics, University of Oregon, USA — Single-photon optomechanics in the strong coupling regime is promising to play a key role in the realization of superpositions of macroscopic objects (for testing the foundations of quantum theory) and enhancing the nonlinear optomechanical interactions (for possible applications in quantum information processing). The stationary/time-independent spectrum of a single-photon interacting with a tiny movable mirror (in the context of cavity quantum optomechanics) can exhibit the signatures of optomechanical interaction as the appearance of multiple side bands in the spectrum. Strong optomechanical coupling and the good cavity limit are the two main conditions that need to be satisfied in order to observe all resonances in the spectrum [J.-Q. Liao et. al., Phys. Rev. A, 85,025803 (2012)]. We investigate the time-dependent (TD) version of the spectrum in the weak mechanical damping limit [Single-photon time-dependent spectrum in quantum optomechanics, I. M. Mirza, S. van Enk, to appear in Phys. Rev. A (2014)], which reveals some novel effects that are not possible to observe otherwise. For instance, the TD spectrum indicates that a sufficient amount of time has to pass before one can observe the fully resolved spectrum, even if the strong coupling and good cavity conditions are respected. Moreover, the TD spectrum also exhibits the order (in time) in which different side bands appear, thus further explaining the different photon-phonon interactions responsible for the distinct resonances.

Tuesday, March 3, 2015 2:30PM - 5:30PM —
Session J36 DAMOP: Bosons in Optical Lattices 211 - Randall Hulet, Rice University

2:30PM J36.00001 Phase diagram of the Bilayer Bose Hubbard Model, YANFEI TANG, VITO SCAROLA, Department of Physics, Virginia Tech, Blacksburg, Virginia 24061, USA — Optical lattices can be tailored to realized a variety of different geometries. We model bosons confined to a bilayer configuration to allow a pseudospin degree of freedom in the layer index. Specifically, we model the Bose-Hubbard model on a bilayer square lattice with variable inter-layer hopping. Without the presence of interlayer hopping, the phase diagram only presents well known superfluid or Mott insulating phases. But interlayer hopping allows coupling of these two states. We find that an interesting incompressible phase emerges at half filling as we increase the interlayer hopping strength. We study the low temperature physics of the new phase and address the nature of pseudospin correlations in observables. We pair our effective theory with a quantum Monte Carlo study.

2:42PM J36.00007 Tunable anisotropic superfluidity in optical Kagome superlattice, AXEL PELSTER, XUE-FENG ZHANG, Univ. of Kaiserslautern, Germany, TAO WANG, Harbin Institute of Technology, China, SEBASTIAN EGGERT, Univ. of Kaiserslautern, Germany — We study the extended Bose-Hubbard model for the optical Kagome superlattice generated by enhancing the long wavelength laser in one direction. By combining Quantum Monte Carlo simulations with the Generalized Effective Potential Landau Theory, we find not only the Mott insulator—superfluid phase transition, but also striped solid phases with non-integer filling factors. Furthermore, we determine with high accuracy the quantum phase diagram for different trap potential offsets. Due to the delicate interplay between onsite repulsion and artificial symmetry breaking, the superfluid density turns out to be anisootropic which reveals its tensorial property. Counterintuitively, the bias of the anisotropy is alternating between $x$- and $y$-direction while tuning the particle number or the hopping strength. Finally, we discuss how to observe such phenomenon experimentally, in particular via time-of-flight absorption measurements.

1 Supported by OPTIMAS and the Deutsche Forschungsgemeinschaft via the SFB/TR49.

3:30PM J36.00006 Minimizing Non-Adiabaticities In Optical Lattice Loading, MICHELE DOLFI, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland, ADRIAN KANTIAN, DPMC-MaNEP, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Geneva, Switzerland, BELA BAUER, Microsoft Research, Station Q, University of California, Santa Barbara, CA 93106, USA, MATTHIAS TROYER, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland — In the quest to reach lower temperatures of ultra-cold gases in optical lattice experiments, we derive an extended mean-field formalism to study the thermodynamical properties of the Bose-Hubbard model. The framework can be viewed as the zero-frequency limit of bosonic dynamical mean-field theory (B-DMFT), but equally well and less accurately than in B-DMFT.

3:18PM J36.00005 ABSTRACT WITHDRAWN
progress on magnetic effects in 2+1 dimensions will be discussed. We propose to implement the quantum rotors which appear in the Hamiltonian formulation using Bose mixtures or p-orbitals. Recent perturbation theory effective Hamiltonian for various Bose-Hubbard models. This correspondence can be exploited for building a lattice gauge theory simulator coupled regime. We discuss the plaquette corrections to the effective theory where link variables are integrated out. We discuss matching with the second-order WEN TSAI, ALEXEI BAZAVOV, JIN ZHANG, UC Riverside — We study the Lattice Gauge Theory of the U(1)-Higgs model in 1+1 dimensions in the strongly density fluctuations, current correlation functions, and excitation spectra are measurable in ultracold atom experiments. 

As the superfluid is rotated it moves with a supercurrent until it develops phase slips which generate vortices. We use a finite temperature strong-coupling approximation on an optical lattice in the presence of an annular trap and a barrier across the annular region which acts as a Josephson junction. In addition, we show how even more complex Josephson junction structures spontaneously arise if the filling is increased to generate Mott regions within the system.

As the superfluid is rotated it moves with a supercurrent until it develops phase slips which generate vortices. We use a finite temperature strong-coupling approximation on an optical lattice in the presence of an annular trap and a barrier across the annular region which acts as a Josephson junction. In addition, we show how even more complex Josephson junction structures spontaneously arise if the filling is increased to generate Mott regions within the system.  

3:54PM J36.00008 Spin Meissner Effect and Chiral Mott Insulators in Quantum Ladders . ALEXANDRU PETRESCU, Yale University USA and Center for Theoretical Physics, Ecole Polytechnique, France, KARYN LE HUR, Center for Theoretical Physics, Ecole Polytechnique and CNRS, France — We introduce generic bosonic models exemplifying that chiral Meissner currents can persist in insulating phases of matter. We first consider interacting bosons on a two-leg ladder. The total density sector can be gapped in a bosonic Mott insulator at odd-integer filling, while the relative density sector remains superfluid due to interchain hopping. Coupling the relative density to gauge fields yields a pseudospin Meissner effect [1]. We show that the same phase arises if the bosons are replaced by spinful fermions confined in Cooper pairs, and find a dual fermionic Mott insulator with spinon currents [2]. We propose two experimental realizations, one with ultracold atoms in the setup of [3], and another with Josephson junction arrays. Finally, we discuss the possibility to explore Laughlin phases in these systems by tuning the magnetic flux and the density of bosons [4].


4:06PM J36.00009 ABSTRACT WITHDRAWN —

4:18PM J36.00010 P-orbital Condensations of Two-species Bose Mixture in Optical Lattice1, JHIH-SHIHI YOU, Department of Physics, National Tsing Hua Univ, I-KANG LIU, Department of Physics and Graduate Institute of Photonics, National Changhua University of Education, DAW-WEI WANG, Department of Physics, National Tsing Hua Univ, SHIH-CHUAN GOU, Department of Physics and Graduate Institute of Photonics, National Changhua University of Education, CONGJUN WU, Department of Physics, University of California, San Diego — We investigate the p-orbital Bose-Einstein condensations (BECs) of two-species mixture in a bipartite optical lattice. A new imaginary-time propagation method is developed to numerically solve the Gross-Pitaevskii equation with truncating states below the p bands, which can be applicable to even higher orbital bands. Our study confirms that the intra-species interactions favor complex time-reversal broken BECs with staggered orbital currents. However, when the inter-species interaction increases, the complex condensate state undergoes a quantum phase transition toward a real-valued TR invariant condensate with staggered spin density structure. We discuss the origin and properties of such phase transition and its implication in the experimental setup.

1 J. S. Y. also acknowledges the support from NSC Grant No. 102-2917-I-007-032.

4:30PM J36.00011 The Abelian Higgs model on Optical Lattice1, YANNICK MEURICE, Univ of Iowa, SHAN-WEN TSAI, ALEXEI BAZAVOV, JIN ZHANG, UC Riverside — We study the Lattice Gauge Theory of the U(1)-Higgs model in 1+1 dimensions in the strongly coupled regime. We discuss the plaquette corrections to the effective theory where link variables are integrated out. We discuss matching with the second-order perturbation theory effective Hamiltonian for various Bose-Hubbard models. This correspondence can be exploited for building a lattice gauge theory simulator on optical lattices. We propose to implement the quantum rotors which appear in the Hamiltonian formulation using Bose mixtures or p-orbitals. Recent progress on magnetic effects in 2+1 dimensions will be discussed.

1Supported by the Army Research Office of the Department of Defense under Award Number W911NF-13-1-0119.

4:42PM J36.00012 Cold-atom quantum simulation of U(1) lattice gauge-Higgs model , KENICHI KASAMATSU, Dept. of Phys. Kinki Univ., YOSHIHITO KUNO, Dept. of Appl. Phys., Nagoya Inst. of Tech., YOSHIRO TAKAHASHI, Dept. of Phys. Kyoto Univ., IKUO ICHINOSE, Dept. of Appl. Phys., Nagoya Inst. of Tech., TETSUO MATSUI, Dept. of Phys. Kinki Univ. — We discuss the possible methods to construct a quantum simulator of the U(1) lattice gauge-Higgs model using cold atoms in an optical lattice. These methods require no severe fine tunings of parameters of atomic-interactions in contrast with the other previous literature. We propose some realistic experimental setups to realize the atomic quantum simulator of the U(1) lattice gauge-Higgs model in a two-dimensional optical lattice. Our target gauge-Higgs model has a nontrivial phase structure, i.e., existence of the phase boundary between confinement and Higgs phases, and this phase boundary is to be observed by cold-atom experiments. As a reference to such experiments, we make numerical simulations of the time-dependent Gross-Pitaevskii equation and observe the real-time dynamics of the atomic simulators. Clarification of the dynamics of this gauge-Higgs model sheds some lights upon various unsolved problems including the inflation process of the early universe.

4:54PM J36.00013 Chiral Bosonic Phases on the Haldane Honeycomb Lattice , IVANA VASIC, Institut fuer Theoretische Physik, Goethe-Universitaet, 60438 Frankfurt/Main, Germany, ALEXANDRU PETRESCU, Department of Physics, Yale University, New Haven, CT 06520, USA and Centre de Physique Theorique, Ecole Polytechnique, CNRS, 91128 Palaiseau, France, KARYN LE HUR, Centre de Physique Theorique, Ecole Polytechnique, CNRS, 91128 Palaiseau Cedex, France, WALTER HOFSTETTER, Institut fuer Theoretische Physik, Goethe-Universitaet, 60438 Frankfurt/Main, Germany — Motivated by its recent realization in an ultracold atom experiment [1], we investigate the honeycomb lattice tight-binding model introduced by Haldane [2], for bosons with local interactions at the average filling of one boson per site [3]. We uncover in the ground state phase diagram three phases: a uniform superfluid (SF), a chiral superfluid (CSF) and a plaquette Mott insulator with local current loops (PMI). Nearest-neighbor and next-nearest neighbor currents distinguish CSF from SF, and the phase transition between them is first order. We apply bosonic dynamical mean field theory and exact diagonalization to obtain the zero temperature phase diagram, complementing numerics with calculations of excitation spectra in strong and weak coupling perturbation theory. Furthermore, we explore the possibility of chiral Mott insulating phases at the average filling of one boson every two sites. The characteristic density fluctuations, current correlation functions, and excitation spectra are measurable in ultracold atom experiments. [1] G. Jotzu et al., arXiv:1406.8784 [2] F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988). [3] Ivana Vasic, Alexandru Petrescu, Karyn Le Hur, Walter Hofstetter, arXiv:1408.1411

5:06PM J36.00014 Strong-coupling theory approach to describe an atomtronic josephson junction on an optical lattice , MANJARI GUPTA, H.R. KRISHNAMURTHY, Center For Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560012, India, J.K. FREERICKS, Department of Physics, Georgetown University, Washington, D.C. 20057, USA — We examine the behavior of a boson superfluid on an optical lattice in the presence of an annular trap and a barrier across the annular region which acts as a Josephson junction. As the superfluid is rotated it moves with a supercurrent until it develops phase slips which generate vortices. We use a finite temperature strong-coupling (t/U) expansion about the mean-field solution of the Bose Hubbard model, as described in our earlier paper Ref. [1] to characterize the device. Although our formalism is in equilibrium, it allows us to study the superfluid current flow and the generation of phase slips. This theory should aid in the further development of atomtronic circuits [2]. In addition, we show how even more complex Josephson junction structures spontaneously arise if the filling is increased to generate Mott regions within the system.

with numerical modelling of the readout process. We have determined the band structure of the BCC optical lattice for all theoretically possible couplings, and find that the band structure for lattices realizable in the lab, differs significantly from that expected for a BCC crystal. As coupling is increased, the lattice becomes increasingly chaotic [1] and it becomes possible to produce band structures that have qualitative similarity to a BCC.


Tuesday, March 3, 2015 2:30PM - 5:18PM —
Session J37 GQI: Focus Session: Quantum Dynamics with Phonons and Photons 212A - Ken Brown, Georgia Institute of Technology

2:30PM J37.00001 Quantum Information Experiments with Trapped Ions at NIST, ANDREW WILSON, National Institute of Standards and Technology, 325 Broadway, Boulder CO 80305 — We present an overview of recent trapped-ion quantum information experiments at NIST. Advancing beyond few-qubit “proof-of-principle” experiments to the many-qubit systems needed for practical quantum simulation and information processing, without compromising on the performance demonstrated with small systems, remains a major challenge. One approach to scalable hardware development is surface-electrode traps. Micro-fabricated planar traps can have a number of useful features, including flexible electrode geometries, integrated microwave delivery, and spatio-temporal tuning of potentials for ion transport and spin-spin interactions. In this talk we report on a number of ongoing investigations with face trapped ions. Experiments feature a multi-zone trap with closely spaced ions in a triangular arrangement (a first step towards 2D arrays of ions with tunable spin-spin interactions), a scheme for smooth transport through a junction in a 2D structure based on switchable RF potentials, and a micro-fabricated photodetector integrated into a trap. We also give a progress report on our latest efforts to improve the fidelity of both optical and microwave 2-qubit gates. This work was supported by IARPA, ONR and the NIST Quantum Information Program. The 3-ion and switchable-RF-junction traps were developed in collaboration with Sandia National Laboratory.

3:06PM J37.00002 Trapped Ion Quantum Computing with Microwaves, JOE RANDALL, University of Sussex, Imperial College, SEBASTIAN WEIDT, MARGARET STERLING, RALPH HANSON, University of Sussex, ANDREW RODRIGUEZ, ANNA WEBB, University of Sussex, HWAJUN TANASANTHI, PRASANNA SRINIVASAN, MICHAEL KRAFT, University of Southampton, JESSICA MACLEAN, CHRIS MELLOR, University of Nottingham, WINFRIED HENSINGR, University of Sussex — To this point, entanglement operations in trapped ion qubits have been predominantly performed with lasers. However, this becomes problematic when scaling to large numbers of qubits due to the challenging engineering required. The use of stable and easily controllable microwaves to drive entanglement gates can overcome this problem. We will present our work towards implementing multi-qubit entanglement gates using microwaves in an experimental setup that produces a static magnetic field gradient of 24 T/m over an ion string. We will first present a scheme for preparing and manipulating dressed-state qubits and qutrits that are highly robust to decoherence from magnetic field fluctuations. We will also present our work experimentally demonstrating motional sideband transitions and Schrödinger cat states using microwaves in conjunction with the magnetic field gradient, as well as sideband cooling to the ground state of motion using dressed-states. Furthermore, we will show our latest results in creating microfabricated ion trap chips towards large scale quantum computing and simulation.

3:18PM J37.00003 Non-Hermitian magnetism and entanglement in dissipative atomic systems, TONY LEE, CHING-KIT CHAN, Harvard/ITAMP, FLORENTINET REITER, Niels Bohr Institute, NIMROD MOISEYEV, Technion — Quantum phase transitions are usually studied in terms of Hermitian Hamiltonians. However, cold-atom experiments can implement non-Hermitian Hamiltonians via weak measurements. We show that the non-Hermitian XY model exhibits quantum phase transitions beyond the framework of Hermitian physics. There is a phase transition already for two atoms. In a 1D chain, the ordered phase is frustrated and has quasi-long-range order despite the absence of a continuous symmetry [1]. The non-Hermitian phase transition also has a lot more entanglement than the Hermitian one [2]. We discuss experimental implementation with trapped ions, cavity QED, and optical lattices. [1] Phys. Rev. X 4, 041001 (2014). [2] arXiv:1409.7067.

3:30PM J37.00004 Entanglement Transfer in a Double Jaynes-Cummings Model, SAMINA MASOOD, University of Houston Clear Lake, Houston TX, ALLEN MILLER, Syracuse University, Syracuse, NY — We compute and analyze the atom-atom entanglement, the entanglement between the two photon modes, and also the entanglement between each atom and each photon mode. The measure of entanglement is the von Neumann entropy. For the case in which the two photon-atom systems have identical properties, but allowing for non-resonant conditions, the sum of the von Neumann entropy. For the case in which the two atom-photon systems have identical properties, but allowing for non-resonant conditions, the sum of the

4:18PM J37.00006 ABSTRACT WITHDRAWN —

4:30PM J37.00007 On Readout of Vibrational Qubits using Quantum Beats, DMYTRO SHYSHLOV, DMITRI BABIKOV, Marquette Univ — Readout of the final states of qubits is a crucial step towards implementing quantum computation in experiment. In this theoretical work we explore the process of readout from vibrational qubits in thiophosphene molecules, SCC12, using quantum beat oscillations. The quantum beats are measured by first exciting the superposition of the qubit-encoding vibrational states to the electronically excited readout state with variable time delay pulses. The resulting oscillation of population of the readout state is then detected as a function of time delay. In principle, fitting the quantum beat signal by an analytical expression should allow extracting the values of probability amplitudes and the relative phases of the vibrational qubit states. However, we found that if this procedure is implemented using the standard analytic expression for quantum beats, a non-negligible phase error is obtained. We discuss the origin and properties of this phase error, and propose a new analytical expression to correct the phase error. The corrected expression fits the quantum beat signal very accurately. We now have a practical approach to read out the final state of vibrational qubits in experiments by combining the analytic expression for fitting with numerical modelling of the readout process.
We study the properties of this generalized entropy and generalized mutual information, and apply this framework to the exact mutual information is complex-valued and the space-like distance and time-like one are determined by the amplitude and the phase of the generalized mutual information between two generic regions of the system which do not have to be space-like separated. We study the generalized mutual information defined using this quantum gravity and condensed matter physics. Based on the proposal of arxiv:1309.6282, we would like to use quantum entanglement between two regions to construct the partially transposed reduced density matrix ρA2 := ρA1 ⊗ ρA2, and correspondingly. We study the process of selective construction of invariants to obtain physically meaningful polynomial invariants for three and four qubit pure states. In this article, we report the exact relations between the concurrence of a two qubit reduced state and corresponding three or four qubit pure state invariants. Firstly, we obtain an analytical expression for concurrence of a given mixed state of two qubits in terms of determinants of negativity fonts in the three or four qubit pure state. For three qubits, a comparison with three angle and squared negativity expressed in terms of determinants of negativity fonts leads to three relations. These three conditions satisfied by the two-way and three-way correlations sum together and lead to well known CKW inequality. When a qubit pair is part of a four qubit pure state, it may be entangled to the rest of the system through two-way, three-way and four-way correlations. Monogamy equalities, satisfied by two-way, three-way and four-way non-local quantum correlations are presented for states belonging to classes of four qubit pure states with distinct entanglement types.

### Session J38 GQI: Focus Session: Entanglement and Mathematics of Quantum Information 212B
- Sean Carroll, California Institute of Technology

2:30PM J38.00001 Entanglement negativity in free-fermion systems, PO-YAO CHANG, XUEDA WEN, SHINSEI RUY, University of Illinois at Urbana-Champaign — We derive a general formula of the logarithmic negativity in free-fermion systems, using the overlap matrix to construct the partially transposed reduced density matrix ρA12 of a subsystem A := A1 ⊃ A2. In particular, we consider the negativity between two adjacent or disjoint regions in three systems: a homogeneous one-dimensional chain, the dimerized Su-Schrieffer-Heeger model, and the integer Quantum Hall state. For the negativity of two adjacent intervals in a homogeneous one-dimensional gas, we find agreement with the conformal field theory [P. Calabrese et al. Phys. Rev. Lett. 109, 130502 (2012)]. On the other hand, the negativity for the integer quantum Hall states satisfies the area law. Our method is applicable to the study of the negativity in any free-fermion systems.

2:42PM J38.00002 Fidelity of recovery and geometric squashed entanglement, KAUSHIK SEHADREESAN, MARK WILDE, Louisiana State University — We define the fidelity of recovery of a tripartite quantum state on systems A, B, and C as a measure of how well one can recover the full state on all three systems if system A is lost and a recovery operation is performed on system A alone. The surprisal of the fidelity of recovery (its negative logarithm) is an information quantity which obeys nearly all of the properties of the conditional quantum mutual information I(A:B|C), including non-negativity, monotonicity under local operations, duality, and a dimension bound. We then define an entanglement measure based on this quantity, which we call the geometric squashed entanglement. We prove that the geometric squashed entanglement is an entanglement monotone, that it vanishes if and only if the state on which it is evaluated is unentangled, and that it reduces to the geometric measure of entanglement if the state is pure. We also show that it is sub-additive, continuous, and normalized on maximally entangled states. Our results for the bipartite case can easily be extended to a multipartite fidelity of recovery and a multipartite geometric squashed entanglement.

### Session J38 212B — Generalized Entanglement Entropy and Space-Time Geometry of Quantum System
- ZHAO YANG, PATRICK HAYDEN, XIAOLIANG QI, Stanford Univ — Entanglement entropy plays a key role in relating quantum information with gravitational wave observables. Based on the proposal of arxiv:1309.6282, we would like to use quantum entanglement between two regions of a quantum system as a measure of the geometrical distance between them. However, since entanglement entropy can only be defined between space-like separated regions, we are forced to treat space and time inhomogeneously. In this work, we propose a generalized entanglement entropy (GEE) which is defined between two generic regions of the system which do not have to be space-like separated. We study the generalized mutual information defined using this generalized entanglement entropy, and demonstrate for several different systems that this provides a reasonable measure of space-time distance. The generalized mutual information is complex-valued and the space-like distance and time-like one are determined by the amplitude and the phase of the generalized mutual information, correspondingly. We study the properties of this generalized entropy and generalized mutual information, and apply this framework to the exact holographic mapping of free fermions in various conditions.
3:18PM J38.00005 Entanglement Spectrum of a Random Partition: Connection with the Anderson Transition, SAGAR VIJAY, LIANG FU, Massachusetts Inst of Tech-MIT — The entanglement spectrum of a topologically-ordered ground-state that is obtained by partitioning the system under consideration into two subsystems which extend throughout the bulk, has been recently shown to be a probe of the quantum critical behavior of the topological phase at the transition to a direct-product state \([1]\). Here, we generalize this notion of a bulk entanglement spectrum to extract universal information about disorder-driven topological phase transitions, by performing an extensive, random partition into two subsystems with probability \(p \in [0, 1]\). We apply our random partitioning procedure to a one-dimensional topological superconductor (TSC), and demonstrate that the phase diagram of the resulting entanglement Hamiltonian describes disorder-driven transitions to a Griffiths phase. \([1]\) T. H. Hsieh and L. Fu, Phys. Rev. Lett. 118, 106801 (2014).

3:30PM J38.00006 The existence of maximally multipartite entangled states of \(N\) particles may depend on their spin, JAY LAWRENCE, University of Chicago and Dartmouth College, MARIO GAETA, ANDREI KLIMOV, University of Guadalajara, Jal., Mexico — Maximally multipartite entangled states (MMES) are defined \([1]\) as pure states of \(N\) particles for which all subsystems consisting of up to half the particles \((k=\lfloor N/2\rfloor)\) are maximally mixed \((\rho_k \sim \frac{1}{2^k})\). Such states exist for two- or three-particle systems (Bell states for \(N=2\) and GHZ states for \(N=3\)), and this holds for any spin. The situation changes for four particles, where MMES states do not exist for spin-1/2 \((\text{dimension } d=2)\), but they do exist for all odd prime dimensions \(d\) or spin states \(s=(d-1)/2\). The latter systems exhibit three types of graph states, the GHZ and cluster states accessible to qubits, which are not MMES, but also a third type, called \(P\) states \([2]\), which are MMES but are not accessible to qubits. We show how the \(P\) states succeed while GHZ and cluster states fail by comparing (i) the reduced states of subsystems, and (ii) the measurement-induced pathways which project Bell states of any two particles. We discuss the possibilities that similar transitions exist for larger systems, for which it is known \([1]\) that MMES do not exist for eight or more qubits. \(1.\) L. Aaroud and N.J. Cerf, Phys. Rev. A 87, 012319 (2013). \(2.\) J. Lawrence, Phys. Rev. A 84, 022338 (2011).

3:42PM J38.00007 Entanglement and coherence in many-body dipolar systems, SUSANNE YELIN, University of Connecticut — The presence of dipoles in atoms and molecules can nonlinearly change the coherent dynamics and entanglement structure in many-body situations. I will present examples for atomic and molecular systems.

4:18PM J38.00008 Entanglement-Assisted Transformations of W-Type States, JIYANG XIAO, ERIC CHITAMBAR, Southern Illinois University - Carbondale — In multipartite systems, it is usually impossible to transform one entangled state into another via local operations and classical communication (LOCC). However, the transformation may become possible with the help of some extra entanglement. This kind of transformation is called entanglement-assisted LOCC (eLOCC). Beyond the bipartite setting, very little is known about eLOCC. We prove the optimal eLOCC probability for transforming a tripartite W-type state \(\frac{1}{\sqrt{2}}(x_{000} + x_{100} + x_{010} + x_{110})\) into a GHZ state \(\sqrt{(x_{011} + x_{101} + x_{110})}\) and a Bell state \(\frac{1}{\sqrt{2}}(x_{000} + x_{100} + x_{010})\) (which is not a GHZ state). We consider eLOCC transformations of a more general W-type state \(\frac{1}{\sqrt{2}(x_{011} + x_{101} + x_{110})}\) into GHZ and cluster states. We demonstrate that the phase diagram of the resulting entanglement Hamiltonian describes disorder-driven transitions to a Griffiths phase. \([1]\) T. H. Hsieh and L. Fu, Phys. Rev. Lett. 118, 106801 (2014).

4:42PM J38.00010 Jordan Algebraic Quantum Categories, MATTHEW GRAYDON, Perimeter Institute, HOWARD BARNUM, University of New Mexico, COZMIN UDULEC, Invenia Technical Computing Corporation, ALEXANDER WILCE, Susquehanna University — State cones in orthodox quantum theory over finite dimensional complex Hilbert spaces enjoy two particularly essential features: homogeneity and self-duality. Orthodox quantum theory is not, however, unique in that regard. Indeed, all finite dimensional formally real Jordan algebras — arenas for generalized quantum theories with close algebraic kinship to the orthodox theory — admit homogeneous self-dual positive cones. We construct categories wherein these theories are unified. The structure of composite systems is cast from universal tensor products of the universal C*-algebras enveloping ambient spaces for the constituent state cones. We develop, in particular, a notion of composition that preserves the local distinction of constituent systems in quaternionic quantum theory. More generally, we explicitly derive the structure of hybrid quantum composites with subsystems of arbitrary Jordan algebraic type.

4:54PM J38.00011 Jacobi – type identities and the underlying quantal algebra, SAMIR LIPOVACA, None — Reference \([1]\) introduced two identities written in terms of single commutators and anticommutators for any three elements of an arbitrary associative algebra where one is a consequence of other which is called the fundamental identity. From the fundamental identity a set of four other identities, represented in terms of double commutators and anticommutators is derived. We will show that three of these identities are in fact the defining identities of the quantal algebra. In this light, \([1]\) did actually derive an underlying quantal algebra for an arbitrary associative algebra from the fundamental identity. Remarkably, the proof of the Theorem 2 showed that the existence of this underlying quantal algebra is equivalent to the associativity condition. A generalization to the super case of the quantal algebra is, in essence, derived in the section 3 of \([1]\).

\([1]\) arXiv:1304.5050v2 [math-ph]

5:06PM J38.00012 Quantum Bochner’s theorem for phase spaces built on projective representations\(^1\), NINNAT DANGNIAM, CHRISTOPHER FERRIE, Univ of New Mexico — Bochner’s theorem gives the necessary and sufficient conditions on a characteristic function such that it corresponds to a true probability density function. In the Wigner phase space picture, quantum Bochner’s theorem gives the necessary and sufficient conditions on the quantum characteristic function such that it corresponds to a valid quantum state and such that its Fourier transform is a true probability density. We extend this theorem to discrete phase space representations which possess enough symmetry to define a generalized Fourier transform.

\(^1\)NSF, Canadian Government
5:18PM J38.00013 Galois-unitary operators that cycle mutually-unbiased bases1. HOAN DANG, Perimeter Institute for Theoretical Physics & University of Waterloo, MARCUS ALPÉBÉY, University of Sydney, INGEMAR BENGTSSON, Stockholms University — Wigner’s theorem states that probability-preserving transformations of quantum states must be either unitary or anti-unitary. However, if we restrict ourselves to a subspace of a Hilbert space, it is possible to generalize the notion of anti-unitaries. Such transformations were recently constructed in search of Symmetric Informationally-Complete (SIC) states. They are called Galois-unitaries (g-unitaries for short), as they are unitaries composed with Galois automorphisms of a chosen number field extension. Despite certain bizarre behaviors of theirs, we show that g-unitaries are indeed useful in the theory of Mutually-Unbiased Bases (MUBs), as they help solve the MUB-cycling problem and provide a construction of MUB-balanced states.

1 HD was supported by the Natural Sciences and Engineering Research Council of Canada and the Vanier Canada Graduate Scholarship

Tuesday, March 3, 2015 2:30PM - 5:30PM –

2:30PM J39.00001 Implementing fault tolerance in a superconducting quantum circuit, RAMI BARENDS, Google, Santa Barbara — The surface code error correction scheme is appealing for superconducting circuits as the fundamental operations have been demonstrated at the fault-tolerant threshold. Here, we present experimental results on the repetition code, a one-dimensional primitive of the surface code which can detect bit-flip errors, implemented on a device consisting of nine Xmon transmon qubits. We discuss the basic mechanics of error detection, show preservation of a Greenberger-Horne-Zeilinger state, and show suppression of environmentally-induced error.

3:06PM J39.00002 Performing repetitive error detection in a superconducting quantum circuit, J. KELLY, UC Santa Barbara, R. BARENDS, A. FOWLER, Google, Santa Barbara, A. MEGRANT, UC Santa Barbara, E. JEFFREY, Google, Santa Barbara, T. WHITE, UC Santa Barbara, D. SANK, J. MUTUS, Google, Santa Barbara, B. CAMPBELL, UC Santa Barbara, Y. CHEN, Google, Santa Barbara, Z. CHEN, B. CHIARO, A. DUNSWORTH, I.-C. HOI, C. NIEL, P. J. O’MALLEY, UC Santa Barbara, P. ROUSHAN, Google, Santa Barbara, C. QUINTANA, A. VAINSENCHER, J. WENNER, A. N. CLELAND, UC Santa Barbara, J. M. MARTINIS, University of California and Google, Santa Barbara — Recently, there has been a large interest in the surface code error correction scheme, as gate and measurement fidelities are near the threshold. If error rates are sufficiently low, increased systems size leads to suppression of logical error. We have combined high fidelity gate and measurements in a single nine qubit device, and use it to perform up to eight rounds of repetitive bit error detection. We demonstrate suppression of environmentally-induced error as compared to a single physical qubit, as well as reduced logical error rates with increasing system size.

3:18PM J39.00003 A Leakage-Resilient Approach to Fault-Tolerant Quantum Computing with Superconducting Elements1. JOYDIP GHOSH, University of Calgary, AUSTIN FOWLER, University of California, Santa Barbara — Superconducting qubits, while promising for scalability and long coherence times, contain more than two energy levels, and therefore are susceptible to errors generated by the leakage of population outside of the computational subspace. Such leakage errors are currently considered to be a prominent roadblock towards fault-tolerant quantum computing with superconducting qubits. Fault-tolerant quantum computing using topological codes is based on sequential measurements of multi-qubit stabilizer operators. In this talk, I propose a leakage-resilient scheme to perform repetitive measurements of multi-qubit stabilizer operators, and then discuss how to use this scheme as an ingredient to develop a leakage-resilient approach for surface code quantum error correction with superconducting circuits. Our protocol is based on SWAP operations between data and ancilla qubits at the end of every cycle, requiring read-out and reset operations on every physical qubit in the system, and thereby preventing persistent leakage errors from occurring.

1 ODNI, IARPA, NSERC, AITF and University of Calgary’s Eyes High Fellowship Program.

3:30PM J39.00004 Characterization of superconducting qubits in a planar lattice1. SRIKANTH SRINIVASAN, ANTONIO CORCOLES, EASWAR MAGESAN, NICHOLAS BRONN, JARED HERTZBERG, JAY GAMBITTA, MATTHIAS STEFFEN, JERRY CHOW, IBM T.J. Watson Research Center — The surface code is a promising implementation for quantum computing because of its relatively lenient thresholds for fault tolerance. The physical layout contains two general classes of qubits, code and syndrome, arranged in a planar lattice. In this talk we present complete characterization of a four qubit planar lattice and discuss the experimental challenges for achieving high fidelity. This includes integrating four independent readouts using parametric amplifiers, gate calibration procedures, and sample design. Careful device design is required for efficient signal delivery without deleterious microwave crosstalk. The low crosstalk is validated through measurements of simultaneous randomized benchmarking on both single and two-qubit entangling gates. This work is a step towards realizing the surface code on a planar lattice.

1 We acknowledge support from IARPA under contract W911NF-10-1-0324.

3:42PM J39.00005 Arbitrary error detection in a planar lattice of the surface code1. ANTONIO CORCOLES, EASWAR MAGESAN, SRIKANTH SRINIVASAN, NICHOLAS BRONN, JARED HERTZBERG, ANDREW CROSS, MATTHIAS STEFFEN, JAY GAMBITTA, JERRY CHOW, IBM T J Watson Res Ctr — We detect arbitrary single-qubit errors on a system of four superconducting qubits arranged in a planar lattice, amenable to the surface code. The error detection protocol is based on the stabilizer formalism and protects a codeword encoded on an entangled two-qubit state by quantum non-demolition parity measurements, ZZ and XX. These parity measurements are performed using the other two qubits acting as syndromes. We introduce a bit- or phase-flip single-qubit error applied to the codeword and show that this error can be revealed uniquely in the syndromes. The -non-trivial- geometric arrangement of the qubits is essential to the surface code algorithm and is therefore extendable throughout the two-dimensional plane, encoding progressively larger logical Hilbert spaces towards a fully scaled fault-tolerant quantum computer.

1 We acknowledge support from IARPA under contract W911NF-10-1-0324.
3:54PM J39.00006 Characterizing Quantum Gates with Iterated Randomized Benchmarking on Superconducting Qubits1. SARAH SHELDON, LEV S. BISHOP, STEFAN FILIPP, MATTHIAS STEFFEN, JERRY M. CHOW, JAY M. GAMBETTA, IBM T.J. Watson Research Center, Yorktown Heights, NY, USA — With coherence times exceeding 40us and single qubit gate fidelities of 0.9996, we find our current calibration schemes and DRAG pulse shaping fall short of the coherence limit. It is therefore necessary to develop new methods of finding and addressing errors in the qubit control. We present a method for characterizing small errors using a variation of interleaved randomized benchmarking to identify sources of systematic errors. Our new scheme, iterative randomized benchmarking, interleaves repetitions of gates in a randomized benchmarking sequence to determine the type of error on the target gate. The scaling of the fidelity with the number of interleaved gates reveals if the gate errors are coherent or incoherent. Experimental data indicates that our system is sensitive to an over-rotation by an angle of \( \pi/128 \). We also apply this technique to identify sources of coherent errors that may be reducing our randomized benchmarking error rates.

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1This work is supported by ARO under contract W911NF-14-1-0124.

4:06PM J39.00007 Detecting and Reducing Gate Leakage in Superconducting Qubits using Randomized Benchmarking. ZHAN, J. KELLY, UC Santa Barbara, R. BAREND, Google, Santa Barbara. B. CAMPBELL, UC Santa Barbara, Y. CHEN, Google, Santa Barbara. B. CHIARO, A. DUNSWORTH, UC Santa Barbara, A. FOWLER, Google, Santa Barbara. I.-C. HOI, UC Santa Barbara. E. JEFFREY, Google, Santa Barbara. A. MGRANT, UC Santa Barbara, J. MUTUS, Google, Santa Barbara. C. NEILL, P.I.J. O’MALLEY, C. QUINTANA, UC Santa Barbara, P. ROUSHAN, D. SANK, Google, Santa Barbara. A. VAINSENCHER, J. WENNER, T. WHITE, UC Santa Barbara. A. N. KOROTKOV, UC Riverside, A.N. CLELAND, UC Santa Barbara, J.M. MARTINIS, University of California and Google, Santa Barbara. — Superconducting qubits are a promising platform for building a quantum computer due to their scalability and ease of control. One potential drawback is the existence of more than two energy levels, which can allow the qubit to leak out of the computational subspace when performing operations. This leakage error is particularly detrimental in the surface code scheme, which leads to correlated errors. We will present a method for characterizing gate leakage rates using randomized benchmarking, and present strategies based on these results for reducing leakage.

4:18PM J39.00008 Efficient State Tomography for Continuous Variable Systems. CHAO SHEN, LUYAO JIANG, STEFAN KRASTANOV, VICTOR V. ALBERT, REINIER HEÈRES, BRIAN VLASTAKIS, ROB SCHOLEKOPF, LIANG JIANG, Yale University — We propose an efficient and error robust scheme for state tomography of a continuous variable system, which is dispersively coupled to a two-level system. Our adaptive tomography protocol offers a significant speed up compared to the conventional Wigner tomography for a practically interesting class of states, such as Schrodinger cat states. In the presence of typical experimental errors, the number of measurements required is still close to the information theoretic limit. Our proposals can be readily implemented in platforms such as superconducting transmon qubit inside a microwave cavity.

4:30PM J39.00009 Implementing gates in a fluxonium-like qubit with suppressed wavefunction overlap. NATHAN EARNEST, YAO LU, DAVID MCKAY, University of Chicago, DAVID CZAPLEWSKI, LEONIDAS OCOLA, Argonne National Lab, DAVID SCHUSTER, University of Chicago. — Superconducting Josephson junction qubits are a promising technology for quantum information processing, but are limited by finite lifetimes. The lifetime of the qubit, according to Fermi’s golden rule, is dictated by the overall overlap of the |0> and |1> wavefunctions and so a long lived qubit may be constructed from states with well-isolated wavefunctions. A “double-well” fluxonium-like qubit [1] with well-separated degenerate ground states is obtained by increasing the qubit energy EJ and decreasing the charging energy EC. This qubit implementation is expected to have T2s similar to a tunable transmon qubit but, due to the isolated wavefunctions, has promise for long T1s that are insensitive to arbitrary forms of noise. This isolation, however, makes performing arbitrary quantum gates more difficult as wavefunction overlap also allows for arbitrary qubit operations. In this presentation, we will discuss methods for performing arbitrary quantum gates, the implications for decoherence due to flux noise, and discuss experimental progress.

4:42PM J39.00010 High-fidelity single-shot Toffoli gate with superconducting elements via quantum control. EHSAN ZAHEDINEJAD, JOYDIP GHOSH, BARRY SANDERS, University of Calgary — A single-shot Toffoli, or controlled-controlled-NOT, gate is desirable for classical and quantum information processing. The Toffoli gate alone is universal for reversible computing and, accompanied by the Hadamard gate, forms a universal gate set for quantum computing. The Toffoli gate is a key ingredient for (non-topological) quantum error correction. Currently Toffoli gates are achieved by decomposing into sequentially implemented single- and two-qubit gates, which requires much longer times and yields lower overall fidelities compared to a single-shot implementation. We develop a quantum-control procedure to directly construct single-shot Toffoli gates and devise a scheme for three nearest-neighbor-coupled superconducting transmon systems that should operate with 99.9% fidelity under realistic conditions. The gate is achieved by a non-greedy quantum control procedure using our enhanced version of the Differential Evolution algorithm.

4:54PM J39.00011 The Design of Control Pulses for Heisenberg Always-On Qubit Models. RUDOLPH MAGYAR, Sandia National Laboratories. — One model for a universal quantum computer is a spin array with constant nearest neighbor interactions and a controlled unidirectional site-specific magnetic field to generate unitary transformations. This system can be described by a Heisenberg spin Hamiltonian and can be simulated for on the order of 50 spins. It has recently been shown that time-dependent density functional inspired methods may be used to relate various spin models of qubits to ones that may be easier to compute numerically allowing potentially the efficient simulation of greater numbers of spins. One of the challenges of such an agenda is the identification of control pulses that produce desired gate operations (CNOT and single qubit phase gates). We apply control theory to design a universal set of pulses for a Heisenberg always-on model Hamiltonian for a few qubits and compute to known pulses when available. We suggest how this approach may be useful to design control pulses in other realistic designs. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Security Administration under contract DE-AC04-94AL85000.

5:06PM J39.00012 Demonstrated control of a Transmon using a Reciprocal Quantum Logic digital circuit - Part 1. MICHA STOUTMORE, JAMES MEDFORD, QUENTIN HERR, OFER NAAMAN, HAROLD HEARNE, JOEL STRAND, ANTHONY PRZYBYSZ, AARON PESETSKI, JOHN PRZYBYSZ, Northrop Grumman Corporation. — We report on experiments in which we used a Reciprocal Quantum Logic circuit to perform Z rotations on a Transmon qubit. Reciprocal Quantum Logic (RQL) [1] is a low-power superconducting digital technology based on paired single-flux quantum voltage pulses. Here we discuss the RQL hardware used in these experiments - an RQL output amplifier [2] whose output is non-return-to-zero (NRZ) encoded 3 mV differential signal, and is primarily intended for transmitting RQL data signals to standard room temperature CMOS hardware. We demonstrate the circuit operation at both 4 K and 20 mK with wide circuit operating margins. [1] J. Appl. Phys. 109, 103903 (2011) [2] Supercond. Sci. Technol. 23, 022044 (2010)
5:18PM J39.00013 Demonstrated control of a Transmon using a Reciprocal Quantum Logic digital circuit - Part 2. JAMES MEDFORD, MICAH STOUTIMORE, QUENTIN HERR, OFER NAAMAN, HAROLD HEARNE, JOEL STRAND, ANTHONY PRZYBYSZ, AARON PESETSKI, JOHN PRZYBYSZ, Northrop Grumman Corporation — We demonstrate coherent manipulation of a 2D asymmetric Transmon qubit using a Reciprocal Quantum Logic (RQL) [1] distributed output amplifier mounted at 20 mK. The RQL amplifier provided active isolation and amplification for signals generated by room temperature equipment. We measured a 30% suppression of the Transmon lifetime when connected to the RQL circuit, which we primarily attributed to static power dissipation associated with the on-chip 50 Ohm source termination of the amplifier. [1] J. Appl. Phys 109, 103903 (2011)

Tuesday, March 3, 2015 2:30PM - 5:30PM – Session J41 DPOLY: Focus Session: Organic Electronics and Photonics, Optical and Electrical Properties 214A - Michael Chabinyc, University of California, Santa Barbara

2:30PM J41.00001 BREAK –

3:06PM J41.00002 Measuring Exciton Diffusion in Conjugated Polymer Films with Super-resolution Microscopy1. SAMUEL PENWELL, LUCAS GINSBERG, RODRIGO NORIEGA MANEZ, NAOMI GINSBERG, UC Berkeley — Conjugated polymers are highly tunable organic semiconductors, which can be solution processed to form thin films, making them prime candidates for organic photovoltaic devices. One of the most important parameters in a conjugated polymer solar cell is the exciton diffusion length, which depends on intermolecular couplings, and is typically on the order of 10 nm. This mean exciton migration can vary dramatically between films and within a single film due to heterogeneities in morphology on length scales of 10’s to 100’s nm. To study the variability of exciton diffusion and morphology within individual conjugated polymer films, we are adapting stimulated emission depletion microscopy, STED is typically used in biology with well-engineered fluorescent labels or on NV-centers in diamond. I will, however, describe how we have demonstrated STED in conjugated polymer films of MEH-PPV and CN-PPV by taking care to first understand the film’s photophysical properties. This new approach provides a way to study exciton diffusion by utilizing subdiffraction optical excitation volumes. In this way, we will obtain a spatiotemporal map of exciton distributions that will help to correlate the energetic landscape to film morphology at the nanoscale. This research is supported in part by the Department of Energy Office of Science Graduate Fellowship Program (DOE SCGF), made possible in part by the American Recovery and Reinvestment Act of 2009, administered by ORISE-ORAU under contract no. DE-AC05-06

3:18PM J41.00003 Probing the exciton coherent size in organic crystals and the effect of polar bonds1. WAI-LUN CHAN, TI WANG, Univ of Kansas — Exciton transport in organic crystals is commonly described by a series of incoherent hopping. This is no longer valid if the transport range is on the order of the exciton coherent size. Recently, it has been proposed that exciton delocalization is responsible for ultrafast charge separation found in bulk heterojunction (BHJ) photovoltaics. However, the coherent exciton transport range has not been measured. Here, by using time-resolved photoemission and zinc phthalocyanine crystals as a model system, we observe a transition from coherent to incoherent transport while the exciton coherent size is decreasing. The electron-vibration interaction is found to be the main driving force that reduces the exciton coherent size. Furthermore, by using phthalocyanine molecules with a polar bond, e.g. titanyl phthalocyanine, we observe an upshift in electron energy as a function of time after photo-excitation. Our observation can be explained by spontaneous exciton dissociation after photoexcitation, which produces a more delocalized charge transfer state. This would explain why BHJ made by ‘push-pull’ polymers or small molecules, which consist of electron-rich and electron-deficient units, often have a better charge separation efficiency.

The work is supported by US National Science Foundation, grant DMR-1351716.

3:30PM J41.00004 Fully three dimensional calculations of c-AFM current flow patterns, including space charge effects, traps and fibrous morphologies, KANOKKORN PIMCHAROEN, PHILLIP DUBURY. Department of Physics and Astronomy, Michigan State University — Organic semiconductors are promising materials for many optoelectronic devices due to their versatile applications and low-cost fabrication, including organic photovoltaics (OPV), light-emitting diodes (OLED), and thin-film transistors (OTFT). The performance of these devices is controlled by charge transport which primarily depends on the nanoscale morphology. Unlike other microscopies, conductive Atomic Force Microscope (c-AFM) is capable of characterizing both nanoscale morphology and local electronic properties simultaneously. With this unique ability, c-AFM has been used extensively to characterize these organic semiconductor devices in the past decade, however the spreading of current from the tip geometry in the presence of traps, which are ubiquitous in these materials, is not well understood. We have developed a fully three dimensional device simulation tool enabling treatment of inhomogeneous systems including c-AFM tip geometry, spatially varying trap distributions, and fibrous morphologies. Results characterizing charge transport in the fibrous morphologies and in the presence of traps will be discussed, including the effect of traps and space charge effects on current spreading from the c-AFM tip.

3:42PM J41.00005 Interface structure of P3HT/SWNT blend and charge separation process on it. KATSUHIKO NISHIMURA, RYOTA JONO, MIKIYA FUJII, KOICHI YAMASHITA, Department of Chemical System Engineering, University of Tokyo and JST, CREST — We investigated the mechanism that suppression of charge recombinations takes place in blends of regioregular Poly-3-HexylThiophene (rrP3HT) and semiconducting Single Walled Carbon Nanotube (scSWNT) only if excess P3HT exists. The rrP3HT/scSWNT blend seems to be suitable for OPV application because rrP3HT is common acceptor material and also can be used for purifying scSWNT and removing metallic one. The suppression of charge recombinations is attributed to unique helical supramolecular structure at P3HT/SWNT interfaces. However, the detailed mechanism of the suppression has not been clarified yet. In this presentation, we show that side chains of P3HT are important in formation of the helical structure rather than alignment of main chains with graphene lattices of SWNT by using semi-empirical quantum chemistry method. Moreover, HOMO levels of P3HT molecules at the interfaces estimated to be lower than those in crystalline domain because of disordered stacking due to formation of the helical structure. This difference in HOMO levels can act as the driving force for escape of charge carriers from the interfaces and can result to the suppression of charge recombinations. [1] S. D. Stranks et. al., Nano. Lett. 11, 66
The conversion of excitons into charge within organic solar cells is complicated by bound electronhole pairs, or charge transfer states at donor/acceptor interfaces. The solar cell requires generating an efficient current. Thus it is necessary that charge transfer is further separated into free charge carriers to be transported to electrode. We focus on the improved the conversion efficiency of bulk-heterojunction organic solar cells. We use dependent density functional theory with CAM-B3LYP/6-31G(d) to study the oscillator strengths, electronic structure, HOMO-LUMO band gap and energy level in several polymer (donor): fullerene (acceptor) blends, such as MDMO-PPV, PCDDBT, PCPDDBT, PBDB3, PTB7 and PTBF2 with PC70BM. To determine the effective physical factor in light energy conversion, we consider (i) charge transfer type excitation generated directly by photoinduced electron transition in the donor/acceptor interface (ii) the factors for controlling the conversion efficiency such as short-circuit current density and closed circuit voltage.

On the theory of Carrier's Electrostatic Interaction near an Interface.

Micheal Watters, Hossein Hashemi, John Kieffer, Univ of Michigan - Ann Arbor  Heterojunction interfaces are common in non-traditional photovoltaic device designs, such as those based on small molecules, polymers and carbon nanotubes [1]. We have developed a number of the effective Hamiltonians for the heterojunction interface region on carrier/exciton energetics using a mixture of both semi-classical and quantum electrostatic methods, ab initio methods, and statistical mechanics. Our theoretical analysis has yielded several useful relationships and numerical recipes that should be considered in device design regardless of the particular materials system. As a demonstration, we highlight these formalisms as applied to carriers and polaron pairs near a C60/subphthalocyanine interface [1]. On the regularly ordered areas of the heterojunction, the effect of the interface is a significant set of corrections to the carrier energies, which in turn directly affects device performance.

2:30PM J42.00001 Phase Transitions on Random Lattices: How Random is Topological Disorder?1, HATEM BARGHATHI, THOMAS VOJTA, Missouri Univ of Sci & Tech — We study the effects of topological (connectivity) disorder on phase transitions. We identify a broad class of random lattices whose disorder fluctuations decay much faster with increasing length scale than those of generic random systems, yielding a wandering exponent of $\omega = (d - 1)/(2d)$ in $d$ dimensions. The stability of clean critical points is thus governed by the criterion $(d + 1)\nu > 2$ rather than the usual Harris criterion $d\nu > 2$, making topological disorder less relevant than generic randomness. The Imry-Ma criterion is also modified, allowing first-order transitions to survive in all dimensions $d > 1$. These results explain a host of puzzling violations of the original criteria for equilibrium and nonequilibrium phase transitions on random lattices. We discuss applications, and we illustrate our theory by computer simulations of random Voronoi and other lattices.

1This work was supported by the NSF under Grant Nos. DMR-1205803 and PHYS-1066293. We acknowledge the hospitality of the Aspen Center for Physics.

2:42PM J42.00002 Shear Jamming in Frictionless Particulate Media1, THIBAULT BERTRAN, COREY S. O’HERN, Yale University, R.P. BEHRINGER, Duke University, BULBUL CHAKRABORTY, Brandeis University, MARK D. SHATTUCK, City College of the City University of New York — We numerically study two-dimensional packings of frictionless bidisperse disks created using compressive and simple shearing protocols. To create jammed packings by compression, we start $N$ particles from random positions and grow their diameters followed by relaxation of particle overlaps using energy minimization. These compressed packings exist over a range of packing fractions $\phi$. As a result, during compression the system may reach a $\phi$ above the minimum value before jamming. If this unjammed packing is then sheared by a strain $\gamma$, it can jam. Using a combination of compression and shearing, we can define jamming protocols as trajectories in the $(\phi, \gamma)$ plane that yield jammed packings. In this plane, we can reach a particular point $(\phi_n, \gamma_n)$ in many ways. We will focus on two protocols: (1) shearing to $\gamma_n$ at $\phi = 0$ followed by compression to $\phi_n$ at $\gamma = \gamma_n$, and (2) compression to $\phi_n$ at $\gamma = 0$ followed by shearing to $\gamma_n$ at $\phi = \phi_n$. For protocol 1, we find that the probability of finding a jammed packing at $\phi$ and $\gamma$, $P(\phi, \gamma) = Q(\phi)$ is independent of $\gamma$. For protocol 2, we use a simple theory to deduce $P(\phi, \gamma)$ from $Q(\phi)$.

1W. M. Keck Foundation Science and Engineering Grant

2:54PM J42.00003 Three Dimensional Characterization of Quantum Vortex Dynamics in Superfluid Helium. DAVID MEICHEL, DANIEL LATHROP, University of Maryland — Vorticity is constrained to line-like topological defects in quantum superfluids, such as liquid Helium below the Lambda transition. We have invented a novel method to disperse fluorescent nanoparticles directly into the superfluid which become trapped on the vortex cores, providing optical tracers. Using a newly constructed multi-camera stereoscopic microscope, we present data dynamically characterizing vortex reconnections and the subsequent emission of Kelvin waves fully in three dimensions. Statistics of thermally driven counterflow will be compared in 3D to previous measurements in projection.

3:06PM J42.00004 Defect-Stabilized Phases in Extensible Active Nematics. GABRIEL REDNER, STEPHEN DECAMP, ZVONIMIR DOGIC, MICHAEL HAGAN, Brandeis University — Active nematics are liquid crystals which are driven out of equilibrium by energy-dissipating active stresses. The equilibrium nematic state is unstable in these materials, leading to beautiful and surprising behaviors including the spontaneous generation of topological defect pairs which stream through the system and later annihilate, yielding a complex, seemingly chaotic dynamical steady-state. In this talk, I will describe the emergence of order from this chaos in the form of previously unknown broken-symmetry phases in which the topological defects themselves undergo orientational ordering. We have identified these defect-ordered phases in two realizations of an active nematic: first, a suspension of extensible bundles of microtubules and molecular motor proteins, and second, a computational model of extending hard rods. I will describe the defect-stabilized phases that manifest in these systems, our current understanding of their origins, and discuss whether such phases may be a general feature of extensible active nematics.

3:18PM J42.00005 Jamming Percolation in Three Dimensions. EIAL TEOMY, Tel Aviv University, ANTIMA GHOSH, Weizmann Institute, YAIR SHOKEF, Tel Aviv University — We introduce a three-dimensional kinetically-constrained model for jamming and glasses [1], and prove that the fraction of frozen states is continuous at the directed-percolation critical density. In agreement with the accepted scenario for jamming- and glass-transitions, this is a mixed-order transition; the discontinuity is accompanied by diverging length- and time-scales. Because one-dimensional directed-percolation paths comprise the backbone of frozen particles, the unfrozen rattlers may use the third dimension to travel between their cages. Thus the dynamics are diffusive on long-time scales even above the critical density for jamming. Our new model is a non-trivial extension of the two-dimensional spiral model [2].


3:30PM J42.00006 Diffuse globally, compute locally: a cyclist approach to modeling long time robot locomotion. TINGNAN ZHANG, DANIEL GOLDMAN, PREDRAG CVITANOVIĆ, Georgia Institute of Technology — To advance autonomous robots we are interested to develop a statistical/dynamical description of diffusive self-propulsion on heterogeneous terrain. We consider a minimal model for such diffusion, the 2-dimensional Lorentz gas, which abstracts the motion of a light, point-like particle bouncing within a large number of heavy scatters (e.g. small robots in a boulder field). We present a precise computation (based on exact periodic orbit theory formula for the diffusion constant) for a periodic billiard wall. For small inter-disk separations, with periodic orbits up to $10^6$, our method is efficient and accurate. For other parameter choices, the boundaries become simple at sufficiently small but widely different scales across the phase space, despite the observed sensitive dependence on initial conditions. However, such scales are often far below the current computational resolution even for low-dimensional dynamical systems.

3:42PM J42.00007 Fractal Geometry of Undriven Dissipative Systems. XIAOWEN CHEN, TAKASHI NISHIKAWA, ADILSON E. MOTTER, Department of Physics and Astronomy, Northwestern University — Traditional studies of chaos in conservative or driven dissipative systems have established a correspondence between sensitive dependence on initial conditions and fractal basin boundaries. Here, I will present on a new type of chaos due to transient interactions with transient chaotic saddles in undriven dissipative systems. I will show that such systems can develop complicated trajectories, but only exhibit fractality and the Wada property at all scales for specific parameter choices at which the dynamics have a degenerate fixed point. For other parameter choices, the boundaries become simple at sufficiently small but widely different scales across the phase space, despite the observed sensitive dependence on initial conditions. However, such scales are often far below the current computational resolution even for low-dimensional dynamical systems.
3:54PM J42.00008 On Path Attractors, Stochastic Bifurcation and Dephasing In Genetic Networks, DAVIT POTOYAN, Rice University — Gene regulatory networks are driven stochastic systems with the noise having two distinct components due to the to birth and death of metabolite molecules and dichotomous nature of gene state switching. Presence of dichotomous gene noise alone has the capacity to significantly perturb the optimal transition paths and steady state probability distributions compared to the macroscopic models and their weak noise approximations. Most importantly dichotomous gene noise can also lead to multimodal distributions due to stochastic bifurcation of the underlying nonlinear dynamical system, which underlies the mechanism of formation of population heterogeneity. In this note we derive approximate path based expression of the time dependent probability of gene circuits which enables deeper exploration of the role of gene noise in formation of epigenetic states and dephasing-like phenomena.

4:06PM J42.00009 Model reduction by manifold boundaries, MARK TRANSTRUM, Brigham Young University — Mathematical models of physical systems can be interpreted as manifolds of predictions embedded in the space of data. For models of complex systems with many parameters, the corresponding model manifold is very high-dimensional but often very thin. This “low effective dimensionality” has been described as a hyper-ribbon and is characteristic of systems exhibiting simple, emergent behavior. I discuss a new model reduction method, the manifold boundary approximation method, which constructs a series of models by iteratively approximating the high-dimensional, thin manifold by its boundary. This model reduction method unifies many different model reduction techniques, such as renormalization group and continuum limits, while greatly expanding the domain of tractable models. I demonstrate with a model of a complex signaling network from systems biology. The method produces a series of approximations which reveal how microscopic parameters are systematically “compressed” into a few macroscopic degrees of freedom, effectively building a bridge between the microscopic and the macroscopic descriptions.

4:18PM J42.00010 Saturation in coupled oscillators, AHMED ROMAN, JAMES HANNA, Virginia Polytechnic Institute and State University — We consider a weakly nonlinear system consisting of a resonantly forced oscillator coupled to an unforced oscillator. It has long been known that, for quadratic nonlinearities and a 2:1 resonance between the oscillators, a perturbative solution of the dynamics exhibits a phenomenon known as saturation. At low forcing, the forced oscillator responds, while the unforced oscillator is quiescent. Above a critical value of the forcing, the forced oscillator’s steady-state amplitude reaches a plateau, while that of the unforced oscillator increases without bound. We show that, contrary to established folklore, saturation is not unique to quadratically nonlinear systems. We present conditions on the form of the nonlinear couplings and resonance that lead to saturation. Our results elucidate a mechanism for localization or diversion of energy in systems of coupled oscillators, and suggest new approaches for the control or suppression of vibrations in engineered systems.

4:30PM J42.00011 Regular and Chaotic Motion of a Piecewise Smooth Bouncer, CAMERON LANGER, BRUCE MILLER, Texas Christian University — The dynamical properties of a particle in a gravitational field colliding with a rigid wall moving with piecewise constant velocity are studied. The linear nature of the wall’s motion permits further analytical investigation than is possible for the system’s sinusoidal counterpart. We consider three distinct collision models: elastic, inelastic with either a constant or velocity dependent restitution coefficient. We confirm the existence of unbounded orbits (Fermi acceleration) in the elastic model, and find regular and chaotic behavior in the inelastic cases. We also examine trajectories wherein the particle experiences an infinite number of collisions in a finite time i.e., the phenomenon of inelastic collapse. We address these “sticking solutions” and their relation to both the overall dynamics and the phenomenon of self-reanimating chaos. Additionally, we investigate the long-term behavior of the system as a function of both initial conditions and parameter values. We find novel bifurcation phenomena not seen in the sinusoidal model. Our investigations reveal that, although the piecewise linear bouncer is a simplified version of the sinusoidal model, it captures essential features of the latter and also exhibits behavior unique to the discontinuous dynamics.

4:42PM J42.00012 Nonlinear Dynamics and Thermodynamics of a One-Dimensional Plasma in Simulation, PANKAJ KUMAR, BRUCE MILLER, Texas Christian Univ — We report on the results of a simulation study of the nonlinear dynamics and the thermodynamics of a single-component one-dimensional plasma with periodic boundary conditions. For a system of the plasma with three particles, we plot the Poincare maps and calculate the largest Lyapunov exponents. The results indicate that the three-particle system exhibits interesting dynamics with the phase-space containing periodic, quasiperiodic, as well as chaotic regions for different initial conditions. Special periodic orbits have been identified and their stabilities have been examined for the three-particle system. The behavior of the system in the thermodynamic limit has been simulated using large versions of the system and the dependences of the pressure, the coupling strength and the largest Lyapunov exponent on the average per-particle kinetic energy are presented. The results of the thermodynamic-limit simulations indicate that the net pressure is equal to the kinetic pressure for all temperatures and there is no phase transition.

4:54PM J42.00013 Evolution of a One-dimensional, Two Component, Universe, YUI SHIOZAWA, BRUCE MILLER, Texas Christian Univ, JEAN-LOUIS ROUET, Universite d’Orleans — While the universe we observe today exhibits local filament-like structures, with stellar clusters and large voids between them, the primordial universe is believed to have been nearly homogeneous with slight variations in matter density. To understand how the observed hierarchical structure was formed, researchers have developed a one-dimensional analogue of the universe that can simulate the evolution of a large number of matter particles. Investigations to date demonstrate that this model reveals structure formation that shares essential features with the three-dimensional observations. In the present work, we have expanded on this concept to include two species of matter, specifically dark matter and luminous matter. In our simulation, luminous matter is treated in a way that loses energy in interaction with itself. The results of the simulations clearly show the formation of a Cantor set like multifractal pattern over time in configuration space as well as in phase space. In contrast with most earlier studies, mass-orientation methods for computing the multifractal dimensions were performed on various subsets of the matter distribution in order to understand the bottom-up structure formation.

5:06PM J42.00014 Cosmology in One Dimension: Fractal Dimensions from Mass Oriented Partitions, BRUCE MILLER, Texas Christian University, JEAN-LOUIS ROUET, Universite d’Orleans, YUI SHIOZAWA, Texas Christian University — The distribution of visible matter in the universe has its origin in the weak fluctuations of density that existed at the epoch of recombination. The hierarchical distribution of the present universe, with its galaxies, clusters and super-clusters of galaxies indicates the absence of a natural length scale. Numerical simulations of a one-dimensional system permit us to closely follow the evolution stage with an initial perturbation in the Hubble flow. The limitation to one dimension removes the necessity to make approximations in calculating the gravitational field and the system dynamics. It is then possible to accurately follow the trajectories of particles for a long time. The simulations show the emergence of a self-similar hierarchical structure in both the phase space and the configuration space and invite the implementation of a multifractal analysis. Here we apply four different methods for computing generalized fractal dimensions Dq of the distribution of particles in configuration space. We first employ the conventional methods based on partitions of equal size and then less familiar methods based on partitions of equal mass. We show that the latter are superior for computing generalized dimensions for indices q < −1 which characterize regions of low density.

Tuesday, March 3, 2015 2:30PM - 5:18PM
Session J43 DPOLY GSOFT: Focus Session: Manipulating Glasses: Mechanics 214C - Daniel Sussman, University of Pennsylvania
Creep experiments were performed for the temperatures ranging from Tg,macroscopic−14°C to Tg,macroscopic+19°C. Time temperature superposition and time thickness superposition were applied to create reduced creep curves, and those were compared with macroscopic data [J. Non-Cryst. Solids. 2002, 307, 790-801]. The results showed that the time temperature superposition was applicable in the glassy relaxation regime to the steady-state plateau regime. However in the long time response of the creep compliance, time thickness superposition failed due to the thickness dependence on the steady-state plateau.

It was observed that the steady state compliance increased with film thickness. The thickness dependence on the plateau stiffening followed a power law of $D_{\text{plateau}} \propto h^{4.16}$, which is greater than observed in organic polymers where the exponents observed range from 0.83 to 2.0 [Macromolecules. 2012, 45 (5), 2453-2459].

1 National Science Foundation Grant No. CHE 1112416 and John R. Bradford Endowment at Texas Tech

3:18PM J43.00003 Effect of temperature on segmental mobility is reduced, but not eliminated during constant strain rate deformation of poly(methyl methacrylate) glasses1. KELLY HEBERT, BENJAMIN BENDING, JOSH RICCI, M.D. EDIGER, Univ of Wisconsin, Madison — Deformation of polymer glasses is typically nonlinear and not understood at a molecular level. During deformation, segmental motion in polymer glasses can be accelerated by over a factor of 1000. While temperature has a big impact on the segmental motion of polymer glasses in the absence of deformation, some workers suggest that segmental mobility in polymer glasses undergoing deformation should be independent of temperature. We have measured segmental mobility in poly(methyl methacrylate) glasses during constant strain rate deformation at four different temperatures using a probe reorientation method. We find that during deformation, the dependence of segmental mobility on temperature is significantly reduced, though not eliminated. This is in qualitative agreement with the work of Chen and Schweizer. We also find that the KWW $\beta$ parameter increases during deformation, indicating a narrower distribution of segmental relaxation times. At a given strain rate, this increase of the KWW $\beta$ parameter is larger at lower temperature.

1 We thank the National Science Foundation (DMR-1404614) for support of this research.

3:30PM J43.00004 Thermally Induced Deformation in Metallic Glass: the Activations and Relaxations1. YUE FAN, Oak Ridge National Laboratory, TAKUYA IWASHITA, TAKESHI EGAMI, University of Tennessee — Thermally induced deformation in metallic glasses was investigated by sampling the potential energy landscape (PEL) and probing the changes in the atomic properties (e.g. energy, displacement, stress). The complete deformation processes consist of two stages: the activation (i.e. trigger, from initial minima to nearby saddle states on PEL), and relaxation (i.e. from saddle states to final minima on PEL). We show that the activation stages are triggered by local rearrangements of a small number of atoms, typically 5 atoms in average. Surprisingly, the individual triggers are invariant of the cooling history or elastic structure of the system. However, the organizations between different trigger centers can be varied and are related to the overall stability of the system. On the other hand, relaxation stages consist of two branches, a localized branch, and a cascade branch. While the localized branch is insensitive to the cooling history the system, the cascade branch is highly related with the processing conditions. In particular, for a faster quenched system, the cascade relaxation is found more prominent than in a slowly quenched system.

1 The work is supported by Department of Energy.

3:42PM J43.00005 An energy landscape description of the mechanical response of model glassy materials1. MINGLEI WANG, KAI ZHANG, MENG FAN, YANHUI LIU, JAN SCHROERS, Yale Univ., MARK SHATTUCK, The City College of the City University of New York, COREY O’HERN, Yale Univ., CENTER FOR RESEARCH ON INTERFACE STRUCTURES AND PHENOMENA TEAM — We perform molecular dynamics simulations of binary Lennard-Jones glasses to determine their mechanical response over a range of cooling rates spanning more than three orders of magnitude. To quantify the mechanical response, we measure the shear and bulk moduli using pure shear and compression deformation modes. To correlate the mechanical response to properties of the energy landscape, we also perform zero-temperature quasistatic pure shear simulations and measure the energy per particle as a function of strain. We show that glasses quenched at slower rates possess more brittle response since they exist in deeper energy minima with wider basins. In contrast, rapidly quenched glasses possess ductile response since they exist in shallow, narrow energy minima, which are easily overcome through applied shear.

1 NSF MRSEC Grant No. DMR-1119826 (K.Z.)
In this talk, I will explore the origin of rigidity of granular solids, and present a new paradigm for emergence of order in these athermal systems. thermal motion provides the mechanism for organization by allowing particles to explore the space of configurations. This well-established paradigm of emergent behavior breaks down for collections of macroscopic objects ranging from grains of sand to asteroids. In this macro-world of particulate systems, thermal motion is absent, and mechanical forces are all important. We lack understanding of the basic, unifying principles that underlie the emergence of order in this world. Behringer, Duke University — Particle systems self-assemble in ways that are sensitive to their environments. Proteins fold, polymers crosslink, and molecular systems form crystals. Granular materials, unlike proteins, polymers or molecules, are not sensitive to temperature, and will only form new structures when they are driven. This raises the question of how a granular state depends on the preparation protocol, and an even more basic question of what is needed to specify a granular state. I will focus on granular systems near jamming, where key state variables include the density and stresses. Systems of frictionless grains are jammed for \( \phi > \phi^* \). For frictional grains the picture changes. For a given strain amplitude, the deformation of the material involves localized plastic events that were identified based on the relative displacement of atoms before and after the shear transformation. We found that the density profiles of cage jumps decay away from the inclusion, which correlates well with the radial dependence of the local deformation of the material. At the same strain amplitude, the plastic deformation becomes more pronounced in the cases of weakly damped dynamics or large time scales of the shear transformation. We showed that the density profiles can be characterized by the universal function of the radial distance multiplied by a dimensionless factor that depends on the friction coefficient and the time scale of the shear event.

**Tuesday, March 3, 2015 2:30PM - 4:54PM**

**Session J44**

**GSNP: Invited Session: Self-assembly in the Macro-World**

214D - Corey O'Hern, Yale University

**2:30PM J44.00001 Self-assembly and the Formation of Structure in Granular Materials**

ROBERT BEHRINGER, Duke University — Particle systems self-assemble in ways that are sensitive to their environments. Proteins fold, polymers crosslink, and molecular systems form crystals. Granular materials, unlike proteins, polymers or molecules, are not sensitive to temperature, and will only form new structures when they are driven. This raises the question of how a granular state depends on the preparation protocol, and an even more basic question of what is needed to specify a granular state. I will focus on granular systems near jamming, where key state variables include the density and stresses. Systems of frictionless grains follow the Liu-Nagel\(^1\) scenario of jamming, with a lowest packing fraction, \( \phi_J \), such that any system with \( \phi < \phi_J \) is unjammed, and all isotropic states (shear stress \( \tau = 0 \)) are jammed for \( \phi > \phi_J \). For frictional grains the picture changes. For a given \( \phi \) in the range \( \phi_S < \phi < \phi_J \) it is possible to have stress-free (un jammed) states, highly anisotropic fragile states, and robustly jammed states. The fragile and strongly jammed states form spontaneously in response to shear. By inference, \( \phi_S \) is not a state variable, but recent experiments\(^2\) indicate that the non-rattler fraction, \( J_{NR} \), is. In \( \phi_S < \phi < \phi_J \) the system response is inherently non-linear; under cyclic shear, the system self-organizes to new steady states via a process that resembles thermal activation, with shear stress replacing energy\(^3\). The activation is provided by shear strain. We observe similar relaxation under cyclic compression. An important question is, what is (are) the organizing principle(s) which govern jamming by shear, and systematic reorganization under cyclic driving? 1. Liu, A. & S. Nagel, Nature 396, 21 (1998). 2. D. Bi et al., Nature 480, 355 (2011). 3. J. Ren et al. Phys. Rev. Lett. 110, 018302 (2013)

1 NSF grants DMR1206351 and DMS1248071, NASA grant NNX10AU10G, and ARO grant W911NF-1-11-0110

**3:06PM J44.00002 Emergent Behavior in the Macro-World: Rigidity of Granular Solids**

BULBUL CHAKRABORTY, Brandeis Univ — Diversity in the natural world emerges from the collective behavior of large numbers of interacting objects. The origin of collectively organized structures over the vast range of length scales from the subatomic to colloidal is the competition between energy and entropy. Thermal motion provides the mechanism for organization by allowing particles to explore the space of configurations. This well-established paradigm of emergent behavior breaks down for collections of macroscopic objects ranging from grains of sand to asteroids. In this macro-world of particulate systems, thermal motion is absent, and mechanical forces are all important. We lack understanding of the basic, unifying principles that underlie the emergence of order in this world. In this talk, I will explore the origin of rigidity of granular solids, and present a new paradigm for emergence of order in these athermal systems.

3 This work has been supported by NSF-DMR 1409093 and by the W. M. Keck foundation
3:30PM J45.00006 Bulk Elastic Fingering in Soft Materials, BAUDOUIN SANTYVES, Harvard University, JOHN BIGGINS, Cambridge University, ZHIYAN WEI, Stanford University, SERGE MORA, Montpellier 2 University, L. MAHADEVAN, Harvard University, ELIS-ABETH BOUCHAUD, ESPCI-PARISTECH, HARVARD UNIVERSITY TEAM, ESPCI-PARISTECH COLLABORATION, CAMBRIDGE UNIVERSITY COLLABORATION — Systematic experiments have been performed in purely elastic polycrylamide gels in Hele-Shaw cells. We have shown that a bulk fingering instability arises in the highly deformable confined elastomers. A systematic study shows that surface tension is not relevant. This instability is sub-critical, with a clear hysteretic behavior. Our experimental observations have been compared very favorably to theoretical and finite element simulations results. In particular, the instability wavelength and the critical front advance have been shown to be proportional to the distance between the two glass plates constituting the cell. A very important feature is that elasticity doesn’t influence this lengthscale, making this instability very generic. We will also show some new results on an elastic counterpart experiment of the famous Saffman-Taylor experiment, where we push a soft gel in a stiff one.

3:42PM J45.00007 Mechanical properties of 3D printed warped membranes, ANDREJ KOSMRLJ, KECHAO XIAO, JAMES C. WEAVER, JOOST J. VLASSAK, DAVID R. NELSON, Harvard University — We explore how a frozen background metric affects the mechanical properties of solid planar membranes. Our focus is on a class of "warped membranes" with a preferred random height profile characterized by random Gaussian variables \( h(q) \) in Fourier space with zero mean and variance \( \langle |h(q)|^2 \rangle \propto q^{-4} \). It has been shown theoretically that in the linear response regime, this quenched random disorder increases the effective bending rigidity, while the Young’s and shear moduli are reduced. Compared to flat plates of the same thickness \( t \), the bending rigidity of warped membranes is increased by a factor \( \sim h_0/t \) while the in-plane elastic moduli are reduced by \( \sim 1/h_0 \), where \( h_0 = \sqrt{\langle |h(x)|^2 \rangle} \) describes the frozen height fluctuations. Interestingly, \( h_0 \) is system size dependent for warped membranes characterized with \( m > 2 \). We present experimental evidence of these predictions, using warped membranes prepared via high resolution 3D printing.

3:54PM J45.00008 Localization in an Idealized Heterogeneous Elastic Sheet, BEKELE GURMESSA, ANDREW B. CROLL, North Dakota State Univ — Localized deformation is ubiquitous in many natural and engineering materials. Often times such deformations are associated to non-homogeneous strain fields in the materials. In this work we demonstrate the response of idealized non-homogeneous elastic sheets to uniaxial compression. The idealized patterned surface layers are created selective ultraviolet/ozone (UVO) treatment of the top surface of polydimethylsiloxane (PDMS) using TEM grid mask. By controlling the exposure time of the UVO, samples ranging from continuous thin films to sets of isolated small plates were created. We show how local strains vary with location in a patterned sample, leading to a complex localization process even at low strains. We also see that continuous regions form isotropic undulations upon compression which persist to high strains, well beyond where localization is observed in the patterned regions. Despite the complexity, the localized deformation profile can be adequately described with a simple elastic model when appropriate local boundary conditions are considered.

4:06PM J45.00009 Primary and secondary bifurcations in compressed elastomeric bilayers with small modulus contrast, ANESIA AUGUSTE, University of Massachusetts Amherst, LIUHUA JIN, ZHIGANG SUO, Harvard University, RYAN C. HAYWARD, University of Massachusetts Amherst — Elastic materials undergo various kinds of elastic instabilities when subjected to compression. The primary bifurcation behavior for a stiff thin film on a thick soft substrate is wrinkling, whereas for a homogeneous material it is creasing. While ideal bilayered systems with large contrasts in modulus and thickness are well understood, many system in nature and engineering contexts are far from this simple case. We have developed an experimental system to systematically vary the modulus contrast, complemented by finite element simulations, to study the primary and secondary bifurcations in compressed bilayers. We find that below a certain strain threshold bilayers can be stable to both wrinkles and creases. For slightly larger contrasts, the primary bifurcation is wrinkling but there are two distinct types of secondary bifurcations: (1) wrinkles that transition into creases without period-doubling; and (2) wrinkles to creases preceded by period doubling. Understanding surface instabilities in such non-ideal bilayer systems provides important insights on the behavior of biological tissues and other systems with a small modulus contrast.

4:18PM J45.00010 The Structural Change of Buckling Depending on the Directional Mechanical Heterogeneity of Top Thin Films, DOKYEONG KWON, Seoul Natl Univ, HYOSEON SUH, University of Chicago, DOMIN KIM, KOOKHEON CHAR, Seoul Natl Univ — Buckling of thin films on elastomeric substrates such as polydimethylsiloxane (PDMS) is the well-known phenomenon in buckling instability originating from the moduli mismatch between a substrate and a thin film placed on the top. Recently, many studies on the microstructure created by the buckling with flat top films have been reported and physics behind them has almost been well received. However, only a few work has been done on the buckling structure with micropatterned top films and buckling mechanics for patterned top films-PDMS bilayers has not yet been studied in detail. Here, we present the buckling of mechanically heterogeneous, patterned top films placed on top of elastomeric PDMS substrates. Mechanically heterogeneous top films were prepared by polystyrene (PS) films with topographic patterns. Buckling instability was induced by applying mechanical stresses to the PS-PDMS bilayer. Resulting buckling structure showed the structural change depending on the alignment of the top films with respect to the buckling direction. The structural change was analyzed with finite element method calculation, giving insights on the buckling mechanics of top film with complicated patterns placed on PDMS substrates.

4:30PM J45.00011 High Aspect Ratio Wrinkles, YU-CHENG CHEN, ALFRED CROSBY, University of Massachusetts Amherst — Buckling-induced surface undulations are widely found in living creatures, for instance, gut villi and the surface of flower petal cells. These undulations provide unique functionalities with their extremely high aspect ratios. For the synthetic systems, sinoidal wrinkles that are induced by buckling a thin film attached on a soft substrate have been proposed to many applied applications. However, the impact of the synthetic wrinkles have been restricted by limited aspect ratios, ranging from 0 to 0.35. Within this range, wrinkled aspect ratio is known to increase with increasing compressive strain until a critical strain is reached, at which point wrinkles transition to localizations, such as folds or period doublings. Inspired by the living creatures, we propose that wrinkles be stabilized in high aspect ratio by manipulating the strain energy in the substrate. We experimentally demonstrate this idea by forming a secondary crosslinking network in the wrinkled surface and successfully achieve aspect ratio as large as 0.8. This work not only provides insights for the mechanism of high aspect ratio structures seen in living creatures, but also demonstrates significant promise for future wrinkle-based applications.

4:42PM J45.00012 Competition between adhesion and inertia during stick-slip peeling of Pressure Sensitive Adhesives, M.-J. DALBE, Laboratoire de Physique de l’ENS de Lyon, CNRS, Université de Lyon, France, R. VILLE, Laboratoire FAST, CNRS, Université Paris-Sud, Orsay, France, M. CICCOTTI, Laboratoire PPMD/SIMM, CNRS, ESPCI ParisTech, Paris, France, P.-P. CORTET, FAST, S. SANTUCCI, Laboratoire de Physique de l’ENS de Lyon, L. VANEL, Institut Lumière Matière, CNRS, Université de Lyon, France — We consider the classical problem of the unstable stick-slip dynamics often observed when peeling a pressure sensitive adhesive, quantifying for the first time experimentally the influence of the peeling angle. This instability is known to be the consequence of a decreasing fracture energy of the adhesive-substrate joint over a certain range of driving velocity: we focus here on the important case where the instability develops at large driving velocity. We show that below a certain rate of film slip, the instability is sub-critical, with a clear hysteretic behavior. Our experimental observations have been compared very favorably to a theoretical model and finite element simulations results. In particular, the instability wavelength and the critical front advance have been shown to be proportional to the distance between the two glass plates constituting the cell. A very important feature is that elasticity doesn’t influence this lengthscale, making this instability very generic. We will also show some new results on an elastic counterpart experiment of the famous Saffman-Taylor experiment, where we push a soft gel in a stiff one.
4:54PM J45.00013 Influence of large strain rheology on the peeling performances of Pressure Sensitive Adhesives. Richard Villey, Matteo Ciccotti, Costantino Creton, Laboratoire SIMM, CNRS, ESPCI ParisTech, Université Pierre et Marie Curie, PSL Research University, Paris, France; Pierre-Philippe Cortet, Laboratoire FAST, CNRS, Université Paris-Sud, Orsay, France; David J. Yarusso, 3M Company, 3M Center, 230-1D-15, St. Paul, MN, 55144-1000, USA — The dependence of adhesion energy of Pressure Sensitive Adhesives (PSA) on peeling velocity reduces to a master curve using a time-temperature superposition principle, usually verified by the linear rheology of polymers. This result has guided models predicting peeling energy of PSA to consider the small strain rheology of the glue only, despite it can experience very large strains before debonding. The argument of the time-temperature superposition principle can actually also be applied to large strains and is thus not a stringent one. To clarify the role of large strain rheology during the peeling of PSA, we present experiments on commercial and custom-made tapes supplied by 3M Company. Small and large strain rheology differences are obtained by changing the glass transition temperature, the cross-linking density and the density of entanglements, yet remaining close to commercial PSA. The rheology influence is decoupled from geometrical effects, by examining the nontrivial dependence of the adhesion energy on the peeling angle. Finally, adhesion energy measurements and visualizations of the process zone, over a large range of peeling velocities, are discussed, in the perspective of building a model for the adherence considering the complete rheology of the glue.

5:06PM J45.00014 What can cracked polymer do? Kexin Jiao, Chuanhong Zhou, Punit Kohli, Department of Chemistry and Biochemistry, Southern Illinois University Carbondale, Anish Pou德尔, Tsuchin Chi, College of Engineering, Southern Illinois University Carbondale — Buckling, delamination, and cracking are very well-known phenomena observed in most thin films. They were theoretically explained by the existence of mechanical instability due to the residue stress generated when a thin film is deposited on substrates or undergoing environmental stress. Buckled structures at micro- or nano-scale have been of great interests and have been used extensively in many applications including particles self-assembling, surface wettability modification, and micro-electronic device fabrication. However, peeling of a layer from a substrate due to delamination or fractures on a thin film due to cracking is mostly taken as an undesirable result. Therefore, strategies are inspired for preventing or removing these often undesired structures. We found that after being heated above its decomposition temperature and then cooled to room temperature, a PDMS thin film showed micro-fibers of 100μm width and up to 1.5 cm in length. By studying the formation mechanism, control of the dimensions and of the growth pattern on a substrate for PDMS micro-fibers were realized. Giving credit to their high flexibility and optical transparency, a PDMS micro-fiber was utilized in high resolution near field imaging achieved by attaching a micro-lens on the fiber. Interestingly, a surface covered by PDMS micro-fibers will turn from superhydrophobic into superhydrophilic by further heating providing potential applications in surface wettability modification. In future, we will investigate and simulate the growth of PDMS micro-fiber and look for more possible applications.

5:18PM J45.00015 Formation of 3He droplets in dilute 3He-4He solid solutions. Chaohuan Huan, University of Florida, Gainesville, USA; Don Canoletta, University of Massachusetts, Amherst, USA; Sung Kim, Liang Yin, Jiang-Sheng Xia, Neil Sullivan, University of Florida, Gainesville, USA — We review the different stages of the formation of 3He droplets in dilute 3He-4He solutions. The studies are interesting because the phase separation in isotopic helium mixtures is a first-order transition with a conserved order parameter. The rate of growth of the droplets as observed in NMR studies [1] is compared with the rates expected for homogeneous nucleation followed by a period of coarsening known as Ostwald ripening.


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Tuesday, March 3, 2015 2:30PM - 5:30PM –
Session J46 DBIO: Invited Session: Physics of Proteins: Integrating Computation with Experiment 217A - Wouter Hoff, Oklahoma State University

2:30PM J46.00001 Protein Folding Transition Paths: Single Molecule Experiments, Theory and Simulations. William Eaton, Laboratory of Chemical Physics, NIDDK, NIH, Bethesda, MD — The transition-path is the tiny fraction of an equilibrium, single-molecule trajectory when the transition over a free-energy barrier occurs between two states. In the case of protein folding, the distribution of transition paths contains all of the mechanistic information on how a protein folds and unfolds. Transition path distributions can now be predicted for fast folding proteins by all-atom molecular dynamics simulations and by an Ising-like theoretical model [1,2]. Experimental information on transition paths should provide the most demanding test of both simulations and theoretical models. However, transition-paths for barrier crossings have never been observed experimentally for any molecular system in solution. Because it is a single molecule property, even determining the average transition-path time is challenging. In this presentation, I will discuss how we use measurements of Förster resonance energy transfer in single molecule fluorescence experiments and a photon-by-photon analysis to measure average transition path times for proteins of different topology and folding rate coefficients using the Gopich/Szabo maximum likelihood method [3,4]. These results, which are surprisingly interesting, are just the first, but important, steps toward measuring intra-molecular distances during individual transition paths. [1] Best, R.B.; Hummer, G.; Eaton, W.A. Native contacts determine protein folding mechanisms in atomistic simulations. Proc. Natl. Acad. Sci. USA 2013, 110, 17874; [2] Henry, E.R.; Best, R.B.; Eaton, W.A. Comparing a simple theoretical model for protein folding with all-atom molecular dynamics simulations. Proc. Natl. Acad. Sci. USA 2013,110, 17880; [3] Chung, H.S.; Mcahe, K.; Louis, J.M.; Eaton, W.A. Single-molecule fluorescence experiments determine protein folding transition path times. Science 2012, 335, 981; [4] Chung, H.S.; Eaton, W.A.Single-molecule fluorescence probes dynamics of barrier crossing. Nature 2013, 502, 685.

3:06PM J46.00002 Exploring the active site structure of photoreceptor proteins by Raman optical activity. Masashi Unno, Saga University — Understanding protein function at the atomic level is a major challenge in a field of biophysics and requires the combined efforts of structural and functional methods. We use photoreceptor proteins as a model system to understand in atomic detail how a chromophore and a protein interact to sense light and send a biological signal. A potential technique for investigating molecular structures is Raman optical activity (ROA), which is a spectroscopic method with a high sensitivity to the structural details of chiral molecules. However, its application to photoreceptor proteins has not been reported. Thus we have constructed ROA spectrometer using near-infrared (NIR) laser excitation at 785 nm. The NIR excitation enables us to measure ROA spectra for a variety of biological samples, including photoreceptor proteins, without fluorescence from the samples. In the present study, we have applied the NIR-ROA to bacteriorhodopsin (BR) and photoactive yellow protein (PYP). BR is a light-driven proton pump and contains a protonated Schiff base of retinal as a chromophore. PYP is a blue light receptor, and this protein has the 4-hydroxycinnamyl chromophore, which is covalently linked to Cys69 through a thiolester bond. We have successfully obtained the ROA spectra of the chromophore within a protein environment. Furthermore, calculations of the ROA spectra utilizing density functional theory provide detailed structural information, such as data on out-of-plane distortions of the chromophore. The structural information obtained from the ROA spectra includes the positions of hydrogen atoms, which are usually not detected in the crystal structures of biological samples.
laboratory frame of reference when using uniformly oriented samples (approximately 1
bilayers provides an excellent tool for such characterizations. Two classes of restraints can be obtained - absolute restraints that constrain the structure to a
are influenced by their native environment. Therefore the characterization of their structure in an environment that models as closely as possible their native
Science

Because a growing
this optimal pH range, a population responds unimodally to a XIP stimulus, and bimodally to CSP; outside this range the response to both signals is suppressed.

in determining how cells respond to the quorum sensing signals: The response to both peptides is sharply tuned to a narrow window of near-neutral pH. Within

the interplay of these variables in regulating the competent state is poorly understood. We are using microfluidics to isolate and control environmental inputs and

Streptococcus mutans
pathogen

results we quantitatively analyzed the immunostaining of purigenic receptors and gap junction channels. The results confirm our hypothesis that collective

stimuli concentrations. Additionally, fibroblast cells exhibit persistent calcium oscillations that increase in regularity with greater stimuli. To interpret these
delivered through microfluidic devices. Our results demonstrate that cancer cells respond faster, generate singular spikes, and are more synchronous across all

a defective multicellular network we have studied the calcium signaling of co-cultured breast cancer cells and fibroblast cells in various concentrations of ATP

stimuli and gap junction communication between the cells. However, just as a well-connected neural network may be compromised by abnormal neurons, a

POTTER, BO SUN, Oregon State University — A communicating multicellular network processes environmental cues into collective cellular dynamics. We

experimental and computational approach to discover novel chemoceptor molecules and compare their binding features, as well as the conformational changes they produce. We first used molecular docking to computationally screen a large chemical library and tested binding strengths of the top-ranking molecules for the E. coli chemoreceptor Tar. Chemotactic properties of the binding molecules were then studied using a specially designed microfluidic device. Novel attractant and antagonist molecules were identified that bind directly with the E. coli chemoreceptor Tar. Molecular dynamics simulations showed that attractant and antagonist binding result in distinct conformational changes in Tar. Differences of antagonist and attractant binding suggest that molecules lacking triggering interaction with the receptor behave as antagonist. For Tar, the triggering interaction is mediated by the hydrogen bonds formed between a donor group in the attractant and the main-chain carbonyls in the fourth helix of Tar. This "bind-and-trigger" mechanism of receptor signaling is verified experimentally by converting an antagonist into an attractant when introducing an NH group into the antagonist compound. Similar conformational changes were also observed in the E. coli Tar system.

Microfluidic study of environmental control of genetic competence in Strep-

cells can be reprogrammed to become pluripotent stem cells [1]. The possible cell fates can be modeled as attractors in a dynamical system, the "epigenetic

both cellular differentiation and reprogramming can be described in the landscape picture as motion from one attractor to another attractor. We perform Monte Carlo simulations in a simple model of the landscape [2]. This model is based on spin glass theory and it can be used to construct a simulated epigenetic landscape starting from the experimental genomic data. We re-analyse data from several cell reprogramming experiments [3-6] and compare with our simulation results. We find that the model can reproduce some of the main features of the dynamics of cell reprogramming.


Collective Calcium Signaling of Defective Multicellular Networks , GARRETT POTTER, BO SUN, Oregon State University — A communicating multicellular network processes environmental cues into collective cellular dynamics. We have previously demonstrated that, when excited by extracellular ATP, fibroblast monolayers generate correlated calcium dynamics modulated by both the stimuli and gap junction communication between the cells. However, just as a well-connected neural network may be compromised by abnormal neurons, a tissue monolayer can also be defective with cancer cells, which typically have down regulated gap junctions. To understand the collective cellular dynamics in a defective multicellular network we have studied the calcium signaling of co-cultured breast cancer cells and fibroblast cells in various concentrations of ATP delivered through microfluidic devices. Our results demonstrate that cancer cells respond faster, generate singular spikes, and are more synchronous across all stimuli concentrations. Additionally, fibroblast cells exhibit persistent calcium oscillations that increase in regularity with greater stimuli. To interpret these results we quantitatively analyzed the immunostaining of purigenic receptors and gap junction channels. The results confirm our hypothesis that collective dynamics are mainly determined by the availability of gap junction communications.

Microfluidic study of environmental control of genetic competence in Strept-
coccus mutans1. MINJUN SON, SEYEDEHDELARAM GHOREISHILANGROUDI, Department of Physics, University of Florida, SANG-JOON AHN, ROBERT BURNE, Department of Oral Biology, University of Florida, STEPHEN HAGEN, Department of Physics, University of Florida — The bacterial pathogen Streptococcus mutans has the ability to enter a transient state of genetic competence in which it can integrate exogenous DNA. It regulates the competent state in response to several environmental inputs that include two quorum sensing peptides (CSP and XIP) as well as pH and other variables. However the interplay of these variables in regulating the competent state is poorly understood. We are using microfluidics to isolate and control environmental inputs and examine how the competence regulatory circuit responds at the single cell level. Our studies reveal that the pH of the growth environment plays a critical role in determining how cells respond to the quorum sensing signals: The response to both peptides is sharply tuned to a narrow window of near-neutral pH. Within this optimal pH range, a population responds unimodally to a XIP stimulus, and bimodally to CSP; outside this range the response to both signals is suppressed. Because a growing S. mutans culture acidifies its medium, our findings suggest that the passage of the pH through the sensitivity window transiently activates the competence circuit. In this way a sharply tuned environmental response gives S. mutans fine control over the duration of its competent state.

3:30PM J47.00004 Discovering novel ligands for understanding molecular mechanism of bacteria chemotaxis , LUHUA LAI, Peking University — In order to understand the molecular mechanism of bacteria chemotaxis, we used a combined experimental and computational approach to discover novel chemoceptor molecules and compare their binding features, as well as the conformational changes they produce. We first used molecular docking to computationally screen a large chemical library and tested binding strengths of the top-ranking molecules for the E. coli chemoreceptor Tar. Chemotactic properties of the binding molecules were then studied using a specially designed microfluidic device. Novel attractant and antagonist molecules were identified that bind directly with the E. coli chemoreceptor Tar. Molecular dynamics simulations showed that attractant and antagonist binding result in distinct conformational changes in Tar. Differences of antagonist and attractant binding suggest that molecules lacking triggering interaction with the receptor behave as antagonist. For Tar, the triggering interaction is mediated by the hydrogen bonds formed between a donor group in the attractant and the main-chain carbonyls in the fourth helix of Tar. This "bind-and-trigger" mechanism of receptor signaling is verified experimentally by converting an antagonist into an attractant when introducing an NH group into the antagonist compound. Similar conformational changes were also observed in the E. coli Tar system.

[1] This work is supported by the NIH under NIDCR awards R01 DE023339.
3:42PM J47.00005 Dynamic information routing in complex networks, Center for Physics and Biology, Rockefeller University, MARC TIMME, Max-Planck Institute for Dynamics and Self-Organization, DEMIAN BATTLAGLIA, Institute of Systems Neuroscience, Aix-Marseille University — Flexible information routing fundamentally underlies the function of many biological and artificial networks. Yet, how information may be specifically communicated and dynamically routed in these systems is not well understood. Here we demonstrate that collective dynamical states systematically control patterns of information sharing and transfer in networks, as measured by delayed mutual information and transfer entropy between activities of a network’s units. For oscillatory networks we analyze how individual unit properties, the connectivity structure and external inputs all provide means to flexibly control information routing. For multi-scale, modular architectures, we resolve communication patterns at all levels and show how local interventions within one sub-network may remotely control the non-local network-wide routing of information. This theory helps understanding information routing patterns across systems where collective dynamics co-occurs with a communication function.

3:54PM J47.00006 Strain induced critical behavior in athermal biopolymer networks, ABHINAV SHARMA, Georg August University, Gottingen, ALBERT LICUP, ROBBIE RENS, MICHAEL SHEINMAN, Vrije Universiteit Amsterdam, KARIN JANSSEN, GIJSE KOENDERINK, AMOLF, Amsterdam, FRED MACKINTOSH, Vrije Universiteit Amsterdam — Biopolymer networks exhibit highly interesting mechanical behavior. An instructive model system is that of a network composed of rope-like filaments—zero resistance to compression but finite resistance to stretching. For networks with connectivity below Maxwell point, there is no elastic modulus for small deformations. However, when networks are subjected to an external strain, stiffness emerges spontaneously beyond a critical strain. We demonstrate that the spontaneous emergence of elasticity is analogous to a continuous phase transition. The critical point is not fixed but depends on the geometry of the underlying network. The elastic behavior near the critical point can be described analogous to that of Magnetization in ferromagnetic material near the curie temperature. Surprisingly, the critical exponents are independent of the dimensionality and depend only on the average connectivity in the network. By including bending interactions in the rope network, we can capture the mechanical behavior of biologically relevant networks. Bending rigidity acts as a coupling constant analogous to the external magnetic field in a ferromagnetic system. We show that nonlinear mechanics of collagen are successfully captured by our framework of regarding nonlinear mechanics as a critical phenomenon.

4:06PM J47.00007 Pattern Learning, Damage and Repair within Biological Neural Networks, THEODORE SIU, KATE FITZGERALD O’NEILL, TROY SHINBROT, Rutgers Univ — Traumatic brain injury (TBI) causes damage to neural networks, potentially leading to disability or even death. Nearly one in ten of these patients die, and most of the remainder suffer from symptoms ranging from headaches and nausea to convulsions and paralysis. In vitro studies to develop treatments for TBI have limited in vivo applicability, and in vitro therapies have even proven to worsen the outcome of TBI patients. We propose that this disconnect between in vitro and in vivo outcomes may be associated with the fact that in vitro tests assess indirect measures of neuronal health, but do not investigate the actual function of neuronal networks. Therefore in this talk, we examine both in vitro and in vivo neuronal networks that actually perform a function: pattern identification. We allow the networks to execute genetic, Hebbian, learning, and, additionally, we examine the effects of damage and subsequent repair within our networks. We show that the length of repaired connections affects the overall pattern learning performance of the network and we propose therapies that may improve function following TBI in clinical settings.

4:18PM J47.00008 In silico evolution of oscillatory dynamics in biochemical networks, MD ZULFIKAR ALI, Clark University, NED S. WINGREEN, Princeton University, RANJAN MUKHOPADHYAY, Clark University — We are studying in silico evolution of complex, oscillatory network dynamics within the framework of a minimal mutational model of protein-protein interactions. In our model we consider two different types of proteins, kinase (activator) and phosphatase (inhibitor). In our model, each protein can either be phosphorylated (active) or unphosphorylated (inactive), represented by binary strings. Active proteins can modify their target based on the Michaelis-Menten kinetics of chemical equation. Reaction rate constants are directly related to sequence dependent protein-protein interaction energies. This model can be studied for non-trivial behavior e.g. oscillations, chaos, multiple stable states. We focus here on biochemical oscillators; some questions we will address within our framework include how the oscillatory dynamics depends on number of protein species, connectivity of the network, whether evolution can readily converge on a stable oscillator if we start with random initial parameters, neutral evolution with additional protein components and general questions of robustness and evolvability.

4:30PM J47.00009 Uncertainty of Prebiotic Scenarios: The Case of the Non-Enzymatic Reverse Tricarboxylic Acid Cycle, DMITRY ZUBAREV, DMITRIJ RAPPOPORT, ALAN ASPURU-GUZIK, Harvard University — We consider the much discussed hypothesis of the primordial nature of the non-enzymatic reverse tricarboxylic acid (rTCA) cycle and describe a modeling approach that quantifies the uncertainty of this hypothesis due to the combinatorial aspect of the constituent chemical transformations. Our results suggest that a) rTCA cycle belongs to a degenerate optimum of auto-catalytic cycles, and b) the set of targets for the investigations of the origin of the common metabolic core should be significantly extended.

This work was supported by a grant from the Simons Foundation (SCOL 291937, Dmitry Zubarev).

4:42PM J47.00010 Extracting Hidden Hierarchies in 3D Distribution Networks, CARL MODES, MARCELO MAGNASCO, Rockefeller University, ELÉNI KATIFORI, Max Planck Institute for Dynamics and Self-Organization — Natural and man-made transport webs are frequently dominated by dense sets of nested cycles. The architecture of these networks—the topology and edge weights—determines how efficiently the networks perform their function. Yet, the set of tools that can characterize such a weighted cycle-rich architecture in a physically relevant, mathematically compact way is sparse. In order to fill this void, we have developed a new algorithm that rests on an abstraction of the physical ‘tiling’ in the case of a two dimensional network to an effective tiling of an abstract surface in space that the network may be thought to sit in. Generically these abstract surfaces are richer than the plane and upon sequential removal of the weakest links by edge weight, neighboring tiles merge and a tree characterizing this merging process results. The properties of this characteristic tree can provide the physical and topological data required to describe the architecture of the network and to build physical models. This new algorithm can be used for automated phenotypic characterization of any weighted network whose structure is dominated by cycles, such as mammalian vasculature in the organs, the root networks of clonal colonies like quaking aspen, or the force networks in jammed granular matter.

4:54PM J47.00011 Dynamic maintenance of stochastic molecular clusters on cell membranes, ANDREW MUGLER, Purdue University, MARTIJN WEHRENS, PIETER REIN TEN WALDE, FOM Institute AMOLF — Clustering of molecules on cell membranes is a widely observed phenomenon. A key example is the oncoprotein Ras. Maintenance of Ras clusters has been linked to proper Ras signaling. Yet, the mechanism by which Ras clusters are maintained remains unclear. Recently it was discovered that activated Ras promotes further Ras activation. We show using particle-based simulation that this positive feedback link is sufficient to produce persistent clusters of active Ras molecules via a dynamic nucleation mechanism. The particle statistics are consistent with experimental observations. Interestingly, our model does not support a Turing regime of macroscopic reaction-diffusion patterning. This means that the clustering we observe is a purely stochastic effect, arising from the coupling of the positive feedback network with the discrete nature of individual molecules. These findings underscore the importance of stochastic and dynamic properties of reaction diffusion systems for biological behavior.
5:06PM J47.00012 Sensing multiple ligands with single receptor1. VIJAY SINGH, ILYA NEMENMAN, Emory University — Cells use surface receptors to measure concentrations of external ligand molecules. Limits on the accuracy of such sensing are well-known for the scenario where concentration of one molecular species is being determined by one receptor [Endre]. However, in more realistic scenarios, a cognate (high-affinity) ligand competes with many non-cognate (low-affinity) ligands for binding to the receptor. We analyze effects of this competition on the accuracy of sensing. We show that maximum-likelihood statistical inference allows determination of concentrations of multiple ligands, cognate and non-cognate, by the same receptor concurrently. While it is unclear if traditional biochemical circuitry downstream of the receptor can implement such inference exactly, we show that an approximate inference can be performed by coupling the receptor to a kinetic proofreading cascade. We characterize the accuracy of such kinetic proofreading sensing in comparison to the exact maximum-likelihood approach.

1We acknowledge the support from the James S. McDonnell Foundation and the Human Frontier Science Program.

5:18PM J47.00013 Dynamic phases in control and information processing biological circuits . SURIYANARAYANAN VAIKUNTHANATHAN, University of Chicago — Recent work using the mathematical framework of large deviation theory has shown that fluctuations about the steady state can have a particularly rich structure even in extremely simple non-equilibrium systems [Phys. Rev. E. 89, 062108, 2014]. In certain instances the fluctuations can encode the presence of a dynamical phase with properties distinct from those of the steady state of the system. The transition between these two regimes is akin to a first order thermodynamic phase transition. Specifically, it implies an extreme sensitivity of the system to changes in certain sets of parameters. I will show that such dynamical phase transitions can serve as a general organizing principle to understand biological circuits that are involved in information processing and control. I will focus on two specific examples: adaptation control in E. coli chemotaxis and ultra sensitive response of the E. coli flagella motor, to illustrate these calculations. This work also elucidates the role played by energy dissipation in ensuring control and suggests general guidelines for the construction of robust non-equilibrium circuits that perform various specified functions.

Tuesday, March 3, 2015 2:30PM - 5:30PM –
Session J48 DBIO: Focus Session: Physics of Cellular Organization

2:30PM J48.00001 Collective Dynamics of Dividing Chemotactic Cells , ANATOLII GELIMSON, RAMIN GOLESTANIAN, Rudolf Peierls Centre for Theoretical Physics, University of Oxford — The large scale behaviour of a population of cells that grow and interact through the concentration field of the chemicals they secrete is studied using dynamical renormalization group methods. The combination of the effective long-range chemotactic interaction and lack of number conservation leads to a rich variety of phase behaviour in the system, which includes a sharp transition from a phase that is controlled by a weakly coupled perturbatively accessible fixed point to a phase controlled by a nonaccessible strong coupling fixed point. For a range of parameters, the perturbatively accessible fixed point has nontrivial critical exponents.

2:42PM J48.00002 Nature’s rheologists: Lymphatic endothelial cells control migration in response to shear stress , GERALD FULLER, ALEX DUNN, VINAY SURYA, Stanford University — Endothelial cells (ECs) line the inner surface of blood and lymphatic vessels and are sensitive to fluid flow as part of their physiological function. EC organization, migration and vessel development are profoundly influenced by shear stresses, with important implications in cardiovascular disease and tumor metastasis. How ECs sense fluid flow is a central and unanswered question in cardiovascular biology. We developed a high-throughput live-cell flow chamber that models the gradients in wall shear stress experienced by ECs in vivo. Live-cell imaging allows us to probe cellular responses to flow, most notably EC migration, which has a key role in vessel remodeling. We find that most EC subtypes, including ECs from the venous, arterial, and microvascular systems, migrate in the flow direction. In contrast, human lymphatic microvascular ECs (hLMVECs) migrate against flow and up spatial gradients in wall shear stress. Further experiments reveal that hLMVECs are sensitive to the magnitude, direction, and the local spatial gradients in wall shear stress. Lastly, recent efforts have aimed to link this directional migration to spatial gradients in cell-mediated small molecule emission that may be linked to the gradient in wall shear stress.

2:54PM J48.00003 Obstructions Inhibit Long-range Motor Motility in Microtubule Bundles . M.W. GRAMLICH, University of Massachusetts - Amherst — Efficient cellular transport along the cytoskeletal network is essential for cell growth and maintenance. Everything from microtubules to plasma membrane components are transported along the cytoskeletal network. Long-range transport is accomplished by molecular motors carrying cargo along a microtubule network. Recently, the role of the microtubule bundle geometry has begun to be explored. Microtubules bundle together in order to efficiently direct transport. Consequently, bundled microtubules introduce a new set of parameters which affect cellular transport, such as bundle spacing or microtubule polarity. Even previously tested parameters need to be re-considered, such as the role of obstructions. In this talk I will focus on the relationship between obstructions and microtubule polarity, and their affects on long-range transport. Microtubule polarity varies from completely uniform, with all plus-ends pointing in the same direction, to completely random. I will quantitatively show how obstructions inhibit long-range motor motility in any bundle, regardless of the distribution of microtubule polarity within the bundle. However, inhibition of long-range transport is greater in mixed polarity bundles. This result has implications for how cells use microtubule polarity to accommodate obstructions in order to efficiently direct transport.

3:06PM J48.00004 Tackling the single molecule counting problem1. STEVE PRESSE, Indiana University - Purdue University Indianapolis — Protein-protein interactions – that give rise to spatiotemporal organization in the cell – are the basis for most biological processes. Quantitatively understanding these interactions is an essential prerequisite for developing mechanistic models of cell biology. However there is currently no routine answer to “how many proteins of type X are in this complex?” in living cells. Here we discuss methods developed in our group (Geoff Rollins, Kostas Tsekovs) for tackling this “single molecule counting problem” starting from photobleaching data and data from a superresolution microscopy technique called PALM (PhotoActivated Localization Microscopy).

1We gratefully acknowledge the NSF (MCB-1412259)

3:18PM J48.00005 C. elegans uses Liquid-Liquid Demixing for the Assembly of Non-Membrane-Bound Compartments. CHRISTOPH A. WEBER, FRANK JUELICHER, Max Planck Institute of the Physics of Complex Systems, ANDRES FELIPE DIAZ DELGADILLO, LOUISE JAWERTH, ANTHONY A. HYMAN, Max Planck Institute of Molecular Cell Biology and Genetics , DEPARTMENT BIOLOGICAL PHYSICS TEAM, HYMAN LAB COLLABORATION — P granules are liquid cytoplasmic RNA/Protein condensates known to determine the germ lineage in Caenorhabditis elegans. They resemble striking similarities with liquid droplets, such as dripping, shearing and wetting. Assuming that P granules are liquid-like we consider how they form in the crowded cytoplasm. Using confocal and light-sheet microscopy, P granule formation in vivo and in vitro is shown to share all hallmarks with a liquid-liquid phase-separation. Specifically, demixing is determined by temperature and concentration, the droplet formation is reversible with respect to temperature quenches and there is evidence for droplet growth due to coalescence and Ostwald-ripening. Liquid-liquid demixing in vivo breaks the paradigmatic view that a molecular machinery is necessary to build up organelles through complex biological pathways. Instead we propose that P granules form following a Flory-Huggins model. Liquid-liquid demixing could also serve as a mechanism for the assembly of non-membrane-bound compartments in other living organisms.
polymerization rate can increase the polymerized-actin content of the patch. We present data for NPF dynamics budding yeast, which confirm some of the
reduced, there is a discontinuous transition from protein pulses to persistent patches. We also find, surprisingly, that in some parameter regimes reducing the
“nucleation-promoting factors” (NPFs) that catalyze actin polymerization, and curvature-generating proteins. We model the dynamics of protein patches in
to bend it, and finally disassemble. The patches contain an initial coat that establishes the endocytic site and binds cargo, polymers of the protein actin,
under Grant R01-GM107667.

5:06PM J48.00012 Pulse Dynamics in Endocytic Protein Patches1, ANDERS CARLSSON, XINXIN WANG, Washington University in St Louis — During the process of endocytosis in yeast, submicron-sized protein patches assemble, exert forces on the membrane
to bend it, and finally disassemble. The patches contain an initial coat that establishes the endocytic site and binds cargo, polymers of the protein actin,
“nucleation-promoting factors” (NPFs) that catalyze actin polymerization, and curvature-generating proteins. We model the dynamics of protein patches in
4:54PM J48.00011 Exploration of locomotion in the ParA/ParB system, LAVISHA JINDAL, ELDON EMBERLY, Simon Fraser University — In many bacteria the ParA/ParB system is responsible for actively segregating DNA during replication. ParB precessively
moves by hydrolyzing DNA bound ParA-ATP forming a depleted ParA region in its wake. Recent in-vitro experiments have shown that a ParB covered bead can
traverse a ParA bound DNA substrate. It has been suggested that the formation of a gradient in ParA leads to diffusion-ratchet like motion of the ParB bead
but its origin and potential consequences requires investigation. We have developed a deterministic model for the in-vitro ParA/ParB system and show that
any amount of spatial noise in ParA can lead to the spontaneous formation of its gradient. The velocity of the bead is independent of this noise but depends
on the scale over which ParA exerts a force on the bead and the scale over which ParB hydrolyzes ParA from the substrate. There is a particular ratio of these
scares at which the velocity is a maximum. We also explore the effects of cooperative vs independent rebinding of ParA to the substrate. Our model shows
how the driving force for ParB originates and highlights necessary conditions for directed motion in the in-vitro system that may provide insight into the in-vivo
behaviour of the ParA/ParB system.

3:54PM J48.00008 Viscoelastic properties of actin networks influence material transport1, SAMANTHA STAM, Biophysical Sciences Graduate Program, University of Chicago, KIMBERLY WEIRICH, James Franck Institute, University of Chicago, MARGARET GARDEL, Department of Physics and James Franck Institute, University of Chicago — Directed flows of cytoplasmatic material are important in a variety of biological processes including assembly of a mitotic spindle, retraction of the cell rear during migration, and asymmetric cell division. Networks of cytoskeletal polymers and molecular motors are known to be involved in these events, but how the network mechanical properties are tuned to perform such functions is not understood. Here, we construct networks of either semiflexible actin filaments or rigid bundles with varying connectivity. We find that solutions of rigid rods, where unimpeded sliding of filaments may enhance transport in comparison to unmoving tracks, are the fastest at transporting network components. Entangled solutions of semiflexible actin filaments also transport material, but the entanglements provide resistance. Increasing the elasticity of the actin networks with crosslinking proteins slows network deformation further. However, the length scale of correlated transport in these networks is increased. Our results reveal how the rigidity and connectivity of biopolymers allows material transport to occur over time and length scales required for physiological processes.

1This work was supported by the U. Chicago MRSEC.

4:06PM J48.00009 Regulation of kinesin-transport by microtubule age and polymerization conditions, JING XU, WINNIE LIANG, Physics, UC Merced, STEPHEN KING, U Central Florida, K. FAYSAL, Physics, UC Merced — Microtubules are fundamental biopolymers in cells, formed via self-assembly (“polymerization”) of tubulin dimers. Microtubule polymerization conditions have been shown to alter the presence of defects in microtubule lattices, including point defects (missing tubulin dimers) and line defects (protofilament disruption). Potential impact of these lattice defects on molecular motor-based transport is not yet understood. Here we investigate the impact of microtubule polymerization conditions on multiple-kinesin transport, using single-molecule-type optical trapping experiments. We find that kinesin-based cargoes pause preferentially at specific locations along individual microtubules, and that the pause frequency and duration is strongly dependent on microtubule age and polymerization condition. Within each polymerization condition and for fresh microtubules, we also observe significant variations in multiple-kinesin travel distances, depending on which microtubules the motors travel along. Taken together, our study suggests an important role of microtubule lattice defect in regulating intracellular transport.

4:18PM J48.00010 Heterogeneity in motor driven transport, ALI TABEL, University of Northern Iowa — I will discuss quantitative analysis of particle tracking data for motor driven vesicles inside an insulin secreting cell. We use this method to study the dynamical and structural heterogeneity inside the cell. I will discuss our effort to explain the origin of observed heterogeneity in intracellular transport. Finally, I will explain how analyzing directional correlations in transport trajectories reveals self-similarity in the diffusion media.

4:54PM J48.00011 Exploration of locomotion in the ParA/ParB system, LAVISHA JINDAL, ELDON EMBERLY, Simon Fraser University — In many bacteria the ParA/ParB system is responsible for actively segregating DNA during replication. ParB precessively
moves by hydrolyzing DNA bound ParA-ATP forming a depleted ParA region in its wake. Recent in-vitro experiments have shown that a ParB covered bead can
traverse a ParA bound DNA substrate. It has been suggested that the formation of a gradient in ParA leads to diffusion-ratchet like motion of the ParB bead
but its origin and potential consequences requires investigation. We have developed a deterministic model for the in-vitro ParA/ParB system and show that
any amount of spatial noise in ParA can lead to the spontaneous formation of its gradient. The velocity of the bead is independent of this noise but depends
on the scale over which ParA exerts a force on the bead and the scale over which ParB hydrolyzes ParA from the substrate. There is a particular ratio of these
scares at which the velocity is a maximum. We also explore the effects of cooperative vs independent rebinding of ParA to the substrate. Our model shows
how the driving force for ParB originates and highlights necessary conditions for directed motion in the in-vitro system that may provide insight into the in-vivo
behaviour of the ParA/ParB system.

5:06PM J48.00012 Pulse Dynamics in Endocytic Protein Patches1, Supported by NIH under Grant R01-GM107667.
at higher ant densities. In comparison, dead ants are always solid-like. oppose the applied stress. In the linear regime, the dynamics is fractal-like with both storage and shear moduli that overlap for over three orders of magnitude to drip and spread like simple liquids, but that can also store energy and maintain a shape like elastic solids. They are an active material where the constituent MICHAEL TENNENBAUM, ZHONGYANG LIU, DAVID HU, Georgia Institute of Technology — Fire ants, and Avalanches, CHARLES REICHARDT, CYNTHIA OLSON REICHARDT, Los Alamos National Laboratory — We examine the mobility and velocity fluctuations of a driven particle moving through an active matter bath of self-mobile particles for varied system densities and activities. The driven particle mobility is strongly non-monotonic and is correlated with distinct spatial-temporal structures that arise in the active media. We identify an activity-induced crystallization regime that is distinct from the higher activity-induced phase-separated cluster regime. The probe particle velocity fluctuation distributions exhibit specific features in the different dynamic regimes. In the cluster phase, we observe telegraph noise, while in the denser active jamming regimes, the probe particle moves in intermittent jumps or avalanches of power-law distributed sizes. 2:42PM J49.00002 Using artificial microswimmers for controlling the motion of passive colloidal particles in straight and asymmetric channels, VYACHESLAV R. MISKO, University of Antwerp — Artificial self-propelled microswimmers capable of autonomous navigation through complex environments provide appealing opportunities for localization, pick-up and delivery of micro- and nanoscopic objects. Such self-driven microswimmers show not only the ability to navigate through the environment but also modify the environment. Using numerical simulations, we investigate active Brownian motion of self-propelled overdamped microswimmers, i.e., Janus spheres illuminated by light, in straight and corrugated channels. We demonstrated that a small fraction of active microswimmers injected in a system of passive colloids are capable of rectifying the passive species (i.e., in asymmetric channels [1]) or separating various species (i.e., in a mixture of passive species [2]). We analyze the effect of autonomous pumping of passive species by active microswimmers in various corrugated channels. [1] Pulak K. Ghosh, Vyacheslav R. Misko, Fabio Marchesoni, and Franco Nori, Phys. Rev. Lett. 110, 268301 (2013). [2] W. Yang, V.R. Misko, K. Nelissen, M. Kong, and F.M. Peeters, Soft Matter 8, 5175 (2012).

2:54PM J49.00003 Visco-elastic Dynamics of an Active Polar Dynamic System, HARALD PLEINER, Max Planck Institute for Polymer Research, Mainz, Germany, DANIEL SVENSEK, Department of Physics, Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia, HELMUT R. BRAND, Theoretische Physik III, Universität Bayreuth, Germany — We study the dynamics of systems with a polar dynamic preferred direction that are embedded in visco-elastic media. Examples include the pattern-forming growth of bacteria and molecular motors. Because the ordered state only exists dynamically, but not statically, the macroscopic variable of choice is the velocity of the active units. The passive visco-elastic medium is described by a relaxing strain tensor. We derive the macroscopic equations for such a system and discuss novel static, reversible and irreversible cross-couplings connected to this two-fluid (velocity-shear) system. The dynamics is rather different compared to the case of passive, static polar order. In particular, we find a complicated normal mode structure that reflects the broken time-reversal symmetry due to the non-equilibrium situation, anisotropy of first sound and a possible second sound excitation due to the active velocity, and various manifestations of the visco-elastic relaxation. We discuss critically the role of the so-called active term in the stress tensor as well as the thermodynamically correct description of the hydrodynamic transport velocities.

3:06PM J49.00004 ABSTRACT WITHDRAWN —

3:18PM J49.00005 Long range self-organization in bacterial swarms, CHONG CHEN, YI LIN WU, The Chinese University of Hong Kong, WU YILIN TEAM — When grown on air-semisolid interface, many bacteria are able to move in groups and expand rapidly, in a manner called swarming. Bacteria swarming displays rich collective behavior. In this work, we focus on the interaction between swarm cells of E. coli and their fluid environment. Using novel tracers, we discovered large scale self-organization in E. coli swarming colonies that spans a distance of millimeters. This long range self-organization most likely results from local interactions. The results provide new insights into the collective behavior in active matter systems.

3:30PM J49.00006 Dynamic Clustering in Suspension of Motile Bacteria, HEPENG ZHANG, XIAO CHEN, XIANG YANG, Shanghai Jiao Tong Univ, China, MINGCHENG YANG, Beijing National Laboratory for Condensed Matter Physics and Key Laboratory of Soft Matter Physics, Institute of Physics, Chinese Academy — Bacteria suspension exhibits a wide range of collective phenomena arising from interactions between individual cells. Here we investigate dynamic clusters of motile bacteria near an air-liquid interface. Cell in a cluster orient its flagella perpendicular to the interface and generate attractive radial fluid flow that leads to cluster formation. Rotating cell also creates tangential forces on neighbors that sets clusters into counter-clockwise rotation. We construct a numerical model of self-propelled particles that interact via pair-wise forces extracted from hydrodynamic calculations; such a model reproduces many properties of observed cluster dynamics.

3:42PM J49.00007 Dynamics and elasticity of fire ant aggregations, ALBERTO FERNANDEZ-NIEVES, MICHAEL TENNENBAUM, ZHONGYANG LIU, DAVID HU, Georgia Institute of Technology — Fire ants, Solenopsis invicta, form aggregations that are able to drip and spread like simple liquids, but that can also store energy and maintain a shape like elastic solids. They are an active material where the constituent particles constantly transform chemical energy into work. We find that fire ant aggregations shear thin and exhibit a stress cutoff below which they are able to oppose the applied stress. In the linear regime, the dynamics is fractal-like with both storage and shear moduli that overlap for over three orders of magnitude and that are power law with frequency. This dynamic behavior, characteristic of polymer gels and the gelation point, gives way to a predominantly elastic regime at higher ant densities. In comparison, dead ants are always solid-like.
Capillary foams: highly stable bubbles formed by synergistic action of particles and immiscible liquid. CARSON MEREDITH, YI ZHANG, SVEN BEHRENS, Georgia Tech — Liquid foams are a familiar part of everyday life from beer and frothed milk to bubble baths; they also play important roles in enhanced oil recovery, lightweight packaging, and insulation. We report a new class of foams, obtained by frothing a suspension of colloidal particles in the presence of a small amount of an immiscible secondary liquid. A unique aspect of the new foams, termed capillary foams, is that suspended particles mediate spreading of a minority liquid around gas bubbles. The resulting mixed particle/liquid coating can stabilize bubbles against coalescence even when the particles alone cannot. We demonstrate the generality of capillary foams by forming them from a diverse set of particle/liquid combinations and rationalize the results with a simple free energy model. In addition to many applications as liquid foams, capillary foams can serve as precursors for hierarchically-structured solids with porosity on different length scales and with significant application potential.
3:06PM J50.00004 Hyperuniformity Length in Experimental Foam and Simulated Point Patterns, ANTHONY CHIECO, ADAM ROTH, University of Pennsylvania, REMI DREYFUS, CNRS-Solvay-UPenn, SALVATORE TORQUATO, Princeton University, DOUGLAS DURIAN, University of Pennsylvania — Systems without long-wavelength number density fluctuations are called hyperuniform (HU). The degree to which a point pattern is HU may be tested in terms of the variance in the number of points inside randomly placed boxes of side length L. If HU then the variance is due solely to fluctuations near the boundary rather than throughout the entire volume of the box. To make this concrete we introduce a hyperuniformity length $\eta$, equal to the width of the boundary where number fluctuations occur. Thus $\eta$ helps characterize the disorder. We show how to deduce $\eta$ from the number of particles, $n$, so that Poisson and Einstein patterns plus those made by the vertices and bubble centroids in 2D foams. A Poisson pattern is one where points are totally random. These are not HU and $\eta$ equals L/2. We coin “Einstein patterns” to be where points in a lattice are independently displaced from their site by a normally distributed amount. These are HU and $\eta$ equals the RMS displacement from the lattice sites. Bubble centroids and vertices are both HU. For these, $\eta$ is less than L/2 and increases slower than linear in L. The centroids are more HU than the vertices, in that $\eta$ increases more slowly.

3:18PM J50.00005 The Response of a 2D Emulsion to Local Perturbations, XIA HONG, CARLOS ORELLANA, ERIC WEEKS, Department of Physics, Emory University, Atlanta, GA — We experimentally perturb a quasi-two-dimensional emulsion packing by inflating an oil droplet into the system in a controlled way. Our samples are oil-in-water emulsion confined between two close-spaced parallel plates, so that the droplets are deformed into pancake shapes. In this system, there is only viscos friction and no static friction between droplets. By imaging the droplets with a video microscopy, we observe rearrangement events induced by the local perturbation. Simultaneously, we measure droplet-droplet contact forces by analyzing the outlines of each droplet in our movies. These allow us to study how the packings with varying degrees of spatial order have different responses to the local perturbation.

3:30PM J50.00006 Simulations of Soft Glassy Matter with Ripening, HYUN JOO HWANG, ROBERT RIGGLEMAN, JOHN CROCKER, University of Pennsylvania — Soft glassy matter (SGM) such as foams, emulsions, and colloids, exhibit interesting rheological properties that have long defied explanation. In particular, the shear modulus of these materials displays weak power law frequency dependence. To understand the origin of this property in more depth, we have built a three-dimensional, modified Bubble Dynamics model. The bubbles interact with a purely repulsive harmonic potential and ripen according to diffusion-based governing equations. An energy minimizer is implemented to quasi-statically relax topological rearrangements in the system as ripening proceeds. Preliminary results show that the model displays expected intermitten particle rearrangements and a weakly frequency-dependent shear modulus behaving like a power law fluid. We find that the anomalous relaxation properties and avalanche-like nature of the rearrangements can be related to different measures of the systems potential energy landscape.

3:42PM J50.00007 Arresting relaxation in Pickering Emulsions, TIM ATHERTON, CHRIS BURKE, Tufts University — Pickering emulsions consist of droplets of one fluid dispersed in a host fluid and stabilized by colloidal particles absorbed at the fluid-fluid interface. Everyday materials such as crude oil and food products like salad dressing are examples of these materials. Particles can stabilize non spherical droplet shapes in these emulsions through the following sequence: first, an isolated droplet is deformed, e.g. by an electric field, increasing the surface area above the equilibrium value; additional particles are then adsorbed to the interface reducing the surface tension. The droplet is then allowed to relax toward a sphere. If more particles were adsorbed than can be accommodated by the surface area of the spherical ground state, relaxation of the droplet is arrested at some non-spherical shape. Because the energetic cost of removing adsorbed particles exceeds the droplet deformation energy, these structures can remain stable over long timescales. In this presentation, we will discuss new results on how chemical reactions can be used to stabilize emulsions and to control their properties in technology and nature.

3:54PM J50.00008 Suppression of Ostwald Ripening by Chemical Reactions, DAVID ZWICKER, Harvard University, ANTHONY A. HYMAN, Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, FRANK JÜLICH, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — Emulsions consisting of droplets immersed in a fluid are typically unstable and coarsen over time. One important coarsening process is Ostwald ripening, which is driven by the surface tension of the droplets. Ostwald ripening must thus be suppressed to stabilize emulsions, e.g. in cosmetic, pharmaceutical, or food products. To study Ostwald ripening, we use microemulsions, which contain stable liquid-like compartments, e.g. germ granules, Cajal-bodies, and centrosomes. Such systems are often driven away from equilibrium by chemical reactions and can thus be called active emulsions. Here, we show that non-equilibrium chemical reactions can suppress Ostwald Ripening, leading to stable, monodisperse emulsions. We derive analytical approximations of the typical droplet size, droplet count, and time scale of the dynamics from a coarse-grained description of the droplet dynamics. We also compare these results to numerical simulations of the continuous concentration fields. Generally, we thus show how chemical reactions can be used to stabilize emulsions and to control their properties in technology and nature.

4:06PM J50.00009 Membrane-mediated colloidal interactions, CASPER VAN DER WEL, DORIS HEINRICH, DANIELA KRAFT, Leiden University — Membrane proteins are known to play a key role in inducing curvature in biological membranes. This curvature leads to interactions between the proteins through minimization of the bending energy of the membrane. Simulations have shown a wide variety of interesting phenomena, for example how curvature influences protein sorting, but little is understood about the underlying physics. We study these membrane-mediated interactions using an experimental model system consisting of micro-sized polymer particles linked to a freestanding lipid membrane (GLV). The particles locally distort the membrane curvature and by that exhibit an attraction. The influence of the curvature distortion on the pairwise interaction is studied systematically by tracking the particles with confocal microscopy.

4:18PM J50.00010 Contact-line deformation around a spherical particle at an anisotropic liquid interface, NESRIN SENBIL, WEI HE, ANTHONY DINSMORE, University of Massachusetts, Amherst — The shape of the contact line around a particle determines its interaction with other particles at liquid interfaces. Thus, the shape of the interface and contact line is significant for self-assembly and many other applications of colloids. In our experiments, we used PDMS-coated millimeter-sized glass spheres to avoid pinning. The contact line around the sphere is observed at initially flat, cylindrical-like and saddle-like shapes with a camera placed perpendicular to the plane of the initially flat interface. Unlike flat interfaces, at anisotropic interfaces, the contact line around the sphere is not circular. Our results demonstrate that the quadrupolar deformation of the contact line ($z_2$) increases with deviatoric curvature (anisotropy) of the interface (D_H). For instance, for a PDMS-coated glass sphere with a diameter 3.2mm, $z_2$ increases from 0 to 0.12mm$^{-1}$, $z_0$ increases from 0 to about 0.3mm. We will discuss the relation among $z_2$, $D_H$, mean contact radius, particle radius, and contact angle and compare to theory. Our results are important to understand the assembly of particles at anisotropically curved interfaces. This work is funded by the NSF through CBET-0967620 and by the Gulf of Mexico Research Initiative through the C-MEDS consortium.

4:30PM J50.00011 The influence of protein aggregation on adsorption kinetics, JOEL ROVNER, NIST — When proteins adsorb to an air-water interface they lower the surface tension and may form an age-dependent viscoelastic film. Protein adsorption to surfaces is relevant to both commercial uses and biological function. The rate at which the surface tension decreases depends strongly on temperature, solution pH, and protein structure. These kinetics also depend on the degree to which the protein is aggregated in solution. Here we explore these differences using Chymotrypsinogen as a model protein whose degree of aggregation is adjusted through controlled heat treatment and measured by chromatography. To study these effects we have used a micropipette tensiometer to produce a spherical-cap bubble whose interfacial pressure was controlled — either steady or oscillating. Short heat treatment produced small soluble aggregates, and these adsorbed faster than the original protein monomer. Longer heat treatment produced somewhat larger soluble aggregates which adsorbed more slowly. These results point to complex interactions during protein adsorption.
Crystal nucleation and structural relaxation, transient domains and dynamic heterogeneity, grain boundaries and polycrystallinity. A stochastic model from which University of California, Berkeley — Materials undergoing glass transitions are often materials that can also crystalize. The qualities of the solid that forms

Grand Ballroom C1 - Eli Ben-Naim, Equilibrium Statistical Mechanics of Liquids, Glasses and Biomolecules

Irwin's knowledge and understanding of the subject were breathtaking.

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LINDENBERG, Univ of California - San Diego — Irwin Oppenheim's early work on Langevin equations, master equations, and Brownian motion was one of the

We consider the problem of constructing dynamic CG models within the context of the Multi-Scale Coarse Graining (MS-CG) method of Voth and coworkers.

Coarse grained (CG) models of molecular systems, with fewer mechanical degrees of freedom than an all-atom model, are used extensively in chemical physics. It is generally accepted that a coarse grained model that accurately describes equilibrium structural properties (as a result of having a well constructed CG potential energy function) does not necessarily exhibit appropriate dynamical behavior when simulated using conservative Hamiltonian motion by stochastic but Markovian dynamics on that surface, such as Langevin or Brownian dynamics. However, depending on the nature of the system and the extent of the coarse graining, a Markovian dynamics for the CG degrees of freedom may not be appropriate.

Dynamic surface tension measurements carried out with conventional methods like pendant drop analysis, Wilhelmy plate, etc are limited in their temporal resolution (>50 ms). In this study, we describe design and application of maximum bubble pressure tensiometry for the measurement of dynamic surface tension effects at extremely short (1-50 ms) timescales. We discuss the ramifications of this nearly unprecedented capability for unraveling physics underlying high speed printing and foaming with small molecule surfactant solutions.

Janus nanoparticles for stable microemulsions with ultra-low IFT values: ILSE NAVA, AGUSTIN DIAZ, YI-HSIEN YU, ZHENDONG CHENG, Texas A&M University — Janus particles are an influential type of materials used in foams, detergents, surfactants and cosmetics. Due to their demonstrated flexibility and non-toxicity, they have the potential to replace molecular surfactants, and thanks to their amphiphilic nature, they can stabilize immiscible biphasic systems. Disk-based Janus particles best perform this stabilization. Graphene has been used to manufacture this class of particles; however, their fabrication in high yield by short and atomically economic syntheses remains a challenge. In this project we report the first synthesis of monolayer disks by a one pot reaction under microwave energy. Using a scalable method, these disks were synthesized, emulsified (in an oil/water system), and chemically reacted to obtain the Janus nanodisks with an efficient method. Our nanosheets production technique is a promising approach for the fabrication of Janus nanodisks via emulsification as it produces IFT (interfacial tension) values in a lower range than that of the molecular surfactants. These ultra-low values, in conjunction with the sheets' salt resistance, temperature resistance, and non-toxicity position Janus particles as the next generation of nanosurfactants.

Maximum bubble pressure tensiometry and foamability: THEODORE WALKER, WILLIAM ABBOTT-KLOSTERMANN, PRASANTH NARAYANAN, VIVEK SHARMA, Chemical Engineering, University of Illinois Chicago — The stability of a freshly created foam is intimately linked with the rate of mass transfer of a surfactant from liquid sub-phase to the interface, and this diffusion- or adsorption-limited mass transfer dictates the so-called foamability. The time dependent variation in surface tension can also become a factor in controlling response to dilational deformations, as kinetic effects due to mass transfer also enter into the description of Gibbs-Marangoni elasticity of surfaces. Dynamic surface tension measurements carried out with conventional methods like pendant drop analysis, Wilhelmy plate, etc are limited in their temporal resolution (>50 ms). In this study, we describe design and application of maximum bubble pressure tensiometry for the measurement of dynamic surface tension effects at extremely short (1-50 ms) timescales. We discuss the ramifications of this nearly unprecedented capability for unraveling physics underlying high speed printing and foaming with small molecule surfactant solutions.

Competing dynamics of vitrification and crystal coarsening: DAVID CHANDLER, University of California, Berkeley — Materials undergoing glass transitions are often materials that can also crystallize. The qualities of the solid that forms depend upon the system's dynamics and experimentalist's protocols. This lecture describes some of the associated phenomena, including competition between crystal nucleation and structural relaxation, transient domains and dynamic heterogeneity, grain boundaries and polycrystallinity. A stochastic model from which all of these phenomena emerge will be presented.

Brownian motion, old and new, and Irwin's role in my academic life: KATJA LINDENBERG, Univ of California - San Diego — Irwin Oppenheim's early work on Langevin equations, master equations, and Brownian motion was one of the earliest and strongest reasons for my change of direction from my PhD work in condensed matter theory to my later and lifelong interest in Brownian motion and, more broadly, statistical mechanics. I will talk about some of my most recent work on subdiffusion, a form of anomalous diffusion that describes random motions in crowded or disordered media where motions are hindered by the medium. On a personal note, I knew Irwin for decades, from the time before he had a family (he was a sworn bachelor...until he met his wife) until shortly before his death. For many years, first alone and then with family, Irwin would spend some portion of the cold Boston winter in warm La Jolla, and we would always get together during these visits. For a period of a number of years we decided to take advantage of these visits to write the definitive text in traditional Thermodynamics. We did not make it past about 2/3 of the project, but it was a great learning experience for me while it lasted. Irwin's knowledge and understanding of the subject were breathtaking.

 session J50.00012: Gravitational Drainage of Anionic and Nonionic Surfactant Mixtures: THEODORE WALKER, UNIVERSITY OF ILLINOIS AT CHICAGO — The stability of a freshly created foam is intimately linked with the rate of mass transfer of a surfactant from liquid sub-phase to the interface, and this diffusion- or adsorption-limited mass transfer dictates the so-called foamability. The time dependent variation in surface tension can also become a factor in controlling response to dilational deformations, as kinetic effects due to mass transfer also enter into the description of Gibbs-Marangoni elasticity of surfaces. Dynamic surface tension measurements carried out with conventional methods like pendant drop analysis, Wilhelmy plate, etc are limited in their temporal resolution (>50 ms). In this study, we describe design and application of maximum bubble pressure tensiometry for the measurement of dynamic surface tension effects at extremely short (1-50 ms) timescales. We discuss the ramifications of this nearly unprecedented capability for unraveling physics underlying high speed printing and foaming with small molecule surfactant solutions.

 session J50.00013: ZrP nanoparticles based fire-fighting foams: LECHENG ZHANG, ZHENDONG CHENG, HAI LI, TEXAS A&M UNIVERSITY — Firefighting foam, as a significant innovation in fire protection, greatly facilitates extinguishments for liquid pool fire. Recently, with developments in LNG industry, high-expansion firefighting foams are also used for extinguishing LNG fire or mitigating LNG leakage. Foam stabilizer, an ingredient in fire-fighting foam, stabilizes foam bubbles and maintains desired foam volume. Conventional foam stabilizers are organic molecules. In this work, we developed a inorganic based ZrP (Zr(HPO4)2·H2O, Zirconium phosphate) plate functionalyzed as firefighting foam stabilizer, improving firefighting foam performance under harsh conditions. Several tests were conducted to indicate performance. The mechanism for the foam stabilization is also proposed.

 session J50.00014: Maximum bubble pressure tensiometry and foamability: THEODORE WALKER, WILLIAM ABBOTT-KLOSTERMANN, PRASANTH NARAYANAN, VIVEK SHARMA, Chemical Engineering, University of Illinois Chicago — The stability of a freshly created foam is intimately linked with the rate of mass transfer of a surfactant from liquid sub-phase to the interface, and this diffusion- or adsorption-limited mass transfer dictates the so-called foamability. The time dependent variation in surface tension can also become a factor in controlling response to dilational deformations, as kinetic effects due to mass transfer also enter into the description of Gibbs-Marangoni elasticity of surfaces. Dynamic surface tension measurements carried out with conventional methods like pendant drop analysis, Wilhelmy plate, etc are limited in their temporal resolution (>50 ms). In this study, we describe design and application of maximum bubble pressure tensiometry for the measurement of dynamic surface tension effects at extremely short (1-50 ms) timescales. We discuss the ramifications of this nearly unprecedented capability for unraveling physics underlying high speed printing and foaming with small molecule surfactant solutions.

 Tuesday, March 3, 2015 2:30PM - 5:30PM –

 Session J51 GSNP GSOFT: Invited Session: Irwin Oppenheim Memorial Session: Non-Equilibrium Statistical Mechanics of Liquids, Glasses and Biomolecules

 Brownian motion, old and new, and Irwin's role in my academic life: KATJA LINDENBERG, Univ of California - San Diego — Irwin Oppenheim's early work on Langevin equations, master equations, and Brownian motion was one of the earliest and strongest reasons for my change of direction from my PhD work in condensed matter theory to my later and lifelong interest in Brownian motion and, more broadly, statistical mechanics. I will talk about some of my most recent work on subdiffusion, a form of anomalous diffusion that describes random motions in crowded or disordered media where motions are hindered by the medium. On a personal note, I knew Irwin for decades, from the time before he had a family (he was a sworn bachelor...until he met his wife) until shortly before his death. For many years, first alone and then with family, Irwin would spend some portion of the cold Boston winter in warm La Jolla, and we would always get together during these visits. For a period of a number of years we decided to take advantage of these visits to write the definitive text in traditional Thermodynamics. We did not make it past about 2/3 of the project, but it was a great learning experience for me while it lasted. Irwin's knowledge and understanding of the subject were breathtaking.
4:18PM J51.00004 Ion Atmosphere Near Nucleic Acids1, UDAYAN MOHANTY, Department of Chemistry, Boston College — We will discuss allatom structure based model that explicitly includes ionic effects, i.e., electrostatic interactions with explicit magnesium ions and implicit KCl that allow us to carry out explicit solvent molecular dynamics simulations of adenine riboswitch and SAMI riboswitch. Our predictions for the excess ions around the riboswitch, and the magnesiumRNA interaction free energy will be compared with experimental data. We will provide upper and lower bounds for preferential interaction coefficient, a statistical mechanical quantity that is a measure of excess ion atmosphere around a polyelectrolyte. We will discuss the role of surface charge density of mobile ions from added salt in determining the counterion release entropy associated with chain collapse. Finally, the Poisson’s ratio of oligomeric DNA will be determined. (Work done in collaboration with R. Hayes, J. Noel, P. Whithford, S. Hennelly, J. Onuchic, and K. Sanbonmatsu.)

1Work supported by fellowship from John Simon Guggenheim Memorial Foundation.

4:54PM J51.00005 The Typical Lengthscale Characterizing the Glass Transition at Lower Temperatures, ITAMAR PROCACCIA, The Weizmann Institute of Science — The existence of a static length scale that grows in accordance with the dramatic slowing down observed at the glass transition is a subject of intense interest. A recent publication compared two proposals for this length scale, one based on the point-to-set correlation technique and the other on the scale where the lowest eigenvalue of the Hessian matrix becomes sensitive to disorder. The conclusion was that both approaches lead to the same length scale, but the former is easier to measure at higher temperatures and the latter at lower temperatures. But even after using both methods together, the range of increase in the observed length scales was limited by the relaxation times reachable by standard molecular dynamics techniques (i.e. about 4-5 orders of magnitude). In this paper we therefore attempt to explore the typical scale at even lower temperatures, testing for this purpose two approaches, one based on the idea of vapor deposition and the other on a swap Monte Carlo technique. We conclude that the first approach does not help in getting to lower temperatures, but the second one does so quite effectively. We can reach a typical lengthscale that grows in accordance with at least 18 orders of magnitude increase in the relaxation time, coming close to the best experimental conditions. We conclude by discussing the relationship between the observed lengthscale and various models of the relaxation time.

Tuesday, March 3, 2015 2:30PM - 5:30PM —
Session J52 Buckley Prize / Apker Award Session Grand Ballroom C2 -

2:30PM J52.00001 Buckley Prize Talk: Electrostatic Control of the Superconductor-Insulator Transition1, ALLEN GOLDMAN, Univ of Minnesota - Minneapolis — The superconductor-insulator transitions (SITs) of ultra-thin films are among the simplest quantum phase transitions. The ground states of systems that have been studied are usually changed by adjusting the level of disorder, by the application of perpendicular and parallel magnetic fields, by altering the chemical composition, and by the seeding of the surface with pair-breaking magnetic impurities. More recently, realizations of the electric field effect have been used to tune SITs. This has been done with devices employing high dielectric constant gate insulators, as well as with electric double layer transistor devices employing ionic liquids as gate insulators. In addition to disordered ultrathin films, cuprates, and metallic interfaces between insulators have also been studied. The SITs of selected systems will be reviewed with particular attention being paid to the results of finite size scaling analyses of the transitions, and the nature of the insulating states found. In the case of the cuprates, the extent to which their phase diagrams can be traversed will be explored. Finally the potential value of electrostatic gating as a tool in the search for new superconductors will be discussed.

3:06PM J52.00002 Buckley Prize Talk: Bosons on the Boundaries: The magnetic field driven superconductor-insulator quantum phase transition . ARTHUR HEBARD, University of Florida — Experiments probing the competition between superconductivity and disorder in two-dimensional (2D) thin-film systems have provided fascinating glimpses into the physics of superconductor-insulator (S-I) quantum phase transitions (QPTs). This talk will address the use of externally applied magnetic fields to tune through the S-I transition of amorphous composite indium oxide (α-InOx) thin films prepared at different stages of disorder. Air-stable α-InOx films are particularly advantageous for these studies: the disorder parameter as measured by the sheet resistance can be reproducibly controlled during deposition and the films are uniformly homogeneous out to macroscopic length scales. Temperature-dependent resistance and current-voltage measurements confirm the power-law decay of the order-parameter correlation function appropriate to a Kosterlitz-Thouless description of phase transitions in 2D systems. Accordingly, the superconducting phase transition temperature Tc is related to the unbinding of vortex-antivortex pairs either by temperature and/or disorder. The application of magnetic fields unveils fundamentally different physics in which, rather than a vortex unbinding transition, a field-tuned QPT emerges with the signature of a disorder-dependent critical field Bc that identifies the delocalization and Bose condensation of field-induced vortices. The concomitant pronounced divergence in resistance, which becomes increasing sharp as the temperature is lowered, marks the boundary between a superconductor harboring both Bose condensed Cooper pairs and localized vortices and an insulator harboring both Bose condensed Cooper pairs and localized Cooper pairs. The data for this putative QPT are well described by finite temperature scaling theory with critical exponent values accurately determined. At higher fields there is a second critical field where the transverse resistance appears to diverge, signaling the unbinding of pairs with the superconducting energy gap simultaneously going to zero and localized single electrons dominating to form a Fermi glass insulator.

3:42PM J52.00003 Buckley Prize Talk: The Superconductor-(Metal)-Insulator Transition . AHARON KAPITULNIK, Stanford University — While the classical theory of phase transitions has been extraordinarily successful, there are several reasons to exercise caution when applying this approach to the zero temperature superconducting transition. First, experimental identification of the relevant phases requires extrapolation to zero temperature, which becomes complicated, especially when one needs to identify sources of dissipation. In addition, since superconductivity may be highly inhomogeneous as appreciable superconducting order parameter may be concentrated in “superconducting puddles” due to disorder and/or spontaneous phase separation, the nature of the quantum phase transition to a superconducting state may be highly anomalous, where the system attempts to optimize the formation of puddles with the Josephson coupling among them to obtain global superconductivity. In this talk we will review some of the consequences of these considerations, emphasizing the possible emergence of anomalous metallic phases close to the superconductor-insulator transition.

4:18PM J52.00004 Buckley Prize Talk: Theory of Quantum Phase Transitions: A 25 year purview . MATTHEW FISHER, UC Santa Barbara — A 25 Purview of Quantum Phase Transitions
4:54PM J52.00005 Leroy Apker Award Talk: Transport measurements of a model cuprate superconductor. MICHAEL VEIT, Univ of Minn - Minneapolis — High-temperature superconductivity in the cuprates has been the subject of intense research since its discovery in 1986 by J. G. Bednorz and K. A. Müller. The fundamental challenge posed by these materials is that they exhibit strong electronic correlations, giving rise to anomalous properties, such as the observation that the resistivity in optimally hole-doped samples is linear in temperature from the superconducting transition temperature up to very high temperatures. The scope of this work was to explore the phase diagram through transport measurements of a model compound. Specifically, the resistivity, magneto-resistance, Hall effect and thermoelectric power were measured for single-crystal samples of HgBa2CuO4+δ (Hg201). The outcome of these measurements is highly surprising. Despite the complexity of the phase diagram, conventional Fermi-liquid metallic behavior is observed in the pseudogap regime below optimal doping.

Tuesday, March 3, 2015 2:30PM - 5:30PM — Session J53 DCMP: Invited Session: Progress in Electrically-Gated Quantum Dot Qubits Grand Ballroom C3 - HongWen Jiang, University of California, Los Angeles

2:30PM J53.00001 Control and Measurement of an Exchange-Only Spin Qubit. JAMES MEDFORD, Harvard University — Gate-defined semiconductor quantum dots have proven to be a versatile testbed for exploring quantum systems and quantum information. We demonstrate the fast all-electrical control of a spin qubit using the two coherent exchange interactions in a triple quantum dot. Our measurements identify the role of nuclear spins from the host GaAs in this system as a mechanism for both dephasing and leakage out of the qubit subspace. We also show that by increasing both exchange interactions in a balanced fashion, we enter a second regime of operation. In this regime, leakage from the subspace has been suppressed, resulting in a spin qubit with a tunable electric dipole moment, which we refer to as the resonant exchange qubit.

3:06PM J53.00002 Silicon based quantum dot hybrid qubits1. DOHUN KIM, University of Wisconsin — The charge and spin degrees of freedom of an electron constitute natural bases for constructing quantum two level systems, or qubits, in semiconductor quantum dots. The quantum dot charge qubit offers a simple architecture and high-speed operation, but generally suffers from fast dephasing due to strong coupling of the environment to the electron’s charge. On the other hand, quantum dot spin qubits have demonstrated long coherence times, but their manipulation is often slower than desired for important future applications. This talk will present experimental progress of a ‘hybrid’ qubit, formed by three electrons in a Si/SiGe double quantum dot, which combines desirable characteristics (speed and coherence) in the past found separately in qubits based on either charge or spin degrees of freedom. Using resonant microwaves, we first discuss qubit operations near the ‘sweet spot’ for charge qubit operation. Along with fast (>GHz) manipulation rates for any rotation axis on the Bloch sphere, we implement two independent topographic characterization schemes in the charge qubit regime: traditional quantum process tomography (QPT) and gate set tomography (GST). We also present resonant qubit operations of the hybrid qubit performed on the same device, DC pulsed gate operations of which were recently demonstrated. We demonstrate three-axis control and the implementation of dynamic decoupling pulse sequences. Performing QPT on the hybrid qubit, we show that AC gating yields π rotation process fidelities higher than 93% for X-axis and 96% for Z-axis rotations, which demonstrates efficient quantum control of semiconductor qubits using resonant microwaves. We discuss a path forward for achieving fidelities better than the threshold for quantum error correction using surface codes.

1This work was supported in part by ARO (W911NF-12-0607), NSF (PHY-1104660), DOE (DE-FG02-03ER46028), and by the Laboratory Directed Research and Development program at Sandia National Laboratories under contract DE-AC04-94AL85000.

3:42PM J53.00003 Electrical control of a long-lived spin qubit in a Si/SiGe quantum dot. ERIKA KAWAKAMI, Kavli Institute of Nanoscience, TU Delft — Electron spins in Si/SiGe quantum dots are one of the most promising candidates for a quantum bit for their potential to scale up and their long dephasing time. We realized coherent control of single electron spin in a single quantum dot (QD) defined in a Si/SiGe 2D electron gas. Spin rotations are achieved by applying microwave excitation to one of the gates, which oscillates the electron wave function back and forth in the gradient field produced by cobalt micromagnets fabricated near the dot. The electron spin is read out in single-shot mode via spin-to-charge conversion and a QD charge sensor. In earlier work [1], both the fidelity of single-spin rotations and the spin echo decay time were limited by a small splitting of the lowest two valleys. By changing the direction and magnitude of the external magnetic field as well as the gate voltages that define the dot potential, we were able to increase the valley splitting and also the difference in Zeeman splittings associated with these two valleys. This has resulted in considerable improvements in the gate fidelity and spin echo decay times. Thanks to the long intrinsic dephasing time T2* ~ 900 ns and Rabi frequency of 1.4 MHz, we now obtain an average single qubit gate fidelity of an electron spin in a Si/SiGe quantum dot of 99 percent, measured via randomized benchmarking. The dephasing time is extended to 70 us for the Hahn echo and up to 400 us with CPMG80. From the dynamical decoupling data, we extract the noise spectral density in the range of 30 kHz-3 MHz. We will discuss the mechanism that induces this noise and is responsible for decoherence. In parallel, we also realized electron spin resonance and coherent single-spin control by second harmonic generation, which means we can drive an electron spin at half the Larmor frequency. Finally, we observe not only single-spin transitions but also transitions whereby both the spin and the valley state are flipped. Altogether, these measurements have significantly increased our understanding and raised the prospects of spin qubits in Si/SiGe quantum dots.

This work has been done in collaboration with T.M. J. Jullien, P. Scarlino, V.V. Dobrovitski, D.R. Ward, D. E. Savage, M. G. Lagally, Mark Friesen, S. N. Coppersmith, M. A. Eriksson, and L. M. K. Vandersypen. This work was supported in part by the Army Research Office (ARO) (W911NF-12-0607), the Foundation for Fundamental Research on Matter (FOM) and the European Research Council (ERC). Development and maintenance of the growth facilities was supported by the Department of Energy (DOE) (DE-FG02-03ER46028). E.K. was supported by a fellowship from the Nakajima Foundation. This research utilized NSF-supported shared facilities at the University of Wisconsin-Madison.


4:18PM J53.00004 Control of Spin States in Triple Quantum Dots. ANDREW SACHRAJDA, National Research Council of Canada — A brief review will be given on coherent behaviour in serial triple quantum dots in AlGaAs/GaAs heterostructure related to multi-spin states. One series of experiments involves the application of coherent superpositions of multi-electron states to the transfer of single spins and two-spin states non-locally between edge quantum dots while maintaining the center quantum dot occupation fixed at one or zero electrons. A second series of experiments involves the identification of coherent leakage mechanisms away from targeted encoded three-spin states qubits. Finally, results will be shown which reveal an unexpected control of the gap at the S-T+ anticrossing by taking advantage of different nuclear dynamic polarization pumping rates.
One- and two-qubit logic using silicon-MOS quantum dots

Andrew Dzurak, UNSW - Australia — Spin qubits in silicon are excellent candidates for scalable quantum information processing [1] due to their long coherence times and the enormous investment in silicon MOS technology. While our Australian effort in Si QC has largely focused on spin qubits based upon phosphorus dopant atoms implanted in Si [2,3], we are also exploring spin qubits based on single electrons confined in SiMOS quantum dots [4]. Such qubits can have long spin lifetimes $T_1 = 2 \text{s}$, while electric field tuning of the conduction-band valley splitting removes problems due to spin-valley mixing [5]. In isotopically enriched Si-28 these SiMOS qubits have a control fidelity of 99.6% [6], consistent with that required for fault-tolerant QC. By gate-voltage tuning the electron $g^*$-factor, the ESR operation frequency can be Stark shifted by >10 MHz [6], allowing individual addressability of many qubits. Most recently we have coupled two SiMOS qubits to realize CNOT gates [7] via either controlled rotation (CROT) or controlled phase (CZ) operations. The speed of the two-qubit CZ-operations is controlled electrically via the detuning energy and over 100 two-qubit gates can be performed within a two-qubit coherence time of 8 $\mu$s.


We acknowledge support from the Australian Research Council (CE11E0001027), the US Army Research Office (W911NF-13-1-0024), and the Australian National Fabrication Facility.
5:45PM K33.00001 GPC BUSINESS MEETING –

Tuesday, March 3, 2015 5:45PM - 6:45PM –
Session K34 GERA: GERA Business Meeting 210A -

5:45PM K34.00001 GERA BUSINESS MEETING –

Tuesday, March 3, 2015 5:45PM - 6:45PM –
Session K36 GQI: GQI Business Meeting 211 -

5:45PM K36.00001 GQI BUSINESS MEETING –

Tuesday, March 3, 2015 5:45PM - 6:45PM –
Session K41 DPOLY: DPOLY Business Meeting 214A -

5:45PM K41.00001 DPOLY BUSINESS MEETING –

Tuesday, March 3, 2015 5:45PM - 6:45PM –
Session K44 GSNP: GSNP Business Meeting 214D -

5:45PM K44.00001 GSNP BUSINESS MEETING –

Tuesday, March 3, 2015 5:45PM - 6:45PM –
Session K47 DBIO: DBIO Business Meeting 217B -

5:45PM K47.00001 DBIO BUSINESS MEETING –

Tuesday, March 3, 2015 5:45PM - 6:45PM –
Session K49 GSOFT: GSÖFT Business Meeting 217D -

5:45PM K49.00001 GSOFT BUSINESS MEETING –

Tuesday, March 3, 2015 5:45PM - 6:45PM –
Session K41 DPOLY: DPOLY - NSF Question and Answer Session on Polymers, Soft Matter, and the Materials Genome Initiative 214A -

6:45PM KA41.00001 DPOLY NSF Q&A –

Wednesday, March 4, 2015 8:00AM - 11:00AM –
Session L1 DMP: Focus Session: Beyond Graphene - Phosphorene III 001A - Yuanbo Zhang, Fudan University

8:00AM L1.00001 Toward Air-Stable Multilayer Phosphorene Thin-Films and Transistors

Joon-Seok Kim, Yingnan Liu, Weinan Zhu, Seohye Kim, Di Wu, Li Tao, Ananth Dodabalapur, Keji Lai, Deji Akinwande, The University of Texas at Austin — Few-layer black phosphorus, also known as phosphorene, has recently rose into scientific limelight due to its promising characteristics for flexible device and optoelectronic applications, such as high mobilities beyond what is achievable in other 2D dichalcogenides. In addition, its direct thickness-dependent bandgap enables optoelectronics from the infrared to visible regions. However, a fundamental challenge lies on its lack of air stability, which is of paramount importance for practical device application. Physical degradation of unprotected phosphorene in a matter of hours in air was obvious from optical and atomic force microscopy (AFM). Moreover, microwave impedance microscopy (MIM) revealed that samples with thin capping layers, though more air-stable, began to degrade from the edges inward within a few days, where the degradation was primarily electronic with minor physical changes. Statistics from phosphorene field-effect transistors (FETs) have shown that double capping with dielectric and hydrophobic fluoropolymer films afford further improved and robust weeks-long air-stability. The simple capping methods represent a facile route for achieving air-stable phosphorene devices that can enable basic studies and potential applications.

1 Support from ARO under contract W911NF-13-1- 0364, ONR under contract N00014-1110190, and the SWAN sponsored by SRC. The microwave imaging work supported by Welch Foundation Grant F-1814. D.A acknowledges the TI/Jack Kilby Faculty Fellowship.
8:12AM L1.00002 Weak Localization in Bulk Black Phosphorus and Few-Layer Phosphorene

YUCHEN DU, ADAM NEAL, HONG ZHOU, PEIDE YE, Purdue University — Most of the recent experimental research on black phosphorus (BP) or phosphorene has been focused on device applications with few systematic studies on electrical transport properties of single-layer or few-layer phosphorene. Here, we report on the magnetotransport experiments on thick BP films and few-layer phosphorene at low temperatures. The observed weak localization is well fitted by the Hikami-Larkin-Nagaoka model where the temperature dependence of the phase coherence length has demonstrated to be a power-law behavior of $T^{-0.7}$. In addition, the temperature dependence of Hall mobility as a function of the film thickness is also examined to uncover the limitation of mobility in few-layer phosphorene with different mechanisms.

8:24AM L1.00003 Passivation of Exfoliated Black Phosphorus Transistors Against Ambient Degradation1

SPENCER WELLS, JOSHUA WOOD, DEEP JARIWALA, KAN-SHENG CHEN, EUNKYUNG CHO, VINOD SANGWAN, XIAOLONG LIU, LINCOLN LAUHON, TOBIN MARKS, MARK HERSAM, Northwestern University — Unencapsulated exfoliated black phosphorus field-effect transistors are found to rapidly degrade upon exposure to ambient conditions, causing large increases in threshold voltage after only 6 h in ambient, followed by a $\sim 10^3$ decrease in FET on/off ratio and mobility after 48 h. Careful investigation into the cause of this degradation suggests that $H_2O$ irreversibly reacts with unprotected, exfoliated BP to form oxidized phosphorus species, as observed by AFM, TEM, XPS, Fourier transform infrared spectroscopy, and electrostatic force microscopy. This interpretation is further supported by the observation that BP degradation occurs more rapidly on hydrophobic octadecyltrichlorosilane self-assembled monolayers as opposed to hydrophilic SiO$_2$, implicating an edge-based intercalation of O$_2$ saturated H$_2$O in BP as the cause of degradation. Atomic layer deposited AlO$_x$ overlayers were found to suppress ambient degradation, allowing encapsulated BP FETs to maintain high on/off ratios of $\sim 10^3$ and mobilities of $\sim 100$ cm$^2$/Vs for over one month in ambient, demonstrating the effective passivation of BP flakes against ambient degradation [1].

1Research supported by the Materials Research Science and Engineering Center of Northwestern University (NSF DMR-1121262), the Office of Naval Research (N00014-14-1-0669), and the Keck Foundation.

8:36AM L1.00004 Imperfect 2D phosphorus, yet an almost perfect semiconductor, EVGENI PENEV, YUANYUE LIU, FANGBO XU, ZHANG ZHANG, BORIS YAKOBSON, Rice Univ — The deep gap states created by defects in semiconductors typically deteriorate the performance of (opto)electronic devices. This has limited the applications of two-dimensional (2D) metal dichalcogenides (MX$_2$) and underscored the need for a new 2D semiconductor without defect-induced deep gap states. The talk will discuss why a 2D mono-elemental semiconductor can be a promising candidate. This is exemplified by a first-principles study of 2D phosphorus (“phosphorene”) [1], a recently fabricated high-mobility semiconductor. Most of the defects, including intrinsic point defects and grain boundaries, are electronically inactive, thanks to the homoelemental bonding, which is not preferred in heterogeneous system such as MX$_2$. Unlike MX$_2$, where the edges create deep gap states and cannot be eliminated by passivation, the edge states of 2D P can be removed from the band gap by hydrogen termination. It is further found that both the type and the concentration of charge carriers in 2D P can be tuned by doping with foreign atoms. The work sheds light on the role of defects on the electronic structure of low-dimensional materials in general.

1Y. Liu, F. Xu, Z. Zhang, E. S. Penev, and B. I. Yakobson, Nano Lett. (2014), DOI: 10.1021/nl5032293

8:48AM L1.00005 Single/Bi-layer Silicene Field-Effect Transistors and their Air-Stability. LI TAO, Microelectronics Research Laboratory, The University of Texas at Austin, Texas 78758, USA, EUGENIO CINQUANTA, CARLO GRAZIANETTI, ALESSANDRO MOLLE, Laboratorio MDM, IMM-CNR, via C. Olivetti 2, Agrate Brianza, I-20864, Italy, DEJI AKINWANDE, Microelectronics Research Center, The University of Texas at Austin, Texas 78758, USA — Silicene, the Si analogue of graphene, has the potential to be a widely tunable 2D material for novel nanoelectronics. Air-stability is a major issue for experimental investigation on siliconene devices, which per this study has been greatly addressed by our encapsulated delamination with native electrodes (SEDNE) approach. SEDNE process preserves silicene/Ag interface during transfer and fabrication, and real-time Raman spectroscopy observes a short time window for Ag-removed silicene device stays intact and gradually degrades. In our predefined experiments, silicene devices exhibit an ambipolar charge transport behavior, corroborating theories on Dirac band in Ag-free silicene. Monolayer silicene device has extracted field-effect mobility within the theoretically predicted range and ON/OFF ratio greater than graphene, whereas bilayer silicene device shows lower mobilities and gate modulation similar to graphene. This work suggests a realistic prospect for improving air-stability of silicene devices and its tunable performance, which can be leveraged for other air-sensitive 2D materials. *Support from U.S. Army Research Office (W911NF-13-0364) and Future Emerging Technologies (270749) under European Commission are appreciated.

9:00AM L1.00006 Black Phosphorus RF Transistor

HAN WANG, Ming Hsieh Dept. EE, USC, XIAOMU WANG, FENGNIAN XIA, Dept. EE, Yale, LUHAO WANG, Ming Hsieh Dept. EE, USC, HAO JIANG, QIANGFEI XIA, Dept. ECE, U Mass, MATTHEW L. CHIN, MADDAN DUBEY, Sens & Elec. Dev. Directorate, US ARL, SHU-JEN HAN, IBM T.J. Wason Cent. — Few-layer and thin film form of layered black phosphorus (BP) has recently emerged as a promising material for applications in high performance thin film electronics and infrared optoelectronics. Layered BP offers a $\sim 0.3\text{ eV}$ bandgap and high mobility, leading to transistor devices with decent on/off ratio and high on-state current density. Here, we demonstrate the GHz frequency operation of black phosphorus field-effect transistor for the first time. BP transistors demonstrated here show excellent current saturation with an on-off ratio exceeding $2 \times 10^{10}$. The S-parameter characterization is performed for the first time on black phosphorus transistors, giving a 12 GHz short-circuit current-gain cut-off frequency and 20 GHz maximum oscillation frequency in 300 nm channel length devices. A current density in excess of 270 mA/mm and DC transconductance above 180 mS/mm are achieved for hole conductions. The results reveal the promising potential of black phosphorus transistors for enabling the next generation thin film transistor technology that can operate in the multi-GHz frequency range and beyond.

9:12AM L1.00007 Phosphorene as a new 2D material for nanoelectronic and optoelectronic applications. PEIDE YE, Purdue University — Phosphorus is one of the most abundant elements preserved in earth, constructing with a fraction of 0.1% of the earth crust. In general, phosphorus has several allotropes including white, red, and black phosphorus. Black phosphorus, though rarely mentioned, is a layered semiconductor and have great potentials in optical and electronic applications. Remarkably, this layered material can be reduced to one single atomic layer in the vertical direction owing to the van der Waals structure, dubbed phosphorene, where the physical properties can be tremendously different from its bulk counterpart and needed to be further explored. In this talk, we trace back to the 100 years research history on black phosphorus from the synthesis to material properties, and extend the topic from black phosphorene to phosphorene. The physical and transport properties are highlighted, aiming at further applications in electronic and optoelectronic devices.
9:48AM L1.00008 The Effect of Gas Absorption on Multilayer Black Phosphorus Field Effect Transistor. XUE LIU, JIN HU, CHUNLEI YUE, NICHOLAS DELLA FERA, ZHIQIANG MAO, JIANG WEI, Tulane University — Multilayer black phosphorus (BP) is drawing much attention recently due to its reported high mobility (up to 1000 cm²/V·s) and on/off ratio (up to 10⁵) as the channel material for field effect transistor (FET). We investigated the interplay between the electrical response of high performing BP-FET and gas adsorbate introduced to its surrounding environment. Different type of gas including CO₂, H₂O, Ethanol, CO, NO, NH₃, etc. has been tested. We observed that the absorption of gas molecules generally reduces the overall on-state conductance of the device with an order of 10 − 100. And such reduction can be fully recovered by purging with inert gas or baking at mild temperature (about 100°C). The absorption dynamics and detailed mechanism are also been investigated. We conclude that multilayer black phosphorus is an excellent material for chemical sensing.

10:00AM L1.00009 Stability and Passivation of Phosphorene Field Effect Transistors. YEXIN DENG, ZHE LUO, Purdue University; XIANFAN XU, Purdue University; PEIDE YE, Purdue University — Phosphorene is a new 2D semiconducting material which has been intensively studied for its physical properties and potential device applications. Its high carrier mobility and thickness-dependent direct band gap make its promising for high-performance field effect transistors and optoelectronic devices. However, even few layer phosphorene films are gradually degraded in air due to its irreversible chemical reactions with oxygen and water in ambient. In order to make stable phosphorene films for real device applications, we systematically studied the different passivation methods including PMMA, 2D hBN, and atomic layer deposited (ALD) dielectrics at different growth conditions. A combination of hBN and ALD could be one of the final solutions for realizing the environmentally stable phosphorene devices.

10:12AM L1.00010 Electrical characterization of fully encapsulated ultra thin black phosphorous-based heterostructures with graphene contacts. AHMET AVSAR, Graphene Research Center, National University of Singapore; IVAN JESUS VERA-MARUN, Graphene Research Center, National University of Singapore; Zernike Institute for Advanced Materials, University of Groningen, The Netherlands; JUN YOUN TAN, Graphene Research Center, National University of Singapore, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan; ANTONIO HELIO CASTRO NETO, BARBAROS ÖZYILMAZ, Graphene Research Center, National University of Singapore — The presence of finite bandgap and high mobility in semiconductor few-layer black phosphorous offers an attractive prospect for using this material in future two-dimensional electronic devices. Here we present for the first time fully encapsulated ultrathin (down to bilayer) black phosphorous field effect transistors in Van der Waals heterostructures to preclude their stability and degradation problems which have limited their potential for applications. Introducing monolayer graphene in our device architecture for one-atom-thick conformal source-drain electrodes enables a chemically inert boron nitride dielectric to tightly seal the black phosphorous surface. This architecture, generally applicable for other sensitive two-dimensional crystals, results in stable transport characteristics which are hysteresis free and identical both under high vacuum and ambient conditions. Remarkably, our graphene electrodes lead to contacts not dominated by thermionic emission, solving the issue of Schottky barrier limited transport in the technologically relevant two-terminal field effect transistor geometry.

10:24AM L1.00011 High Mobility Two-Dimensional Electron Gas in Black Phosphorus. LIKAI LI, Fudan University, GUO JUN YE, University of Science and Technology of China; VY TRAN, Washington University in St. Louis; St. Louis, GUORUI CHEN, Fudan University; HUICHAO WANG, JIAN YANG, Washington University in St. Louis, St. Louis, XIANHUI CHEN, University of Science and Technology of China, YUANBO ZHANG, Fudan University — Black phosphorus has recently emerged as a new member in the family of two-dimensional (2D) atomic crystals. It is a semiconductor with a tunable bandgap and high carrier mobility — material properties that are important for potential opto-electronic and high-speed device applications. In this work, we achieve a record-high carrier mobility in black phosphorus by placing it on hexagonal boron nitride (h-BN) substrate. The exceptional mobility of the 2D electron gas created at the interface allows us to observe quantum oscillations for the first time in this material. The temperature and magnetic field dependence of the oscillations yields crucial information about the black phosphorous 2DEG, such as cyclotron mass of the charge carriers and their lifetime. Our results pave the way to future research on quantum transport in black phosphorus.

10:36AM L1.00012 Oxidation pathways in Phosphorene: an ab-initio investigation. MATHEUS PAES LIMA, ADALBERTO FAZZIO, ANTONIO JOSÉ ROQUE DA SILVA, University of São Paulo — Phosphorene is a recently isolated single layer of Black Phosphorus. In this 2D material, the combination of a direct band gap with a high charge carrier mobility opens up the possibility of its use in nano devices. However, the exposure of Black Phosphorus to air leads to its fast degradation, which indicates the relevance to understand its oxidation processes. In the present work we investigate the initial steps of the oxidation process, focusing on the interaction of a single O₂ molecule with the phosphorene layer. We show that the existence of oxidation pathways having only a single barrier of 0.13eV occurring between the free O₂ (triplet) and the triplet-singlet potential energy surface (PES) crossing point. We estimate a room temperature triplet-singlet transition probability of P₁→₀ = 0.015, using the Landau-Zener model. Once the O₂ switches to the singlet PES, there is an oxygen incorporation with an energy gain of 4.2eV with respect to the PES crossing point, with the O₂ molecule spontaneously dissociating without any barrier. In this process, the final geometry has one O bonded to a P lone pair, and the other located between two P atoms. Our investigations were performed with DFT calculations at the GGA level as implemented in the VASP code.

10:48AM L1.00013 Tunability of Band Gap in Multilayer Phosphorene by External Electric Fields and Electron Dopings. SEUNG SU BAIK, HYOU NG JOON CHOI, Center for Computational Studies of Advanced Electronic Materials (CCSAEMP) and Department of Physics, Yonsei University, Korea — Black phosphorus (BP) and its two-dimensional derivative phosphorene are rapidly emerging nanoelectronic materials with potential applicability to field effect transistors and optoelectronic devices. Unlike the gapless semiconductor graphene, multilayer BP has a substantial band gap of ~ 0.2 eV and the band-gap size is reportedly varied by external electric fields. To explore the extensibility of such band-gap modulation, we have investigated electronic band structures of multilayer BP by using the first-principles density-functional method as implemented in the SIESTA code. By controlling the electron doping concentrations and the resultant electric fields therefrom, we examine the manageability of the band-gap size and the anisotropic carrier mobility. This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2013-C3-062).

Wednesday, March 4, 2015 8:00AM - 11:00AM — Session L2 DMP: Focus Session: Beyond Graphene - Spin and Magnetic Properties 001B - Jun Zhu, Pennsylvania State University
8:00AM L2.00001 Indirect exchange interaction in 3D Dirac semimetals, A. Mellnik, J. S. Lee, A. Richardella et al.; NANCY SANDLER, SERGIO ULLOA, Ohio University — 3D Dirac semimetals are new three-dimensional materials with linear band crossings —Dirac points— at distinctive locations in the Brillouin zone. They are predicted to have fascinating properties such as the chiral anomaly and surface Fermi arcs. Na$_2$Bi and Cd$_3$As$_2$ are two prototypical examples that have been characterized experimentally [1]. Breaking of time reversal symmetry splits the Dirac points into Weyl points, which are protected by the underlying crystal symmetry. We study the indirect exchange interaction, between two magnetic impurities in these materials. We present results on the behavior of the interaction as a function of the inter-impurity separation in the Dirac phase. We also analyze the transition into the Weyl phase, by introducing perturbations that can be induced by external fields. [1] Science 343, 864; arXiv:1312.7624; Nat. Commun. 5, 3786; PRL 113, 027603.

1Supported by NSF-MWN/CIAM.

8:12AM L2.00002 First-principles study of magnetic properties of two-dimensional semi conductors ABX$_3$\(^3\), A. Kandala, A. Richardella, S.-Y. Xu, M. Neupane, A. Mellnik, A. Kandala, J. S. Lee, D. M. Zhang, M. Z. Hasan and D. C. Ralph. We acknowledge funding from the DARPA Meso program, ONR and C-SPIN (under sponsorship of MARCO and DARPA).

8:24AM L2.00003 Structure and magnetism of the van der Waals bonded ferromagnet CrI$_3$, M. Neupane, A. Richardella, S.-Y. Xu, M. Neupane, A. Mellnik, A. Kandala, J. S. Lee, D. M. Zhang, M. Z. Hasan and D. C. Ralph. We acknowledge funding from the DARPA Meso program, ONR and C-SPIN (under sponsorship of MARCO and DARPA).

8:36AM L2.00004 Topological Spintronics: Materials, Phenomena and Devices, NITIN SAMARTH, Penn State University — The two-dimensional surface states of three-dimensional topological insulators such as Bi$_2$Se$_3$ and (Bi,Sb)$_2$Te$_3$ possess a spin texture that can potentially be exploited for spintronics applications. We provide a perspective on the emergence of “topological spintronics,” demonstrating how this spin texture can be engineered using either quantum tunneling between surfaces [1] or by breaking time-reversal symmetry [2]. We then discuss recent experiments that show striking spintronic phenomena useful for proof-of-concept devices, including a spin-orbit torque of record efficiency at room temperature [3] and an electrically-gated “giant anisotropic magnetoresistance” at low temperature [4].

This work was carried out in collaboration with A. Richardella, S.-Y. Xu, M. Neupane, A. Mellnik, A. Kandala, J. S. Lee, D. M. Zhang, M. Z. Hasan and D. C. Ralph. We acknowledge funding from the DARPA Meso program, ONR and C-SPIN (under sponsorship of MARCO and DARPA).

1Research supported by the US Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

9:00AM L2.00005 Thermodynamic Stability of Topological Insulators, DEMET USANMAZ, PINKU NATH, JOSE J. PLATA, Department of Mechanical Engineering and Materials Science, Duke University, Durham, North Carolina 27708, USA, GIUS L.W. HART, Department of Physics and Astronomy, Brigham Young University, Provo, UT 84602, MARCO B. NARDELLI, Department of Physics and Department of Chemistry, University of North Texas, Denton, Texas 76203, USA, STEFANO CURTAROLO, Materials Science, Electrical Engineering, Physics, and Chemistry, Duke University, Durham, North Carolina 27708, USA, CENTER FOR MATERIALS GENOMICS TEAM, G. L. W. HART COLLABORATION, M. B. NARDELLI COLLABORATION — Well known three-dimensional TIs such as Bi$_2$Te$_3$, Bi$_2$Se$_3$, Bi$_2$Te$_2$Se, Sb$_2$Te$_3$Se have been the subject of research due to potential application for spintronic devices. TIs have large bulk band gap and metallic surface states at the special time-reversal-invariant momentum (TRIM) points of the Brillouin zone. These fascinating properties constitute the current carry along the surface and not conduct current through the bulk. Creating heterostructures of TIs has recently been demonstrated to be advantageous for controlling electronic properties. In addition to the importance of the electronic properties of materials, thermodynamic stability is the key for manufacturability of materials. Guided by cluster expansion, we have investigated the thermodynamic stability of TI interfaces.

9:24AM L2.00006 A Field-effect Transistor based on Two-dimensional Topological Insulators, WOLfgang Vandenbergh, MASSIMO FISCHETTI, The University of Texas at Dallas — Monolayer tin functionalized with iodine (iodostannanane) is a two-dimensional topological insulator and iodostannanane ribbons have a very high mobility when the Fermi level is in the bandgap. For wide ribbons, the mobility and the conductivity decrease by several orders of magnitude when the Fermi level is in the conduction or valence band[1]. We show how this property can be exploited to make a topological-insulator field-effect transistor (TIFET) by gating the iodostannanane. We simulate the TIFET's electrical characteristics invoking a drift-diffusion like approximation and introducing a simplified model for the conductivity of the topological insulator. The TIFET is shown to have input and output characteristics similar to those of conventional field-effect transistors with an on/off ratio exceeding three orders of magnitude. Furthermore, the on-current is very high enabling high-speed operation and the amount charge in the channel is small making TIFETs interesting for low-power applications.


1We acknowledge the support of Nanoelectronics Research Initiative’s (NRI’s) Southwest Academy of Nanoelectronics (SWAN).
9:36AM L2.00007 Magneto-optical studies of MoS$_2$\textsuperscript{1}, MUMTAZ MURAT ARIK, ALOK MUKHERJEE, PAYAM TAHERI, HUI XING, HAO ZENG, JOHN CERNE, State Univ of NY - Buffalo — We report infrared and visible (0.100 – 2.75 eV) magneto-optical measurements on high quality monolayer MoS$_2$ prepared by sulfurizing MoO$_3$ films. Reflection, photoluminescence, and magneto-optical Kerr spectra of MoS$_2$ on different substrates are measured at magnetic fields up to 7 T and temperatures down to 10 K. In the visible reflection spectrum we observe the A1 and B1 excitonic transitions. While the A1 strength is independent of magnetic field, the B1 amplitude increases by a factor of 1.5 at 5 T. This work is supported by NSF-DMR1006078.

9:48AM L2.00008 Valley contrasting chiral phonons in monolayer hexagonal systems\textsuperscript{1}, LIFA ZHANG, QIAN NIU, Univ of Texas, Austin — In monolayer hexagonal lattice systems, two inequivalent valleys appear in the reciprocal lattice space. With inversion symmetry breaking, we find valley dependent chiral phonons which are circularly polarized with carrying spin angular momentum and ionic magnetic moment. At valleys, light and heavy phonons are found and evolve in intervallley electronic scattering. Under three-fold rotation operation, phonons have pseudo angular momentum, which include spin and orbital parts. From conservation of pseudo angular momentum, momentum and energy, the selection rules in valleytronics are obtained. Due to chiral valley phonons, one can observe polarized infrared photoluminescence and phonon valley coherence by infrared excitation. There is also a valley dependent phonon Berry curvature which can result a valley phonon Hall effect. The valley-dependent chiral phonon, together with its spin angular momentum, pseudo angular momentum, infrared polarized photoluminescence, phonon valley coherence and valley Hall effect, will form a basis for valley-based phonics applications.

\textsuperscript{1}We acknowledge support from DOE-DMSE (DE-FG03-02ER45958), NBRPC (2012CB-921300), NSFC (91121004), and the Welch Foundation (F-1255)

10:00AM L2.00009 Thickness dependence of spin polarization and electronic structure of ultra-thin films of MoS$_2$ and related transition-metal dichalcogenides, TAY-RONG CHANG, National Tsing Hua U., Taiwan, HSIN LIN, National University of Singapore, HORNG-TAY JENG, National Tsing Hua U., Taiwan, ARUN BANSIL, Northwestern U. — Thickness dependence of electronic structures of transition-metal dichalcogenides (TMDs) MX$_2$ (M=Mo or W, X=S, Se or Te) is investigated using first-principles calculations. When spin-orbit coupling (SOC) is included in the computations, the electronic structure of monolayer MX$_2$ films exhibits significant band splittings due to the breaking of spatial inversion symmetry. In particular, spin-split states appear around the valence band maximum with nearly 100% out-of-the-plane spin polarization with the spin oriented oppositely at the K and K’ symmetry points in the Brillouin zone. For bilayer films, the spin-polarization can be tuned by an out-of-the-plane electric field, and the spin-polarized states are weakly coupled between the layers with small $\xi_{\perp}$ dispersion. We confirm a transition from an indirect to a direct band gap as the thickness is reduced to a monolayer in MoX$_2$, in agreement with recent experimental findings. Our study provides insights into the thickness dependence of electronic structure and the degree of spin polarization of the valence bands in ultra-thin TMD films and their viability for spintronics applications.

10:12AM L2.00010 RKKY interaction in transition-metal dichalcogenide nanoflakes\textsuperscript{1}, OSCAR AVALOS-OVANDO, DIEGO MASTROGIUSEPPE, SERGIO ULLOA, Ohio University — Transition metal dichalcogenides (TMDs) are layered crystals with unique electronic and optical properties, and are promising candidates for a new generation of semiconductor-based devices, mainly when exfoliated to one or a few layers. The process of exfoliation often produces nanoscale samples – flakes – with different shapes and boundaries. These flakes might have applications as quantum dots with novel characteristics. One interesting topic relates to the presence of magnetic impurities and their interaction. In combination with strong spin-orbit coupling and valley degrees of freedom, TMDs might have a great impact in the field of spintronics. Using an effective low-energy two-orbital tight-binding model, we study the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between two magnetic impurities in 2D TMD nanoflakes. We consider different geometries and terminations, analyzing the effect of the sample size. Our results show the behavior of the interaction for impurities sitting at different positions in the flake, and its possible tunability with the electron/hole concentration. The magnetic impurities can be intrinsic to the sample production process or can be introduced extrinsically. Our results can be tested with local probes, such as spin-polarized STM.

\textsuperscript{1}Supported by NSF DMR MWN/CIAM

10:24AM L2.00011 Two-dimensional Mineral [Pb$_2$Bi$_3$][AuTe$_2$]: High mobility Charge Carriers in Single-atom-thick Layers\textsuperscript{1}, LEI FANG, Department of Chemistry, Northwestern University, J. IM, C. STOUMPOS, F. SHI, V. DRAVID, Northwestern University, M. LEROUX, Argonne National Laboratory, A. FREEMAN, Northwestern University, W.-K. KWOK, D.-Y. CHUNG, Argonne National Laboratory, M. KANATZIDIS, Northwestern University — We report that [Pb$_2$Bi$_3$][AuTe$_2$], known as a naturally occurring mineral buckhornite, hosts 2D carriers in single-atom-thick layers. The structure is composed of stacking layers of weakly coupled [Pb$_2$Bi$_3$] and [AuTe$_2$] sheets. The insulating [Pb$_2$Bi$_3$] sheet inhibits interlayer charge hopping and confines the carriers in the basal plane of the single-atom-thick [AuTe$_2$] layer. Magneto-transport measurements and theoretical calculations show a property of multiband semimetal with compensated density of electrons and holes, which exhibit high hole carrier mobility of 1360 cm$^2$/Vs. This material possesses an extremely large anisotropy $10^4$, comparable to benchmark materials graphite. The electronic structure features linear band dispersion at the Fermi level and ultrahigh Fermi velocities of 10$^4$ m/s which are virtually identical to that of graphene. The weak interlayer coupling gives rise to the highly cleavable property of single crystal specimens, indicating a prospect for monolayer system.

\textsuperscript{1}This research was supported by the DoE, BES, under Contract No. DE-AC02-06CH11357, and NUANCE Center at the Northwestern University

10:36AM L2.00012 Giant spin-splitting and orbital angular momentum in triangular lattice, SEHOON OH, HYOUNG JOON CHOI, Department of Physics, IPAP, and Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University, Seoul, Korea — We study the spin-splitting in triangular-lattice materials including Au (111) surface and transition-metal dichalcogenides quantitatively as well as qualitatively using tight-binding calculations and first-principles calculations. To analyze the spin-splitting of the bands, we calculate the orbital angular momentum (OAM) and consider the symmetry of the system. We confirm that the giant spin-splitting results from the presence of significant local OAMs and strong spin-orbit interactions in the vicinity of high-atomic number elements. This work was supported by NRF of KOREA (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2013-C3-062).
10:48AM L2.00013 Excitonic and marginal Fermi liquid instabilities in 2D and 3D Dirac semimetals, JOSE GONZALEZ, Instituto de Estructura de la Materia (CSIC), Madrid, Spain — We study the quantum electrodynamics of 2D and 3D Dirac semimetals by means of a self-consistent resolution of the Schwinger-Dyson equations, aiming to obtain the respective phase diagrams in terms of the relative strength of the Coulomb interaction and the number N of Dirac fermions. In this framework, 2D Dirac semimetals have just a strong-coupling instability characterized by exciton condensation (and dynamical generation of mass) that we find at a critical coupling well above the estimates made with RPA screening (large-N approximation), thus explaining the absence of that instability in free-standing graphene samples. On the other hand, we show that 3D Dirac semimetals have a richer phase diagram, with a strong-coupling instability leading to dynamical mass generation up to N = 4 and a line of critical points for larger values of N characterized by the vanishing of the electron quasiparticle weight in the low-energy limit. Such a marginal Fermi liquid boundary marks the transition to a kind of strange metal that can still be defined in terms of electron quasiparticles, but with parameters that have large imaginary parts implying an increasing deviation at strong coupling from the conventional Fermi liquid picture.

Wednesday, March 4, 2015 8:00AM - 11:00AM — Session L3 GSNP: Topics in Statistical Physics II

8:00AM L3.00001 Concept of Linear Thermal Circulator Based on Coriolis forces1, HUANAN LI, TSAMPIKOS KOTTOS, Wesleyan University — Directional transport and the creation of non-reciprocal devices that control the flow of energy and/or mass at predefined directions have been posing always fascinating challenges. In this contribution, we show that the presence of a Coriolis force in a rotating linear lattice imposes a non-reciprocal propagation of the phononic heat carriers. Using this effect we propose the concept of Coriolis linear thermal circulator which can control the circulation of a heat current. A simple model of three coupled harmonic masses on a rotating platform allow us to demonstrate giant circulating rectification effects for moderate values of the angular velocities of the platform.

1This work was partly sponsored by a NSF DMR-1306984 grant and by an AFOSR MURI grant FA9550-14-1-0037.

8:12AM L3.00002 Magnetically driven quantum heat engine1, ENRIQUE MUNOZ, Pontificia Universidad Catolica de Chile, FRANCISCO PENA, Pontificia Universidad Catolica de Valparaiso — In analogy with classical thermodynamics, a quantum heat engine generates useful mechanical work from heat, by means of a reversible sequence of transformations (trajectories), where the “working substance” is of quantum mechanical nature. Several theoretical implementations for a quantum heat engine have been discussed in the literature, such as entangled states in a qubit, quantum mechanical versions of the Otto cycle, and photocells. In this work [1], we propose yet a different alternative by introducing the concept of a magnetically driven quantum heat engine. We studied the efficiency of such system, by considering as the “working substance” a single nonrelativistic particle trapped in a cylindrical potential well, as a model for a semiconductor quantum dot, in the presence of an external magnetic field. The trajectories are driven by a quasistatic modulation of the external magnetic-field intensity, while the system is in contact with macroscopic thermostats. The external magnetic field modulation allows to modify the effective geometric confinement, in analogy with a piston in a classical gas.


8:24AM L3.00003 ABSTRACT WITHDRAWN —

8:36AM L3.00004 Why are all dualities conformal? Theory and practical consequences, SEYYED MOHAMMAD SADEGH VAEZI, ZOHARN NUSSINOV, Washington University, GERARDO ORTIZ, Indiana University, Bloomington — We relate duality mappings to the “Babbage equation” F(F(z)) = z with F a map linking weak to strong coupling theories. Under fairly general conditions F may only be a specific conformal transformation of the fractional linear type. This deep general result has enormous practical consequences. For example, one can establish that weak and strong coupling expansions are trivially related, i.e., one needs to generate only one of them while the other is automatically determined through a set of linear constraints. The latter partially solve or, equivalently, localize the computational complexity to a simple fraction of the coefficients, and as a bonus those relations encode non-trivial equalities between different geometric constructions. We illustrate our findings by examining various models including, but not limited to, ferromagnetic and spin-glass type Ising models on hypercubic lattices.

8:48AM L3.00005 ABSTRACT WITHDRAWN —

9:00AM L3.00006 Quantifying the Effects of Noise on Diffuse Interface Models: Cahn-Hilliard-Cook equations, SPENCER FIEFER, BASKAR GANAPATHYSUBRAMANIAN, Iowa State Univ — We present an investigation into the dynamics of phase separation through numerical simulations of the Cahn-Hilliard-Cook (CHC) equation. This model is an extension of the well-known Cahn-Hilliard equation, perturbed by an additive white noise. Studies have shown that random fluctuations are critical for proper resolution of physical phenomena. This is especially true for phase critical systems. We explore the transient behavior of the solution space for varying levels of noise. This is enabled by our massively scalable finite element-based numerical framework. We briefly examine the interplay between noise level and discretization (spatial and temporal) in obtaining statistically consistent solutions. We show that the added noise accelerates progress towards phase separation, but retards dynamics throughout subsequent coarsening. We identify a scaling exponent relating morphology metrics with the level of noise. We observe a very clear scaling effect of finite domain size, which is observed to be offset by increasing levels of noise. Domain scaling reveals a clear microstructural asymmetry at various stages of the evolution for lower noise levels. In contrast, higher noise levels tend to produce more uniform morphologies.
9:12AM L3.00007 Definitions of temperature in non-extensive systems¹, SERGIO DAVIS, GONZALO GUTIERREZ, Departamento de Física, Facultad de Ciencias, Universidad de Chile — Superstatistics (Beck and Cohen, 2003) is a proposed formalism for explaining the presence of non-Boltzmann distributions in Nature for systems out of equilibrium. The superstatistical ensemble is a superposition of canonical ensembles according to

\[ P(\vec{r}, \vec{p} | H) = \int dB P(\beta | H) \exp(-\beta H(\vec{r}, \vec{p})) Z(\beta), \] 

with \( P(\beta | H) \) the probability density for the inverse temperature parameter \( \beta \). In this work we show that, in order for this formalism to be internally consistent, it is impossible to have a definition of \( \beta \) as an observable which is valid across all “superstatistical” ensembles. In other words, the shape of the ensemble cannot be determined by measuring temperature, only by measuring energy. Our results also reveal that energy and temperature are not in the same footing as observables for non-canonical ensembles.

¹Funding from FONDECYT 1140514

9:24AM L3.00008 Non-reciprocal acoustic transport in media with spectral asymmetry and losses, ANDREA KLEEMAN, RAHUL DEORA, HUANAN LI, FRED ELLIS, TSAMPIKOS KOTTOS, Department of Physics, Wesleyan University, Middletown CT-06459, USA, ILYA VITEBSKIY, The Air Force Research Laboratory, Sensors Directorate, Wright Patterson AFB, OH 45433 USA — We propose a novel scheme for acoustic isolators, which rely on the interplay of spectral asymmetry and distributed losses. The spectral asymmetry is imposed to the system via a flow, which is moving inside a corrugated waveguide with a constant velocity. A result of this asymmetry is that left and right moving acoustic waves have different group velocities. Then, depending on the direction of the incident acoustic signal, inherent losses result in different level of attenuation of the transmitted signal. The outgoing acoustic wave has the same frequency characteristics as the incoming one. An experimental realization of our proposal is also discussed.

9:36AM L3.00009 Density reconstruction via maximum entropy method, AUSTIN MCDONALD, RAYMOND ATTA-FYNN, Department of Physics, University of Texas at Arlington, PARTHAPRATIM BISWAS, Department of Physics and Astronomy, The University of Southern Mississippi — We demonstrate an application of the maximum entropy principle by employing the Shannon entropy functional to reconstruct functions that are otherwise non-trivial to reproduce by existing reconstruction techniques. Specifically, we present the reconstruction of the Dirac comb by maximizing the Shannon entropy subject to the moment constraints using Monte-Carlo type and population-based approaches. The results are compared with the existing results in the literature and the convergence properties of the resulting distributions are examined in relation to the number of input moments.

9:48AM L3.00010 Density of Yang-Lee zeros in the thermodynamic limit using Tensor RG¹, ARTUR GARCIA-SAEZ, TZU-CHIEH WEI, Yang Institute for Theoretical Physics and Department of Physics and Astronomy, Stony Brook University — The partition function of ferromagnets in a lattice is represented as a Tensor Network and efficiently contracted using an iterative RG process. The density of Yang-Lee zeros on the complex field plane is obtained from accurate calculations of the free energy and local observables in an effective thermodynamic limit. We illustrate this approach studying the distribution of Yang-Lee zeros for the Ising model in 2D and 3D square lattices.

¹This work was supported in part by the National Science Foundation.

10:00AM L3.00011 Entanglement Thermalization and Local Conservation Laws, LIANGSHENG ZHANG, Princeton University, HYUNGWON KIM, Rutgers University, DAVID HUSE, Princeton University — We study the thermalization of entanglement entropy in one-dimensional spin chains under the unitary dynamics of a nonintegrable Hamiltonian or periodic driving by Floquet operators. Using full diagonalization of the Hamiltonian matrix and the Floquet operators, we analyze the time evolution of entanglement entropy starting from various initial conditions, including initial states with entanglement in excess of the thermal equilibrium value. It is found that the thermalization of entanglement entropy is coupled to local conservation laws when approaching equilibrium, and the absence of conservation laws in the Floquet system allows the entanglement entropy to thermalize more rapidly than it does in the corresponding Hamiltonian.

10:12AM L3.00012 Phase transitions in a confined monolayer of magnetized beads, JULIEN SCHOCK-MEL, Univ de Liege — We present experimental results obtained with a model experimental system dedicated to the study of 2D phase transitions. The system is composed of millimetric beads interacting through magnetic dipole-dipole interaction. Due to the confinement, repulsive interactions tend to order the system. In addition, the system is submitted to a controlled mechanical agitation which produce an erratic motion of the beads and thus creates disorder. Controlling the competition between interaction energy and entropy, allows us to explore different structures of 2 dimensional systems. At first, the melting of a two dimensional crystal is studied. As predicted by the KTHNY theory, a two stage melting is observed, including the so-called hexatic phase (see results in Phys. Rev. E.87, 062201 (2013)). Afterward, the behavior of binary systems is studied. In particular, the effect of the grains polydispersity on the order is analyzed.

10:24AM L3.00013 Complex Pole Approach in Thermodynamic Description of Fluid Mixtures with Small Number of Molecules, TIMUR ASLYAMOV, Moscow Inst of Phys & Tech, OLEG DINARIEV, Schlumberger Moscow Research Center — Physically consistent description of equilibrium small molecular systems requires the extension of thermodynamics. The reason is the absence of thermodynamic limit, which is mandatory for the applicability of classical thermodynamics. New theoretical method of complex pole decomposition for the statistical description of small multicomponent molecular systems is implemented. Similar approach has been previously developed and applied in nuclear physics for finite systems of nucleons. We have significantly transformed and extended the original formulation to make it work for multicomponent molecular mixtures in small systems. The aim of this research is to provide new comprehensive description of small equilibrium molecular systems with numerous scientific and industrial applications for artificial and natural materials with nanopores. Several cases for molecular systems in small cavities are studied. In particular size-dependent additional pressure for small systems is evaluated analytically and numerically. The obtained results are in correspondence to published experimental data and molecular dynamics simulations.
Heterogeneous dynamics and stretched exponential decay of spatio-temporal correlations for Coulomb-interacting particles in confined geometries, AMIT GHOSAL, BISWARUP ASH, Indian Institute of Science Education and Research-Kolkata, Mohanpur Campus, India-741252, JAYDEEP CHAKRABORTI, S. N. Bose National Centre for Basic Sciences, Kolkata, India-700098 — We investigate the dynamics of Coulomb-interacting confined particles over a range of temperatures capturing the crossover from a Wigner molecule to a liquid-like phase. Dynamical signatures, derived from the Van-Hove correlations, develop pivotal understanding of the phases as well as the intervening crossover, which are inaccessible from the study of static correlations alone. The motion of the particles shows frustrations, produces heterogeneities depending on the observation time-scales and temperatures and results into a non-Gaussian behavior. The extent and nature of the departure of the behavior of spatio-temporal correlations from the conventional wisdom depends crucially on the symmetry of the confinements. In particular, we find that the decay of correlations follow a stretched-exponential form in traps that lack any symmetry. Our data offers a broad support to a theoretical model that integrates the non-Gaussian behavior arising from the convolution of Gaussian fluctuations weighted by appropriate diffusivities, consistent with local dynamics. The richness of information from the dynamic correlation will be shown to improve the understanding of melting in confined systems in a powerful manner.

Current-driven complex dynamics of single-layer epitaxial islands on substrates, DWAIPAYAN DASGUPTA, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — We study theoretically the current-driven dynamics of isolated single-layer epitaxial islands on crystalline substrates, which provides important guidance toward surface nanopatterning approaches based on the current-driven assembly of such islands. We develop and validate a fully nonlinear model for the islands’ driven morphological evolution on elastic substrates of face-centered cubic crystals in the regime where diffusional mass transport is limited to the island edge. For islands on (110)-, (100)-, and (111)-oriented substrate surfaces, we report a transition in the asymptotic states reached by such driven island dynamics from steady to oscillatory, mediated by Hopf bifurcation. We characterize the bifurcation and explore the dependence of the stable time-periodic state beyond the Hopf point on the misorientation angle between the applied electric field and fast edge diffusion directions, the strength of the edge diffusional anisotropy, and the island size. For islands larger than a critical size, depending on the orientation of the substrate surface, we observe fingering and necking instabilities in the island morphology. We carry out a comprehensive numerical simulation study and explore the complexity of the driven island dynamics with the variation of the problem parameters.

Experimental Signatures of Orbital Fluctuations in Iron Based Superconductors, WEI-CHENG LEE, Binghamton University - SUNY — Understanding the high temperature superconductivity has been one of main subjects in the condensed matter physics. The discovery of new classes of high-temperature superconductors, iron pnictides in 2008, launched an international wave of research in the past few years. While the magnetic interactions are certainly important in these materials, there have been significant evidences suggesting that the orbital degrees of freedom could play an important role as well. In this talk, I will demonstrate that the orbital degrees of freedom do play a significant role in physical properties of iron-based superconductors. At the level of single particle properties, while the orbital order in the quasi-1D dxy and dzy bands has been proposed to be a possible driving mechanism for the structural phase transition, our study shows that the fluctuations associated with the orbital order could further drive a non-Fermi liquid behavior in the critical region of the orbital ordering phase transition. I will show that this non-Fermi liquid behavior could induce a zero-bias anomaly in the point contact spectroscopy, which has been observed in a variety of iron based superconductors. As for the magnetic properties, we also find that the orbital order and fluctuations can qualitatively change the nature of the spin excitation spectrum, giving rise to the novel incommensurate-to-commensurate transformation observed in a recent neutron scattering measurement. In the superconducting state, we predict that a new collective excitation, termed as orbital resonance mode, could exist generally in the iron-based superconductors, which in principle can be measured by Raman spectroscopy. Our findings offer a new perspective on the pairing mechanism of iron based superconductors, and suggest that orbital degrees of freedom could provide a new route to high temperature superconductivity.

Orbital-selective Correlation Effects in Alkali Metal Iron Pnictides, WEICHENG LV, Rice University, RONG YU, Renmin University of China, JIAN-XIN ZHU, Los Alamos National Laboratory, QMIAO SI, Rice University — There is growing evidence for the substantial electronic correlations in the iron based superconductors. In particular, recent experiments have revealed strong orbital-selective correlation effects in the series of alkali metal iron pnictides AFe2As2 (A = K, Rb, Cs). Among the important questions is how these systems, with a 3d-electron filling n = 5.5 per site, differs from the parent iron pnictides, which has n = 6. Here, we address these issues in a five-orbital Hubbard model with filling n = 5.5, using the U(1) slave-spin method. As the lattice parameters increase from K to Rb, then to Cs, we are able to identify the systematics in the orbital-selective Mott behavior as the correlation effects are enhanced due to the reduced bandwidth. We discuss the implications of our results for the quasiparticle mass as well as for the spin spectral weight.

Spin and Orbital Nematic Susceptibility of Iron Based Superconductors. CHRISTOPHER BISHOP, SHUHUA LIANG, ANAMITRA MUKHERJEE, NIRAVKUMAR PATEL, ELBIO DAGOTTO, ADRIANA MOREO, Univ of Tennessee, Knoxville — The spin and orbital nematic susceptibility of the iron-based superconductors are calculated in the undoped limit using a three-orbital (xz, yz, xy) spin-fermion model that includes spin, orbital, and lattice degrees of freedom [1]. The results are in very good agreement with experiments by J-H. Chu et al., Science 337, 710 (2012). Recently, Raman scattering experiments[2] indicate a Curie-Weiss behavior of the orbital nematic susceptibility in BaFe2As2 and Sr(Fe1−xCox)2As2. This behavior is observed in our numerical simulations after considering the coupling between the spin and orbital nematic order parameters. A Landau-Ginzburg formalism is used to analytically derive equations for both the spin and orbital susceptibility that fit well the numerical data. [1] S. Liang et al., arXiv:1405.6395 (2014), to appear in PRB. [2] Y.-X. Yang, et al., “Raman scattering as a probe of charge nematic fluctuations in iron based superconductors,” JPS Conf. Proc. 3, 015001, 2014.

1National Science Foundation Grant No. DMR-1104386
9:00AM L.00004 Diverging Nematic Susceptibility, Physical Meaning of $T^*$ scale, and Pseudogap in the Spin Fermon Model for Pnictides, SHUHUA LIANG, ANAMITA MUKHERJEE, NIRVUKUMAR PATEL, CHRIS BISHOP, ELBIO DAGOTTO, ADRIANA MOREO, Univ of Tennessee, Knoxville — Using Monte Carlo simulations including the lattice degree of freedom [1], for the first time the nematic susceptibility of the spin fermion model for the pnictides is calculated [2]. The results are in very good agreement with experiments by J.-H. Chu et al., Science 337, 710 (2012). Our study suggests a nematicity in the spin fermion model primarily originating on magnetism, but with the lattice/orbital also playing an important role by boosting up critical temperatures and separating the structural $T_S$ and Néel $T_N$ transitions. At $T > T_S$, Curie-Weiss behavior is observed with a characteristic temperature $T^*$ being the $T_N$ of the purely electronic system. In this regime, a pseudogap in the density of states and short-range magnetic order is observed.


9:12AM L.00005 Symmetry of reentrant tetragonal phase in Ba$_{1-x}$Na$_x$Fe$_2$As$_2$: Magnetic versus orbital ordering mechanism, DMITRY KHAYALIYIN, ISIS facility, Rutherford Appleton Laboratory, STEPHEN LOVESEY, Diamond Light Source Ltd, PASCAL MANUEL, ISIS facility, Rutherford Appleton Laboratory, FRANK KRUGER, London Centre for Nanotechnology, University College London, STEPHAN ROSENKRANZ, JARED ALLRED, OMAR CHMAISSEM, RAY OSBORN, Materials Science Division, Argonne National Laboratory — Magneto-structural phase transitions in Ba$_{1-x}$Fe$_2$As$_2$ ( $A$ = K, Na) materials have been analyzed for both magnetically and orbitally driven mechanisms, using symmetry methods formulated within the Landau theory of phase transitions. Both mechanisms predict identical orthorhombic space group symmetries for the magnetic and nematic phases observed over much of the phase diagram, but they predict different tetragonal space-group symmetries for the newly discovered reentrant tetragonal phase in Ba$_{1-x}$Na$_x$Fe$_2$As$_2$ ($x \sim 0.25$). In a magnetic scenario, magnetic order with moments along the $c$-axis, as found experimentally, does not allow any type of orbital order, but in an orbital scenario, we have determined two possible orbital patterns, specified by $P4/mnc1$ and $H221$ space groups, which do not require atomic displacements relative to the parent $H/mmm$1 symmetry and, in consequence, are indistinguishable in conventional diffraction experiments. We demonstrate that the three possible space groups are however, distinct in resonant X-ray Bragg diffraction patterns created by Templeton & Templeton scattering. This provides an experimental method of distinguishing between magnetic and orbital models.

9:24AM L.00006 The phase diagram of Sr$_{1-x}$Na$_x$Fe$_2$As$_2$: evidence of magnetic C4 phase universality, K.M. TADDEI, Northern Illinois University, J.M. ALLRED, Argonne National Laboratory (ANL), D.E. BUGARIS, ANL, M. KROGSTAD, Northern Illinois University, S. ROSENKRANZ, R. OSBORN, H. CLAUS, D.Y. CHUNG, ANL, S.H. LAPIDUS, ANL Advanced Photon Source. M.G. KANATZIDIS, ANL and Northwestern University, O. CHMAISSEM, ANL and Northern Illinois University — Determination of the nature of superconductivity in the high $T_c$ iron based superconductors requires understanding the material’s magnetic behavior out of which superconductivity arises. The apparent competition between superconductivity and magnetism in these materials and the appearance of superconductivity upon suppression of magnetism suggests magnetic fluctuations as a possible superconducting pairing mechanism. A recent study of the sodium doped barium 122 system which established the existence of a new magnetic phase near the Fermi level of the electron and hole bands and is determined by the electron filling. We find that within an itinerant approach the magnetic susceptibility introduces the anisotropy of the magnetization of the striped antiferromagnetic state by lifting the degeneracy of all three components of the magnetization.

9:36AM L.00007 Enhancement of superconductivity near a nematic quantum critical point, SAMUEL LEDERER, Stanford Univ, YONATAN SCHATTNER, EREZ BERG, Weizmann Institute of Science, STEVEN KIVELSON, Stanford Univ — In both the hole-doped cuprate and iron-based high temperature superconductors, there is evidence of a nematic quantum critical point at a critical doping near the “optimal doping” at which the superconducting $T_c$ is maximal. Thus motivated by experiments, but without pretense that the theory is directly applicable to these materials, we consider a low $T_c$ metallic superconductor weakly coupled to the soft fluctuations associated with proximity to a nematic quantum critical point. We show that a dynamical Efros-Slatkin model remains valid outside of a parametrically narrow interval about the nematic quantum critical point; 2) in 2D, the symmetry of the superconducting state (d-wave, s-wave) is typically determined by the non-critical interactions, but $T_c$ is enhanced by the nematic fluctuations in all channels; 3) in 2D, this enhancement grows rapidly upon approach to criticality up to the point at which the weak coupling approach breaks down, but in 3D the enhancement is much weaker. Finally, we note some consequences of the nematicity-mediated pairing interaction, such as highly anisotropic gap functions and non-local collective modes.

9:48AM L.00008 Manifestation of nematic degrees of freedom in the Raman response function of iron pnictides, UNA KARAHASANOVIC, JOERG SCHMALIAN, Karlsruhe Institute of Technology — The electronic nematic phase in pnictides, characterized by the broken C4 symmetry, is believed to be generated by the presence of magnetic fluctuations associated with the striped phase, and occurs as a thin sliver in the phase diagram, above the magnetic transition temperature. Detecting the presence of nematic degrees of freedom in iron-based superconductors is a difficult task, since it involves measuring four spin correlation functions. We show that the nematic degrees of freedom manifest themselves in the experimentally measurable Raman response function, which is a density-density correlation weighted by an appropriate form factor. We calculate the Raman response function in the large $N$ limit by considering Aslamazov-Larkin type of diagrams that contain series of inserted boxed-like diagrams that resemble the nematic coupling constant of the theory. These diagrams effectively account for collisions between spin fluctuations. We demonstrate that the Raman response function diverges at the structural phase transition.

10:00AM L.00009 Magnetic and orbital ordering in the iron-based superconductors: role of spin-orbit coupling, FELIX AHN, Institut für Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany, JOHANNES KNOlle, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, RAFAEL FERNANDES, School of Physics and Astronomy, University of Minnesota, Minneapolis, USA, ILYA EREMIN, Institut für Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany — We analyze the magnetic ordering in the iron-based superconductors in presence of spin-orbit coupling. Based on several tight-binding parametrizations of the 3d electron states we show how the spin-orbit coupling introduces the anisotropy of the magnetization of the striped antiferromagnetic state by lifting the degeneracy of all three components of the magnetization $m_x$, $m_y$, and $m_z$. The orientation of the magnetic moment is determined by the contribution of the xy, zz, and yz orbitals to the electronic states near the Fermi level of the electron and hole bands and is determined by the electron filling. We find that within an itinerant approach the magnetic ordering is most favorable along the wavevector of the striped AF state. This appears to be a natural consequence of the spin-orbit coupling in the striped AF state where the ferro-orbital order of the $xz$ and $yz$ orbitals is only a consequence of the striped AF order. We further analyze the role of spin-orbit coupling for the C4 magnetic structure where SDW order parameters with both wavevectors, $Q_{x} = (\pi, 0)$ and $Q_{y} = (0, \pi)$, coexist.

10:12AM L.00010 ABSTRACT WITHDRAWN

10:24AM L.00011 ABSTRACT WITHDRAWN
The work is supported by NSFC and the Ministry of Science and Technology of China.

Wednesday, March 4, 2015 8:00AM - 11:00AM
Session L6 DMP: Focus Session: Phononic And Mechanical Phenomena In Nanostructures
006A - Michael Scheibner, University of California, Merced

8:00AM L6.00001 Coherent phonon modulation by nanoscale acoustically mismatched interface
SHANGJIE YU, MIN QING. Univ of Maryland-College Park — Precise engineering of phonon spectrum by material design is essential for in-depth understanding of fundamental physical phenomena as well as new technology breakthrough. When phonons propagate through two different constituents, their mismatched interface can coherently modulate phonon spectrum. In this talk, we will demonstrate the phonon characteristics can be precisely tailored through nanoscale interfacial coupling by investigating acoustically mismatched core-shell hetero-nanostructures with ultrafast pump-probe technique. Coherent phonon coupling between core and shell through their interface has been experimentally revealed, which agrees well with theoretical simulation. This interfacial phonon coupling also represents a unique fingerprint of complex nanostructures.

8:12AM L6.00002 Acoustic vibrations of complex metal nanostructures
AFTAB AHMED, Argonne National Laboratory, ANNA KLJINKOVA, EUGENIA KUMACHEVA, University of Toronto, Canada, JEFFREY GUEST, Argonne National Laboratory — Coherent acoustic vibrations of plasmonic nanoparticles modulate light at ultra-high frequencies. Plasmonic nanoparticles are of particular interest because of their high absorption cross sections, and offer wide range of applications including sensing and nano-mechanical devices. Here we show acoustic vibrations of complex metal nanostructure using a femtosecond pump-probe technique. The studied nanostructure is composed of an octahedral core (Au) and cubic shell (Ag). Unique elastic properties and complex geometries of the two metals provide a richer transient absorption spectrum than that of a simple nanocube of similar dimensions. Further, two different vibrational modes are detected as compared to the single-probe wavelengths. Numerical simulations were carried out to explain our experimental findings and to study the dynamics of the complex structure. Dependence of the excited modes on the pump wavelength is also investigated. These oscillations provide insights into the mechanical properties of the material at nanoscale.

8:24AM L6.00003 Slow light using crystal lattice vibrations in coupled quantum dots
ANDREW JACOBS, JOSHUA CASARA, CAMERON JENNINGS, MARK KERFOOT, MICHAEL SCHEIBNER, University of California, Merced — Phonons can induce an optical transparency in crystal structures, as was recently shown in an experimental study of asymmetric coupled quantum dots [1]. This transparency occurs due to Fano-type quantum interference between the discrete interdot exciton and continuum single dot-like polariton states. Here, we study this phonon-induced optical transparency as an avenue for slowing light. We find that slowdown factors up to 80,000 are possible, corresponding to a time delay of order 1 ps for a photon passing through a single coupled quantum dot pair. The optical slowdown is sensitive to both the Fano asymmetry factor and the homogeneous linewidth of the interdot exciton–we discuss the tunability of the slowdown factor using either parameter. Lastly, we investigate the effect of charge fluctuations, which are found to decrease the amount of optical slowdown. The experimentally measured interdot exciton linewidth is then used to theoretically infer the maximum possible optical transparency and slowdown factor without fluctuations present. [1] M. L. Kerfoot et al., Nat. Commun. 5, 3299 (2014).

8:36AM L6.00004 Phononic frequency combs through nonlinear resonances
RU-WEN PENG, Nanjing University, LU-SHUAI CAO, Universitat Hamburg, DONG-XIANG QI, MU WANG, Nanjing University, PETER SCHMELCHER, Universitat Hamburg — It is well known that optical frequency combs have become important coherent optical sources with diverging applications, ranging from optical frequency metrology to ultracold gases. In this work, we explore an analogue of optical frequency combs in driven nonlinear phononic systems, and present a mechanism for generating phononic frequency combs through nonlinear resonances. In the underlying process, a set of phonon modes is simultaneously excited by the external driving which yields frequency combs with an array of discrete and equidistant spectral lines of each nonlinearly excited phonon mode. Frequency combs through nonlinear resonance of different orders are investigated, and in particular the possibility of correlation tailoring in higher-order cases is revealed. We suggest that our results can be applied in various nonlinear acoustic processes, such as phonon harvesting, and can also be generalized to other nonlinear systems. Reference: L. S. Cao, D. X. Qi, R. W. Peng, Mu Wang and P. Schmelcher, Phys. Rev. Lett. 112, 075505 (2014).

8:48AM L6.00005 Low Frequency Thermal Conductivity in Micro Phononic Crystals
VIRGILIO ANJOS, ALISON ARANTES, Univ Federal de Juiz de Fora — We study theoretically the cumulative thermal conductivity of a micro phononic crystal at low temperature regime. The phononic crystal considered presents carbon microtubes inclusions arranged periodically in a two-dimensional square lattice embedded in soft elastic matrix. Moderate and high impedance mismatch are considered concerning the material composition. The low frequency phonon spectra (up to tens of GHz) are obtained solving the generalized wave equation for inhomogeneous media within the Plane Wave Expansion method. We consider low temperatures in order to increase the participation of GHz thermal phonons. We observed suppression in the cumulative thermal conductivity at the band gap region and thus a reduction of thermal conductivity of the phononic crystal when compared with the bulk matrix.

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9:00AM L6.00006 ABSTRACT WITHDRAWN —
9:12AM L6.00007 How intermixing and anharmonicity enhances interfacial thermal conductance?1 CARLOS POLANCO, JINGJIE ZHANG, NAM LE, ROUZBEH RASTGARKAFSGHARKOLAEI, PAMELA NORRIS, AVIK GHOSH, Univ of Virginia — The thermal conductance at an interface, whether ballistic or diffusive, can be expressed as a product of the number of conducting channels (M) and their average transmission (T). The common expectation is that interfacial defects reduce T and thus hurt the conductance. This is however at odds with recent simulations showing that a thin intermixing layer can in fact enhance the conductance. We argue that such an enhancement occurs when the increase in number of modes outweighs the reduction in their average transmission. The new channels open as a result of (a) the random interfacial structure that relaxes the conservation rules for the transverse momentum and promotes transitions between formerly symmetry disallowed channels; and (b) inelastic scattering through phonon-phonon interactions that allow modes beyond the contact cut-off frequency to contribute to transport. We use these results to build a back of the envelope model for interfacial conductance that depends on the mixing distribution, the anharmonic strength, the phonon polarization and wavelength. Non-Equilibrium Green’s Function (NEGF) as well as Molecular Dynamics (MD) simulations on Si/mixed layer/Ge, as well as simpler FCC crystals support our results.

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9:24AM L6.00008 Interfacial thermal transport and phonon-phonon conversion at the graphene-boron nitride lateral interface, ZHUN-YONG ONG, GANG ZHANG, YONG-WEI ZHANG, Inst of High Perform Comp — Using the nonequilibrium Green’s function method, we compute the thermal boundary conductance of a monolayer graphene-boron-nitride (Gr-BN) lateral heterostructure with an armchair interface. At 300 K, the thermal conductance of the Gr-BN interface is computed to be 3.5 nW/nm² or equivalent to approximately 200 nm of BN. The application of a strain, parallel or normal to the interface, also reduces the interfacial thermal resistance by improving the transmission of acoustic phonons. We do a modal decomposition of the phonon transmission spectrum and identify the phonon scattering channels responsible for heat transfer at the interface. We show that at low frequencies, interfacial heat transfer is dominated by the longitudinal, transverse and flexural acoustic phonons while at higher frequencies, it is mostly by longitudinal acoustic and optical phonons. Our work sheds light on the mechanism of phonon-phonon conversion at the interface of 2D lateral heterostructures and how it can be modified via the application of strain.


9:36AM L6.00009 Thermoelectric transport through a quantum nanoelectromechanical system and its backaction, HANGBO ZHOU, Natl Univ of Singapore, JUZAR THINGNA, University of Augsburg, JIAN-SHENG WANG, BAOVEN LI, Natl Univ of Singapore — In recent years, nanoelectromechanical systems (NEMS) have been in the limelight of intense experimental and theoretical investigation due to their potential applications in quantum-controlled devices. In this work we study the thermoelectric transport through a single electron transistor (SET) coupled to a quantum nano mechanical resonator (NR). The effects of the quantum NR on the thermoelectric current are investigated with special emphasis on how the SET-NR coupling strength plays a role in such a NEMS. We find that the SET-NR coupling is not only able to suppress or enhance the thermoelectric current but can also switch its direction. The effect of the NR on the thermoelectric coefficients of the SET are studied and we find that even a small SET-NR coupling could dramatically suppress the figure of merits 2ZT. Lastly, we investigate the backaction of electronic current on the NR and possible routes of heating or cooling the NR are discussed. We find that by appropriately tuning the gate voltage the backaction can be eliminated, which could find possible applications to enhance the sensitivity of detection devices.

9:48AM L6.00010 Emergence of Chaos in nano-electromechanical shuttles with hard-wall collision: Nonanalytic charge transport1 HEE CHUL PARK, Korea Institute for Advanced Study, KANG-HUN AHN, Department of physics, Chungnam National University — We develop a theory for charge transport in nano-electromechanical shuttles in the presence of hard-wall collision. We show that, in certain regimes, the time-averaged charge current is not predictable and is not an analytic function of applied voltage. The rectified electric current and its non-analyticity emerge from a non-Markovian process in the presence of the hard-wall collision, which causes chaotic motion of the shuttle.

1This work was supported by research fund of KIAS and Chungnam National University. Computations was supported by the CAC of KIAS.

10:00AM L6.00011 Nonlinearity-induced synchronization enhancement in micromechanical oscillators, JEFFREY R. GUEST, DARIO ANTONIO, DAVID A. CZAPLEWSKI, DANIEL LÓPEZ, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL, USA, SEBASTIÁN I. ARROYO, DAMIAN H. ZANETTE, Centro Atómico Bariloche and Instituto Balseiro, 8400 Bariloche, Río Negro, Argentina — An autonomous oscillator synchronizes to an external harmonic force only when the forcing frequency lies within a certain interval around the oscillator’s natural frequency. Under ordinary conditions, the width of this “synchronization range” decreases when the oscillator’s self-sustained amplitude grows, constraining synchronized motion of micro- and nanomechanical resonators to narrow frequency and amplitude bounds. In this talk, we will show that nonlinearity in the oscillator can be exploited to manifest a regime where the synchronization range increases with increasing oscillation amplitude. We demonstrate this regime experimentally with a self-sustained micromechanical oscillator, revealing an increase in the synchronization range by orders of magnitude over that expected for a linear oscillator. We provide analytical results which show that nonlinearities are the key determinants of this enhancement. Our results suggest a new strategy to enhance synchronization of micromechanical oscillators by capitalizing on their intrinsic nonlinear dynamics.

10:12AM L6.00012 Fluctuation Reduction in a Si Micromechanical Resonator Tuned to Nonlinear Internal Resonance, B. SCOTT STRACHAN, Michigan State Univ, DAVID CZAPLEWSKI, CHANGYAO CHEN, Argonne National Labs, MARK DYKMAN, Michigan State Univ, DANIEL LÓPEZ, Argonne National Labs, STEVEN SHAW, Michigan State Univ — We describe experimental and theoretical results on an unusual behavior of fluctuations when the system exhibits internal resonance. We study the fundamental flexural mode (FFM) of a Si microbeam. The FFM is electrically actuated and detected. It is resonantly nonlinearly coupled to another mode, which is not directly accessible and has a frequency nearly 3 times the FFM frequency. Both the FFM and the passive mode have long lifetimes. We find that the passive mode can be a “sink” for fluctuations of the FFM. This explains the recently observed dramatic decrease of these fluctuations at nonlinear resonance [1]. The re-distribution of the vibration amplitudes and the fluctuations is reminiscent of what happens at level anti-crossing in quantum mechanics. However, here it is different because of interplay of the dependence of the vibration frequency of the FFM on its amplitude due to internal nonlinearity and the nonlinear resonance with the passive mode. We study both the response of the system to external resonant driving and also the behavior of the system in the presence of a feedback loop. The experimental and theoretical results are in good agreement. [1] D. Antonio, Nat. Comm., 3, 806 (2012).
10:24AM L6.00013 Dynamical properties of single crystalline 4H-SiC micro-cantilevers and determination of Poisson’s ratio and density of 4H-SiC thin film. FENG ZHAO, ALLEN LIM, QUAN TRAN, School of Engineering and Computer Science, Washington State University Vancouver — As a wide bandgap semiconductor, single crystalline 4H-polytype silicon carbide (4H-SiC) is a very attractive material for microelectromechanical systems (MEMS) with operation in harsh environments such as high temperature, radiation, chemical/biomedical, etc. Fabrication and performance prediction of 4H-SiC MEMS require releasing of thin films as well as an accurate value of its important material properties including density and Poisson’s ratio. However, releasing single crystal 4H-SiC microstructures is extremely challenging due to the very inert chemical resistance of 4H-SiC (practically only etched by molten KOH above 600 °C). Although density and Poisson’s ratio in bulk 4H-SiC form have been known, they may not be the same in thin film with the thickness in the order of micrometers for MEMS systems. In this paper, we successfully released single crystal 4H-SiC to fabricate suspended micro-cantilever structures using a recently developed surface micromachining technique. The dynamical properties of these cantilevers including resonant frequency and force-distance were characterized, from which the density and Poisson’s ratio of 4H-SiC thin film were determined.

10:36AM L6.00014 Structural and Mechanical Properties of (Co/Cu) Co-doped Nano ZnO1. OZGUR OZTURK, ELIF ASIKUZUN, Kastamonu University, DOGAN AKCAY, LUTFI ARDA, Bahcesehir University, AHMET TOLGA TASC1, ABDULKADIR SENOL, Kastamonu University, SEVIM SENOL, CABIR TERZIOGLU, Abant Izzet Baysal University — Zn1−xCoxCoxO (x=0.0, 0.01, 0.02, 0.03, 0.04, and 0.05) solutions were prepared by co-precipitation method with subsequent calcination at 800 °C. The crystal structures, phases, sizes and microstructure of Zn1−xCoxCoxO powder samples were characterized by using X-Ray Diffraction (XRD) and Scanning Electron Microscopy (SEM). Microhardness values of all B doped ZnO powders were measured by using Vickers hardness tester. The experimental microhardness data were used to determine elastic modules, yield strength, and fracture toughness value of the samples. Additionally, the experimental results were analyzed using the various theoretical models namely, Kick’s Law, Elastic/Plastic Deformation (EPD) models, Proportional Specimen Resistance (PSR), and Hays-Kendall (HK) approach. The Vickers microhardness measurements revealed that hardness of Zn1−xBxO powder samples increased with B doping.

1This research has been partially supported by Scientific and Technological Council of Turkey (Project No. 114F259) and partially supported by Kastamonu University Scientific Research Projects Coordination Department under the Grant No. KUBAP-03/2013-41.

10:48AM L6.00015 The structural and mechanical behaviours of Boron-doped ZnO nanostructures1. ABDULKADIR SENOL, Department of Physics, Abant Izzet Baysal University, 14280 Bolu, Turkey, SEVIM DEMIROZU SENOL, Department of Chemistry, Abant Izzet Baysal University, 14280 Bolu, Turkey, OZGUR OZTURK, ELIF ASIKUZUN, AHMET TOLGA TASC1, ABDULKADIR SENOL, Kastamonu University, 37100 Kastamonu, Turkey, CABIR TERZIOGLU, Department of Physics, Abant Izzet Baysal University, 14280 Bolu, Turkey — Undoped and Boron (B)-doped Zinc Oxide (ZnO) nanoparticles were synthesized by Hydrothermal method. The structural and mechanical behaviours of B doped ZnO (Zn1−xBxO, x=0, 0.05, 0.07, 0.11) were systematically examined. The crystal structure, phases, sizes and microstructure of Zn1−xBxO powder samples characterized by using X-Ray Diffraction (XRD) and Scanning Electron Microscopy (SEM). Microhardness values of all B doped ZnO powders were measured by using Vickers hardness tester. The experimental microhardness data were used to determine elastic modules, yield strength, and fracture toughness value of the samples. Additionally, the experimental results were analyzed using the various theoretical models namely, Kick’s Law, Elastic/Plastic Deformation (EPD) models, Proportional Specimen Resistance (PSR), and Hays-Kendall (HK) approach. The Vickers microhardness measurements revealed that hardness of Zn1−xBxO powder samples increased with B doping.

1This research partially supported by Abant Izzet Baysal University Scientific Research Projects Coordination Department under the Grant No. BAP-2013.03.02.609.

Wednesday, March 4, 2015 8:00AM - 10:48AM – Session L7 DMP DCMP: Focus Session: Topological Superconductivity and Majorana Fermions

8:00AM L7.00001 Multiple signatures of topological phase transitions in a finite superconducting nanowire with intrinsic interactions1. Y.-H. CHAN, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan, CHING-KAI CHIU, Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada V6T 1Z1, KUEI SUN, Department of Physics, The University of Texas at Dallas, Richardson, Texas 75080-3021, USA — We study a finite chain model with spinless fermions that describes a pair wave superconductor with intrinsic interactions. By systematically tracking various physical quantities such as ground state energy, compressibility, entanglement spectrum, Cooper pair size, and pair condensate density, we obtain multi-signature of topological phase transitions between strong and weak pairing states. Some of the signatures are stable against finite-size effects. In addition, we explore the possibility of the topological transition at fixed volume, number of particles, and number of condensed pairs. The results would help explore a fundamental question: whether or not must a topological phase transition accompany with the change of extensive thermodynamic quantities?

8:12AM L7.00002 Effect of coupling to Majorana bound states on Kondo physics in a strongly correlated quantum-dot device1. TATHAGATA CHOWDHURY, KEVIN INGERSENT, Univ of Florida - Gainesville — Majorana bound states in spinless fermions is an intriguing possibility that is a key ingredient of Majorana bound states in Kondo physics. In order to test the theory, we have designed a quantum dot model with spinless fermions interacting with a Majorana bound state. We have studied the ground state structure of the system and found that the Majorana bound state, when added to the system, changes the ground state energy and the entanglement spectrum.

1Supported by NSF Grant DMR-1107814

8:24AM L7.00003 Classification of reflection symmetry protected topological semimetals and nodal superconductors, CHING-KAI CHIU, University of British Columbia, ANDREAS SCHNYDER, Max Planck Institute Stuttgart — The topological classification of insulators, semimetals, and superconductors in terms of nonspatial symmetries is well understood, less is known about topological states protected by crystalline symmetries, such as mirror reflections and rotations. In this work, we systematically classify topological semimetals and nodal superconductors that are protected, not only by nonspatial (i.e., global) symmetries, but also by a crystal reflection symmetry. We find that the classification crucially depends on (i) the codimension of the Fermi surface (nodal line or point) of the semimetal (superconductor), (ii) whether the mirror symmetry commutes or anticommutes with the nonspatial symmetries and (iii) how the Fermi surfaces (nodal lines or points) transform under the mirror reflection and nonspatial symmetries. The classification is derived by examining all possible symmetry-allowed mass terms that can be added to the Bloch or Bogoliubov-de Gennes Hamiltonian in a given symmetry class and by explicitly deriving topological invariants.
8:36AM L7.00004 Signatures of topological phase transition from fluctuating vortices in superconducting doped topological insulators. PEDRO LOPES, UNICAMP-Univ de Campinas, POUYAN GAHEMI, Physics Department, City College of the City University of New York — We study the interplay between low energy vortex bound modes in superconducting doped topological insulators and dynamical fluctuations of the vortex position. We show how this interaction leads to corrections in the local density of states close to the vortex core, signaling a topological vortex phase transition. We also present a detailed analysis of the low energy vortex bound modes, with analytic and numerical approximations, which may be used to access the quantities of physical interest.

8:48AM L7.00005 Quantum interference of edge supercurrents in a two-dimensional topological insulator1. GRIGORY TKACHOV, PABLO BURSET, BJOERN TRAUZETTEL, EWELINA HANKIEWICZ, Wurzburg University — Josephson weak links made of two-dimensional topological insulators (TIs) exhibit magnetic oscillations of the supercurrent that are reminiscent of those in superconducting quantum interference devices. We propose a microscopic theory of such a TI SQUID effect1. The key ingredient of our model is the exact treatment of the influence of an external magnetic field on the edge supercurrents. We show that this effect has the form of a 1D Doppler effect that describes the flux-controlled interference of the edge currents with superimposed suppression of Andreev reflection. Both long and short junctions are discussed. In particular, for long junctions the theory shows a temperature-driven crossover from the normal $\Phi_0$-periodic SQUID pattern to a $2\Phi_0$-quasiperiodic pattern consisting of a series of alternating even and odd peaks (where $\Phi_0=hc/2e$ is the magnetic flux quantum). The predicted even-odd effect is the signature of gapless (protected) Andreev bound states with a sawtooth dependence on the magnetic flux. Our findings may shed some light on the recently observed even-odd interference pattern in InAs/GaSb-based TI Josephson junctions, suggesting new operation regimes for nano-SQUIDs.

1 GT. acknowledges financial support of the German Research Foundation (DFG Grant No TK60/1-1). This work was also supported by DFG FOR 1162, SPP1066, IST research unit “Topotronics” and the ENB graduate school “Topological insulators.”

9:00AM L7.00006 Topologically stable gapless phases in nonsymmorphic superconductors. SHINGO KOBAYASHI, MASATOSHI SATO, Department of Applied Physics, Nagoya University — Nontivial node structures are a salient feature in the unconventional superconductors (SCs), providing valuable clues to an understanding of the symmetry of Cooper pairs. In the presence of spin-orbital coupling, the node structures are determined by the group theory [1] where the symmetry operation in a crystal lattice is followed by spin. Such a node is stabilized by crystal symmetry. Especially, as the counterexample of the Blount’s theorem, Micklitz and Norman indicated that there exists a stable line node in nonsymmorphic SCs with odd parity [2]. In our previous study [3], we found that the topological classification not only includes the Blount’s theorem but also updates the instability of line node via the bulk-boundary correspondence. In this talk, taking into account the nonperiodic boundary condition on a tight-binding Hamiltonian, we extend the topological node stability to nonsymmorphic SCs and show that the stable line node suggested by Micklitz and Norman is also the topological object.


9:12AM L7.00007 Dynamical Generation of Floquet Majorana Flat Bands in s-Wave Superconductors. AMRIT POUDIL, Dartmouth College, GERARDO ORTIZ, Indiana University, Bloomington, LORENZA VIOLA, Dartmouth College — We present techniques to dynamically engineer flat bands of symmetry-protected Majorana edge modes in s-wave superconductors. Specifically, we show how time-dependent periodic control may be employed for designing time-independent effective Hamiltonians, which support Floquet Majorana flat bands, starting from topologically trivial equilibrium conditions. In the first approach, a suitably chosen modulation of the chemical potential simultaneously induces Majorana states with strong Rashba spin-orbit coupling. We focus, in particular, on the role of confinement effects in long ballistic junctions. In the normal regime, scattering at the two contacts gives rise to two distinct features in conductance, Fabry-Perot resonances and Fano dips. The latter arise in the presence of a strong Zeeman field $B$ that removes a spin sector in the leads (helical leads), but not in the central region. Conversely, a helical central region between non-helical leads exhibits helical gaps of half-quantum conductance, with superimposed helical Fabry-Perot oscillations. These normal features translate into distinct subgap states when the leads become superconducting. In particular, Fabry-Perot resonances within the helical gap become parity-protected zero-energy states (parity crossings related to Yu-Shiba-Rusinov bound states), well below the critical field $B_c$, at which the superconducting leads become topological. As a function of Zeeman field or Fermi energy, these zero-modes oscillate around zero energy, forming characteristic loops, which evolve continuously into Majorana bound states as $B$ exceeds $B_c$.

9:24AM L7.00008 Superconducting States in Doped Topological Materials. MASATOSHI SATO, Department of Applied Physics, Nagoya University — There are considerable interests in topological superconductivity in condensed matter physics. In this talk, we will present our recent works on topological superconductors and the related phenomena. In particular, I will discuss how topological non-trivial structures in normal states may provide non-trivial quantum phenomena in the superconducting states. As examples, I will discuss odd parity superconductors, superconducting states in doped topological insulators and Weyl semi-metals. In the latter case, I will show how synergy effects of symmetry and surface states in the normal states may provide non-trivial quantum phenomena in the superconducting states.

9:36AM L7.00009 SNS junctions in nanowires with spin-orbit coupling: role of confinement and helicity on the sub-gap spectrum. JORGE CAYAYO, Consejo Superior de Investigaciones Científicas (CSIC) - Spain, ELSA PRADA, Universidad Autónoma de Madrid (UAM) - Spain, PABLO SÁNCHEZ-RODRÍGUEZ, CONSEJO Superior de Investigaciones Científicas (CSIC) - Spain — We study normal transport and the sub-gap spectrum of superconductor-normal-superconductor (SNS) junctions made of semiconducting nanowires with strong Rashba spin-orbit coupling. We focus, in particular, on the role of confinement effects in long ballistic junctions. In the normal regime, scattering at the two contacts gives rise to two distinct features in conductance, Fabry-Perot resonances and Fano dips. The latter arise in the presence of a strong Zeeman field $B$ that removes a spin sector in the leads (helical leads), but not in the central region. Conversely, a helical central region between non-helical leads exhibits helical gaps of half-quantum conductance, with superimposed helical Fabry-Perot oscillations. These normal features translate into distinct subgap states when the leads become superconducting. In particular, Fabry-Perot resonances within the helical gap become parity-protected zero-energy states (parity crossings related to Yu-Shiba-Rusinov bound states), well below the critical field $B_c$, at which the superconducting leads become topological. As a function of Zeeman field or Fermi energy, these zero-modes oscillate around zero energy, forming characteristic loops, which evolve continuously into Majorana bound states as $B$ exceeds $B_c$.

9:48AM L7.00010 Observation of topologically protected surface states in a Bi-Pd superconductor. MASATO SAKANO, Quantum-Phase Electronics Center (QPEC) and Department of Applied Physics, The University of Tokyo, KENJIRO OKAWA, MANABU KANOU, Materials and Structures Laboratory, Tokyo Institute of Technology, HARUHIKO SANJO, Quantum-Phase Electronics Center (QPEC) and Department of Applied Physics, The University of Tokyo, TAICHI OKUDA, Hiroshima Synchrotron Radiation Center, Hiroshima University, TAKAO SASAGAWA, Materials and Structures Laboratory, Tokyo Institute of Technology, KYOKO ISHIZAKA, Quantum-Phase Electronics Center (QPEC) and Department of Applied Physics, The University of Tokyo — A layered Bi-Pd superconductor is investigated by spin- and angle-resolved photoemission spectroscopy. Beside the spin-degenerate bulk bands, several spin-polarized surface bands, some of which crossing the Fermi level, are clearly observed. These surface states are evaluated to be topologically protected, based on the $Z_2$ invariant analysis in analogy to 3-dimensional strong topological insulators. It indicates that this material is likely to be a topological superconductor realized without any carrier doping or applying pressure.
10:00AM L7.00011 Surface transport coefficients for three-dimensional topological superconductors\textsuperscript{1}, HONG-YI XIE, YANG-ZHI CHOU, MATTHEW FOSTER, Rice Univ — We argue that surface spin and thermal conductivities of three-dimensional topological superconductors are universal and topologically-quantized at low temperature. For a bulk winding number $\nu$, there are $|\nu|$ “colors” of surface Majorana fermions. Localization corrections to surface transport coefficients vanish due to time-reversal symmetry (TRS). We argue that Altshuler-Aronov interaction corrections vanish because TRS forbids color or spin Friedel oscillations. We confirm this within a perturbative expansion in the interactions, and to lowest order in a large-$|\nu|$ expansion. We suggest that 3D topological superconductors are a closer analog of the 2D quantum Hall effect than 3D topological insulators.

\textsuperscript{1}This research was supported by the Welch Foundation under Grant No.C-1809 and by an Alfred P. Sloan Research Fellowship (BR2014-035)

10:12AM L7.00012 Majorana fermion from weak topological superconductivity: application to SrTiO\textsubscript{3} and KTaO\textsubscript{3}, SUK BUM CHUNG, Seoul Natl Univ, CHEUNG CHAN, HONG YAO, Institute for Advanced Study, Tsinghua University — Much of the current experimental efforts for detecting Majorana zero modes centered on probing the boundary of quantum wires with strong spin-orbit coupling. It is possible to realize the same type of Majorana zero mode at crystalline dislocation in the 2D superconductor, which has non-zero weak topological indices. Unlike at an Abrikosov vortex, at such a dislocation, there will not be midgap states other than the Majorana zero mode that can complicate the experimental detection. We will show that, using the anisotropic dispersion of the Ti / Ta t2g orbitals, such a weak topological superconductivity can be realized when the surface 2DEG of SrTiO\textsubscript{3} or KTaO\textsubscript{3} becomes superconducting.

10:24AM L7.00013 Probing Majorana-like states in quantum dots and quantum rings\textsuperscript{1}, IGOR ZUTIC, BENEDIKT SCHARF, Department of Physics, University at Buffalo, SUNY, Buffalo, NY 14260, USA — Engineering topological superconductivity in semiconductor structures offers fascinating ways to obtain and study Majorana modes in a condensed matter context. Here, we theoretically investigate topological superconductivity in quantum dots and quantum rings [1]. Using both analytical as well as numerical methods, we calculate the quasiparticle excitation spectra in these structures and the corresponding excitation amplitudes and charge densities. In the topological regime, we can observe the chiral edge modes localized at the boundaries and possessing finite energy in quantum dots and quantum rings. By applying a magnetic field which is expelled from the quantum ring, but which creates a flux that is an odd integer multiple of $\Phi_0/2 = \hbar/2e$, Majorana modes, that is, (approximately) degenerate edge modes with zero energy and zero charge density, become possible in the topological regime. Furthermore, we investigate finite-size effects that split these degenerate edge modes as well as the effect of a magnetic field penetrating into the superconducting region that can under certain circumstances still support edge modes with approximately zero energy and charge.

\textsuperscript{1}We acknowledge support from U.S. ONR N000141310754, DFG Grant No. SCHA 1899/1-1, and DOE-BES DE-SC0004890.

10:36AM L7.00014 Superconducting tunneling studies on thin film gold nanowires coupled to a BCS superconductor\textsuperscript{1}, PENG WEI, Department of Physics and Francis Bitter Magnet Lab, MIT, FERHAT KATMIS, CUI-ZU CHANG, Francis Bitter Magnet Lab, MIT, PATRICK LEE, Department of Physics, MIT, JAGADEESH MOODERA, Department of Physics and Francis Bitter Magnet Lab, MIT — The nanowire patterned out of (111)-oriented gold thin film is an excellent candidate for hosting Majorana bound states (MBS) when it is coupled to an s-wave superconductor [1]. The robust MBS is guaranteed by the large Rashba spin-orbit coupling (SOC) of gold surface state, as well as by large spatial separations between the two MBS in fabricated micrometer size long nanowires. In addition, being able to produce complex nanowire circuit, our approach is better streamlined for achieving the braiding circuit of Majorana fermions. We present our experimental approach of growing high quality hetero-layers consisting of epitaxial (111)-oriented gold thin film on vanadium using molecular beam epitaxy (MBE). Unique lithography processes are developed to pattern the top gold thin film into nanowires with a width around 100nm without damaging the hetero-layers such as its topography or superconducting behavior. Superconducting tunneling studies are performed over the gold nanowire using lithographically fabricated planar tunnel junctions. These tunneling characteristics will be discussed.


Wednesday, March 4, 2015 8:00AM - 10:48AM

Session L8 DCMP: Modeling and Measurement of Surface Morphology 006C - Mina Yoon, Oak Ridge National Laboratory

8:00AM L8.00001 A Computational Investigation of Random Angle Grain Boundaries for CdTe Solar Cells, CHRISTOPHER BUURMA, University of Illinois at Chicago, MARIA CHAN, Argonne National Laboratory, ROBERT KLIE, SIVALINGAM SIVANANTHAN, University of Illinois at Chicago, DOE BRIDGE COLLABORATION — Grain boundaries (GB) in poly-CdTe solar cells play an important role in species diffusion, segregation, defect formation, and carrier recombination. Many studies on GBs in CdTe focus on either entire grain-boundary networks found in complete poly-CdTe devices, those exhibiting high symmetry such as the coincident site lattice (CSL) or symmetric tilt or twist, or on very small scale Scanning-Tunneling Electron Microscope (STEM) viewable interfaces and dislocations. The topic of this talk is a comprehensive survey of the grain boundary parameter space regardless of the degree of symmetry found and whether the STEM channeling condition is satisfied. Our survey encompasses both near-CSL or vicinal grain boundaries decorated with nearby dislocations, as well as mixed tilt and twist interfaces with all possible symmetrically inequivalent grain boundary planes. Atomistic calculations using a Stillinger-Weber potential will be presented on a large representative sample of random-angle GBs. Trends in interfacial energies and atomistic structures as a function of tilt/twist/displacement parameters will be investigated. First principles density functional theory (DFT) calculations will be performed on a subset of these GBs to reveal their electronic structures and their implications towards PV performance. DoE Sunshot program contract DOE DEEE005956. Use of the Center for Nanoscale Materials was supported by the USDoE, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.
8:12AM L8.00002 The surface morphology of CuFeS$_2$: A hybrid-exchange density functional study$^{1}$, VICENT HUAIR-YU CHEN, Department of Physics, Imperial College London, London SW7 2AZ, United Kingdom, RUTH MARTINEZ CASADO, Department of Theoretical Condensed Matter Physics, Autonomous University of Madrid, 28049 Madrid, Spain, GIUSEPPE MALLIA, NICHOLAS HARRISON, Thomas Young Centre, Department of Chemistry, Imperial College London, London SW7 2AZ, United Kingdom — The surface morphology of CuFeS$_2$ has been determined using hybrid-exchange density functional theory calculations. The (110) surface is identified to be the most stable non-polar surface with a surface energy of 0.58 Jm$^{-1}$. The polar (112)/(112) surface pair is shown to be remarkably stable and thermodynamically preferred to the (110) surface if certain defects are included. The stability of the polar (112)/(112) surface pair is attributed to a combination of geometric and electronic mechanisms localised to the (112) surface which combine to neutralise the electrostatic dipole perpendicular to the surface. The former entails a partial reversal of the surface atomic layer sequence while the latter involves dispersion of charge from the subsurface anions to neighbouring cations. Because of its stability, (112) and (112) facets always form a significant portion of the Wulff construction regardless of the growth conditions.

$^{1}$VHC was supported by the CDT in Theory and Simulation of Materials at Imperial College funded by EPSRC grant EP/G036888/1. In addition, this work was supported by the Rio Tinto Centre for Advanced Mineral Recovery at Imperial College London.

8:24AM L8.00003 Characterizing Submonolayer Growth of 6P on Mica: Capture Zone Distributions vs. Growth Exponents and the Role of Hot Precursors$^{1}$, T.L. EINSTEIN, JOSUE MORALES-CIFUENTES, Univ of Maryland-College Park, ALBERTO PIMPINELLI, Rice Quantum Institute — Analyzing capture-zone distributions (CZD) using the generalized Wigner distribution (GWD) has proved a powerful way to access the critical nucleus size$^{2}$. Of the several systems to which the GWD has been applied, we consider 6P on mica, for which Winkler’s group found $i \approx 3$. Subsequently they measured the growth exponent $\alpha$ (island density $\propto F^\alpha$, for flux $F$) of this system and found good scaling but different values at small and large $F$, which they attributed to DLA and ALA dynamics, but with larger values of $i$ than found from the CZD analysis. We investigate this result in some detail. The third talk of this group describes a new universal relation between $\alpha$ and the characteristic exponent $\beta$ of the GWD. The second talk reports the results of a proposed model that takes long-known transient ballistic adsorption into account, for the first time in a quantitative way$^{3}$. We find several intermediate scaling regimes, with distinctive values of $\alpha$ and an effective activation energy. One of these, rather than ALA, gives the best fit of the experimental data and a value of $i$ consistent with the CZD analysis.

$^{1}$Work at UMD supported by NSF CHE 13-05892
$^{3}$JRM-C, TLE, & AP, PRL, in press

8:36AM L8.00004 How Hot Precursor Modify Island Nucleation: A Rate-Equation Model$^{1}$, JOSUE MORALES-CIFUENTES, T.L. EINSTEIN, Univ of Maryland-College Park, ALBERTO PIMPINELLI, Rice Quantum Institute — We describe the analysis, based on rate equations, of the hot precursor model mentioned in the previous talk$^{4}$. Two key parameters are the competing times of ballistic monomers decaying into thermalized monomers vs. being captured by an island, which naturally define a “thermalization” scale for the system. We interpret the energies and dimensionless parameters used in the model, and provide both an implicit analytic solution and a convenient asymptotic approximation. Further analysis reveals novel scaling regimes and nonmonotonic crossovers between them. To test our model, we applied it to experiments on parahexaphenyl (6P) on sputtered mica$^{5}$. With the resulting parameters, the curves derived from our analytic treatment account very well for the data at the 4 different temperatures. The fit shows that the high-flux regime corresponds not to ALA (attachment-limited aggregation) or HMA (hot monomer aggregation) but rather to an intermediate scaling regime related to DLA (diffusion-limited aggregation). We hope this work stimulates further experimental investigations.

$^{1}$Work at UMD supported by NSF CHE 13-05892
$^{2}$J.R. Morales-Cifuentes, T.L. Einstein, & A. Pimpinelli, PRL, in press

8:48AM L8.00005 Scaling and Exponent Equalities in Island Nucleation: Novel Results and Application to Organic Films Alberto Pimpinelli, Levent Tumbek, and Adolf Winkler$^{1}$, ALBERTO PIMPINELLI, Rice Quantum Institute, LEVENT TUMBEK, ADOLF WINKLER, Graz Univ of Technol. — As discussed in the first talk, the scaling of the island density with the flux $F$ and/or the capture zone distribution (CZD) can be used to determine the size of the critical nucleus $i$, but so far an analytic function for CZD exists only for diffusion-limited aggregation (DLA). For CZD the scaling function is $P_i(s) = a_i s^\beta \exp(-b_i s^2)$, with $\beta = i + 2$. We have extended the analytic description of the CZD in terms of $P_i$ also to attachment-limited aggregation (ALA); in this case we obtain $\beta = (i + 3)/2$. Furthermore, we could demonstrate that the general relationship $\alpha \beta = i$ holds, independent of the aggregation mechanism$^{6}$. This important exponent equality should help to better characterize nucleation and growth of thin films.

$^{1}$Work at Graz supported by Austrian Science Fund (FWF), Project No. P 23530

9:00AM L8.00006 A spatio-temporal model of wrinkling in photopolymerised networks, MATTHEW HENNESSY, ALESSANDRA VITALE, PAUL STAVRINOU, OMAR MATAR, JOAO CABRAL, Imperial College London — Photopolymerisation is a common solidification process whereby crosslinked polymer networks are created by illuminating a monomer-rich bath with collimated light. In addition, photopolymerisation is extensively employed industrially and shows exceptional promise for advanced three-dimensional patterning of functional surfaces. Under conditions of strong optical attenuation and limited mass and thermal diffusion, photopolymerisation occurs in a localised region which propagates from the illuminated surface into the bulk as a travelling wave with a planar wavefront. Under specific conditions that we set out to map, this planar wavefront may become unstable and the surface of the resulting gel can acquire a wrinkled morphology. We believe this instability is mechanical in nature and arises from compressive stresses that are generated during frontal photopolymerisation. In this talk, we will present a novel mathematical model that captures both the photopolymerisation with wrinkling processes. We show that by coupling photopolymerisation with wrinkling in a controlled manner, a number of interesting and industrially relevant patterns can be achieved.
9:12AM L8.00007 Ginzburg-Landau theory of the bcc-liquid interface kinetic coefficient. KUO-AN WU, Department of Physics, National Tsing-Hua University, Hsinchu, Taiwan, JEFFREY HOYT, Department of Materials Science and Engineering and Brockhouse Institute for Materials Research, McMaster University, Hamilton, Canada, ALAIN KARMA, Physics Department and Center for Interdisciplinary Research on Complex Systems, Northeastern University, Boston, USA — We extend the Ginzburg-Landau (GL) theory of atomically rough bcc-liquid interfaces outside of equilibrium to derive an analytical expression for the kinetic coefficient $\mu_i$. The kinetic coefficient is expressed as a spatial integral along the normal direction of a sum of gradient square terms corresponding to different nonlinear density wave profiles. Anisotropy arises naturally from the dependence of those profiles on the angles between the principal reciprocal lattice vectors $\mathbf{K}$ and $\mathbf{n}$. Values of the kinetic coefficient for the (100), (110) and (111) interfaces are compared quantitatively to the prediction of linear Mikhail-Chernov (MC) theory and previous MD simulation studies of crystallization kinetics for a classical model of Fe. The GL theory predicts a similar expression for $\mu$ as the MC theory but yields a better agreement with MD simulations for both its magnitude and anisotropy due to a fully nonlinear description of density wave profiles across the solid-liquid interface. In particular, the overall magnitude of $\mu$ predicted by GL theory is an order of magnitude larger than predicted by the MC theory. GL theory is also used to derive an inverse relation between $\mu$ and the solid-liquid interfacial free-energy.

9:24AM L8.00008 Island Dynamics Model for Mound Formation: Effect of a Step-Edge Barrier. CHRISTIAN RATCSCH, UCLA, DIONISIOS MARGETIS, University of Maryland, FREDERIC GIBOU, UCSB — We have developed an island dynamics model for epitaxial growth with the level-set technique, where islands are treated as continuous in the x-y-plane, while individual atomic layers are resolved in the z-direction. Atoms are treated as a mean field quantity by solving a diffusion equation. We will discuss an analytic derivation for the proper expression for the equilibrium adatom density at the step edge in the presence of a step-edge barrier. The effect of an additional step-edge barrier is incorporated via a mixed Robin-type boundary condition for the diffusion equation. We will present a numerical scheme to solve such a boundary condition on a fixed grid with moving boundaries. We will show how the inclusion of the step-edge barrier leads to the formation of mounds that become progressively steeper as the step-edge barrier increases. Finally, we will discuss how we can include the effect of downward funneling in our model, and how it leads to the stabilization of the slope of the mounds.

9:36AM L8.00009 In-situ probing and modeling atomic layer deposition processes on Ge surface. YUANXIA ZHENG, SUNGWOOK HONG, Penn State Univ, BRUCE RAYNER, Kurt J. Lesker Company, SUMAN DATTA, ADRI VAN DUIN, ROMAN ENGEL-HERBERT, Penn State Univ — Germanium (Ge) is a promising CMOS compatible channel material with a low effective-mass of holes. One of the major challenges in developing Ge-FETs is integrating a high-quality gate stack on Ge. A direct high-k dielectric deposition like HfO$_2$ on Ge has resulted in poor electrical characteristics of the semiconductor-dielectric interface. 1 GeO$_2$/Ge interface has been found low in interface-trap density, but its quality rapidly degrades when deposited with high deposition rates. Ultrathin GeO$_2$ layers on Ge(001) are known to enhance dopant incorporation. 2 This work focuses on deposition of GeO$_2$ on Ge(001) by atomic layer deposition (ALD) processes. We use (a) in-situ spectroscopic ellipsometry for real-time monitoring of atomic-layer-deposition (ALD) processes on Ge, (b) ex-situ X-ray photoelectron spectroscopy (XPS) to probe the interface chemistry, and (c) reactive force field (ReaxFF) simulations to directly model the growth kinetics and interface formation. A strong surface-chemistry dependence (hydrogenated Ge vs oxidized Ge) has been found in the Al$_2$O$_3$-ALD nucleation (Trimethylaluminum+H$_2$O), which is well reproduced by ReaxFF simulation. Furthermore, both experiments and simulations revealed that the Al$_2$O$_3$ capping on GeO$_2$/Ge interface prevents oxygen diffusion into Ge, and therefore stabilizes the interface. 1 [1] Appl. Phys. Lett. 87, 032107 (2005). 2 J. Appl. Phys. 106, 104117 (2009). 3 2012 Symp. VLSI Technol. 2011~2012 (2012).

9:48AM L8.00010 Structural evolution of Ag nanoparticles during electron driven synthesis of Ag filaments on Ag$_2$WO$_4$. In situ observation and theoretical supporting evidence. EDISON Z. DA SILVA, Institute of Physics, University of Campinas, Unicamp, WYLLAMANIEY DA SILVA PEREIRA, INCTMN-UFScar, Universidade Federal de Sao Carlos, JUAN ANDRES, LOURDES GRACIA, Departament de Quimica Fisica i Analítica, Universitat Jaume I, MIGUEL SAN-MIGUEL, Instituto of Chemistry - University of Campinas, ELSON LONGO, INCTMN-UNESP, Universidade Estadual Paulista, VALERIA M. LONGO, INCTMN-USP, Universidade de Sao Paulo, Instituto de Fisica de Sao Carlos — $\alpha$-Ag$_2$WO$_4$ crystals irradiated by an electron beam from an electron microscope under high vacuum, nucleate metallic Ag, and form Ag metallic nanowires on the $\alpha$-crystals surface. In order to understand this interesting and complex behavior of the formation and growth of Ag nanowires on $\alpha$-Ag$_2$WO$_4$ we investigated by detailed in situ transmission electron microscopy (TEM), field emission scanning electron microscopy (FE-SEM) studies, density functional theory calculations and ab initio molecular dynamics (MD) simulations. First principle calculations point out that Ag-3 and Ag-4 atoms, located on the (100) surface, are the most energetically favorable to undergo the diffusion process to form metallic Ag. Ab initio MD simulations and nudged elastic band (NEB) method were used to investigate the minimum energy pathways for diffusion of Ag atoms to outward sites on the (100) surface. The results point out that the injection of electrons decreases the activation barrier for this diffusion step and this unusual behavior results from the presence of a lower energy barrier process.

1 Financial support FAPESP, Project 2010/16970-4, grant (2013/2032-7), calculations performed at CENAPAD-SP.

10:00AM L8.00011 Kinetic Transition of Crystal Morphology from Nanoparticles to Dendrites during Electron Beam Induced Deposition of Gold. JEUNG HUN PARK, Univ of California Los Angeles and IBM T. J. Watson Research Center, NICHOLAS SCHNEIDER, HAIM BAU, Univ of Pennsylvania, SUNEEL KODAMBAKA, Univ of California Los Angeles, FRANCES ROSS, IBM T. J. Watson Research Center — We studied the kinetic transition from compact nanoparticle to dendritic morphology during electron beam-induced Au deposition using in situ liquid cell-based transmission electron microscopy. Radiolysis of water by electrons generates radicals and molecular species. Hydrated electrons and hydrogen and hydroxide radicals can act as reducing agents and initiate the reduction of the water-soluble precursor, HAuCl$_4$, resulting in the precipitation of Au as nanostructures. We tracked nucleation, growth, and morphological transition of Au from movies recorded in situ, as a function of irradiated dose and liquid thickness. We identified several distinct regimes that depend on the irradiation time: (1) nucleation; (2) linear volumetric growth; (3) formation of dendritic structures; (4) coalescence and dissolution. A diffusion and reaction model for the radiolytic species and metal ions in the confined geometry of the irradiated volume is used to understand the nucleation sites and morphological transitions. We finally describe how nanoparticles can be made to grow in a stepwise manner by switching the supply of Au ions on and off electrochemically, and discuss possibilities for creating more complex nanostructures.

2 This research was partially funded by the National Science Foundation (DMR-1310639, CMMI-1129722, and CBET-1066573).

10:12AM L8.00012 Possible detection of surface melting on solid hydrogen by TOF-SIMS. TAKU SUZUKI, National Institute for Materials Science — The molecular hydrogens form the simplest of all molecular solids. Thus, the irradiation effect of ion beams on quench-condensed hydrogen film is conceptually the simplest of all molecular condensed systems and therefore is an ideal benchmark system for testing theories. However, the number of studies concerning ion beam irradiation effect on solid hydrogen is quite limited. In the present study, we have investigated secondary ion emission from quench-condensed hydrogen films under ion beam irradiation. To prepare the quench-condensed hydrogen films, we developed ultra-high vacuum (UHV) – compatible cryostat, which enables such heating to 4 K. The UHV chamber was equipped with an ion gun with an electrostatic deflector for chopping and an electrostatic energy analyzer. The continuous 2 keV He$^+$ ion beam was utilized for ion scanning spectroscopy (ISS), while the ion beam was chopped for time-of-flight secondary ion mass spectroscopy (TOF-SIMS). The sample was prepared by the exposure of a polycrystalline H$_2$. We found the enhancement of the H$^+$ ion emission with decreasing the sample temperature. The enhancement of the secondary H$^+$ ion emission is most likely related with the solid-liquid phase transition.
10:24AM L8.00013 Surface nanopatterning using electric-field-driven assembly of single-layer epitaxial islands, ASHISH KUMAR, DWAIYEAR DASGUPTA, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — We report a systematic simulation study of an approach to surface nanopatterning based on electric-field-driven assembly of single-layer epitaxial islands on face-centered cubic crystalline substrates. We have developed and validated a fully nonlinear driven island evolution model with diffusional mass transport limited to the island edges and accounting for edge diffusional anisotropy and island coalescence and break-up. For islands on (110), (100), and (111)-oriented substrate surfaces, we report formation of complex nanomodels starting from two different types of initial configurations: a single island with larger-than-critical size and an assembly of relatively small islands, which undergo a sequence of coalescence and break-up events. For both initial configurations, we study the dependence of the nanopattern features on the duration of application of the electric field, the strength of edge diffusional anisotropy, and the misorientation angle between a fast edge diffusion direction and the applied electric field direction. For assemblies of islands, we also study the resulting nanopattern dependence on the intrinsic geometrical parameters of the assembly. We report entire classes of complex patterns formed as the above parameters are varied.

10:36AM L8.00014 Nonlinear Analysis of Secondary Ripple Formation on Surfaces of Stressed Crystalline Solids, LIN DU, DWAIYEAR DASGUPTA, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — The competition between surface energy and elastic strain energy in surfaces of stressed crystalline solids is responsible for Asaro-Tiller/Grinfeld (surface cracking) morphological instabilities. Using linear stability theory (LST), we have predicted that properly directed and sufficiently strong electric fields and thermal gradients can inhibit such instabilities; we validate the LST predictions based on self-consistent dynamical simulations according to a fully nonlinear surface evolution model. The simulations also reveal that long-wavelength perturbations from the planar surface morphology can trigger a tip-splitting instability, which causes formation of a pattern of secondary ripples that is beyond the scope of LST. Based on weakly nonlinear analysis, we have developed a theory that can explain the occurrence of such rippling instabilities and predict the number of ripples that form on the surface as a function of perturbation wavelength. The theory predicts the critical wavelength for the onset of secondary ripple formation and the external field strength requirement for planar surface stabilization. The conclusions of the theory are validated by comparisons with the results of the self-consistent numerical simulations.

Wednesday, March 4, 2015 8:00AM - 10:48AM
Session L9 DCMP: Semiconductor Atomic Structure, Lattice Properties, and Phase Transitions
006D - Matthew Stone, Oak Ridge National Laboratory

8:00AM L9.00001 Structure and dynamics of CdTe studied by X-ray and neutron scattering, MATTHEW STONE, JENNIFER NIEDZIELA, Oak Ridge National Laboratory — We present x-ray diffraction and inelastic neutron scattering studies of the structure and lattice dynamics of commercial CdTe. We also present complementary density functional theory calculations. The X-ray data show a subtle structural transition is present near 80 K, which manifests also in the measured phonon density of states. Refinement of the structure above and below the transition temperature shows no change to the long-range ordered structure. The inelastic neutron scattering studies were performed using an isotopically un-enriched sample of CdTe, which possesses a high cross section for thermal neutron absorption. The neutron portion of the study was performed with a thin-plate geometry in the reflection condition at the ARCS instrument at the SNS, showing the high flux of the instrument makes possible lattice dynamics studies of materials with high thermal neutron absorption. Single crystal and powder inelastic neutron scattering measurements will be presented. Current interpretation of the nature of the transition and future studies will be discussed.

8:12AM L9.00002 First-principles calculations of phonons and Raman spectra in monoclinic CsSnCl$_3$, LING-YI HUANG, WALTER LAMBRECHT, Case Western Reserve Univ — Halide perovskites have recently attracted attention for photovoltaic applications. While CsSnCl$_3$ in the perovskite structure is less suitable for solar cells because of its higher band gap than the iodides, it is still of interest as the end member of mixed CsSn(I$_{1-x}$Cl$_x$)$_3$ and addition of Cl has been found to increase solar cell efficiencies. The other reason this material is interesting is that at 390 K it undergoes a phase transition to a monoclinic structure with even larger band gap, which differs from the yellow phase occuring for CsSnI$_3$. Understanding the various possible phase transitions and structures in the trihalides is important for the long-term stability of these materials in solar cells. Raman data exist on monoclinic CsSnCl$_3$ material since the late 80s but have in the past not been compared with first-principles calculations of the phonons in this material. We present calculations of the phonons at the Γ point using density functional perturbation theory using the abinit program. A symmetry analysis is presented and the calculated phonon modes are compared with experimental data and previous attempts to classify the modes as internal to the SnCl$_3$ tetrahedra and lattice modes. Supported by DOE.

8:24AM L9.00003 Application of Quantum Monte Carlo Methods to Describe the Properties of Manganese Oxide Polymorphs, JOSHUA SCHILLER, ELIF ERTEKIN, Univ of Illinois - Urbana — First-principles descriptions of the properties of correlated materials such as transition metal oxides has been a long-standing challenge. Manganese oxide is one such example: according to both conventional and hybrid functional density functional theory, the zinc blende polymorph is predicted to be lower in energy than the rock salt polymorph that occurs in nature. While the correct energy ordering can be obtained in density functional approaches by careful selection of modeling parameters, we present here an alternative approach based on quantum Monte Carlo methods, which are a suite of stochastic tools for solution of the many-body Schrodinger equation. Due to its direct treatment of electron correlation, the QMC method offers the possibility of parameter-free, high-accuracy, systematically improvable analysis. In manganese oxide, we find that the QMC methodology is able to accurately reproduce relative phase energies, lattice constants, and band gaps without the use of adjustable parameters. Additionally, statistical analysis of the many-body wave functions from QMC provides some diagnostic assessments to reveal the physics that may be missing from other modeling approaches.

8:36AM L9.00004 ABSTRACT WITHDRAWN
8:48AM L9.00005 ABSTRACT WITHDRAWN
Harmonic Approximation was applied successfully to determine the Gibbs free energy of MnFeSi, which is linearly proportional to the Latent heat \( L \) of magnetization. Experimentally \( L \) can be determined with techniques such as Differential Scanning Calorimetry. In our study we use VASP in addition to the Phonopy package, to determine the finite temperature properties of the system. Quasi Harmonic Approximation was applied successfully to determine the Gibbs free energy of MnFeSi-P, \( \text{P}_{0.66} \). Hence we show a phase transition around 425 K. From the temperature derivative of \( G \), the specific heat was obtained and finally the latent heat was obtained.

Institude for Basic Sciences, Kyung Hee University, Seoul, Korea — Using ab initio density functional calculations, we investigate the structural and electronic properties of the ordered crystalline and disordered amorphous phases of a GeTe material, which would be used for phase change random access memory. In order to understand the mechanism of shear-induced phase transition and the key factors effecting the transition, we performed molecular dynamics simulations on a GeTe material. The shear-induced phase transition would not occur without change of lattice structure — contrarily to Ce. Our study of Pu shows that the most important effect originating the differentiation between the equilibrium densities of its allotropes is the competition between the Peierls effect and the Madelung interaction. However, the proper treatment of electron correlation effects is crucial to reach good agreement with experiment. A similar interplay between kinetic and elastic interactions in the formation of Si-IV. Combining nanoscratching and micro-Raman spectroscopy, shear effect on Si-I to Si-IV phase transition has been studied qualitatively and quantitatively. A clear evolution of phase transition of silicon has been recorded. The stability of Si-IV has been analyzed by analyzing an in-situ Raman measurement under various temperatures.

National Natural Science Foundation of China (11274372)
**10:12AM L9.00012 Temperature Dependence of Brillouin Light Scattering Spectra of Acoustic Phonons in Silicon**

This work is supported by National Science Foundation (NSF) Thermal Transport Processes Program under grant CBET-1336968.

**10:24AM L9.00013 Diffuse X-ray Scattering as a Tool to Characterize Morphology of Multilayered Structures of Ultra-small (Submonolayer) Quantum Dots**

This work is supported by DOE, BES award DE-SC000379.

**10:36AM L9.00014 Brillouin Light Scattering study of patterned TiN/SiOC:H/Si structures**

**Wednesday, March 4, 2015 8:00AM - 11:00AM —**

Session L10 DCMP: Two Dimensional Topological Insulators: Experiments

**8:00AM L10.00001 Emergence and coupling of topological surface states in tunable TI-non TI heterostructures**

**8:12AM L10.00002 Effect of in-plane magnetic field and strain to quantization in 2D topological insulator: application to InAs/GaSb Quantum Wells**

**8:24AM L10.00003 ABSTRACT WITHDRAWN**
8:36AM L10.00044 Tuning the Fermi level through the Dirac point of giant Rashba semiconductor BiTeI*1, DERRICK VANGENNEP, D.L. MASLOW, J.J. HAMLIN, Dept. of Physics, Univ. of Florida, S. MAITH, Dept. of Physics, Univ. of Florida and NHMFL, Tallahassee, FL, D. GRAFT, S.W. TOZER, NHMFL, Tallahassee, FL, C. MARTIN, Dept. of Physics, Univ. of Florida and Ramapo Coll., NJ, H. BERGER, Inst. of Cond. Mat. Physics, École Poly. Féd. de Lausanne — We report measurements of Shubnikov-de Haas oscillations in the giant Rashba semiconductor BiTeI under pressure. We observe one high frequency oscillation at all pressures and one low frequency oscillation that emerges between ~0.3 - 0.7 GPa indicating the appearance of a second small Fermi surface. BiTeI has a conduction band bottom that is split into two sub-bands due to the strong Rashba coupling, resulting in a “Dirac point.” Our results suggest that the chemical potential starts below the Dirac point in the conduction band at ambient pressure and moves upward across it as pressure is increased. We present a simple model that captures this effect and can be used to understand the pressure dependence of our sample parameters. The parameters extracted via our model support the notion that pressure brings the system closer to the predicted topological quantum phase transition.

*1Supported by NNSA-NA0001979 (DG and SWT), NSF DMR-1157490 (SM), NSF DMR-0908029 and NSF DMR-1308972 (DLI).

8:48AM L10.00005 Magnetic field-induced breakdown of helical conduction in an InAs/GaSb bilayer, DMITRY PIKULIN, Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada V6T 1Z1, TIMO HYART, Department of Physics and Nanoscience Center, University of Jyväskyla, P.O. Box 35 (YFL), FI-40014 University of Jyväskyla, Finland, SHUO MI, Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands, JAKUB TWORZYDLO, Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Hoza 69, 00-681 Warsaw, Poland, MICHAEL WIMMER, Kavli Institute of Nanoscience, Delft University of Technology, P.O. Box 5046, 2600 GA Delft, The Netherlands, CARLO BEENAKKER, Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands — We calculate the conductance of a two-dimensional bilayer with inverted electron-hole bands, to study the sensitivity of the quantum spin Hall insulator (with helical edge conduction) to the combination of the perpendicular magnetic field in presence of disorder. The characteristic breakdown field for helical edge conduction splits into two fields with increasing disorder, a field $B_\tau$ for the transition into a quantum Hall insulator (supporting chiral edge conduction) and a smaller field $B_\sigma$, for the transition to bulk conduction in a quasi-massless state. The spatial separation of the inverted bands, typical for broken-gap InAs/GaSb quantum wells, is essential for the magnetic-field induced bulk conduction — there is no such regime in HgTe quantum wells.

9:00AM L10.00006 HgTe/CdTe heterostructure under perturbations preserving time-reversal symmetry: a density functional theory study, PAULO PIQUINI, JONAS ANVERSA, Universidade Federal de Uberlândia, ADALBERTO FAZZIO, Universidade de São Paulo — The Dirac-like spin states at the interfaces of HgTe/CdTe heterostructures are predicted to be robust against perturbations preserving time-reversal symmetry. However, these perturbations will certainly affect these interface states. In this work we use the density functional theory to study the behavior of these interface states under external pressure and electric fields. Differently from the three-dimensional topological insulators, the HgTe/CdTe interface states present fully in-plane Rashba-like spin texture. Further, biaxial external pressures and electric fields perpendicular to the interfaces are seen to change the energetics and dispersion of the protected states, modifying the energy ordering of the crossing of the polarized interface states inside the band structure, and altering their Fermi velocities while not changing the topological phase.

9:12AM L10.00007 Search for emergent superlattice dispersion in a topological insulator heterostructure*1, ILYA BELIOPOLSKI, Princeton Univ, NIKESH KOIRALA, Rutgers University, SUYANG XU, MADHAB NEUPANE, GUANG BIAN, NASSER ALIDOUSS, Princeton University, SEONGSHIK OH, Rutgers University, ZAHID HASAN, Princeton University — Crystals are typically offered to us by nature and we must search among them to find ones with useful properties. Here, we consider a more aggressive approach to materials engineering whereby we build nanometer-scale periodic arrays of different crystal lattices. Such a lattice of lattices mimics the behavior of ‘directly engineered’ electronic properties in an emergent superlattice band structure. To our knowledge, no such superlattice dispersion has yet been observed. However, the discovery of topological insulators offers a natural route to engineering a superlattice band structure. Moreover, a topological insulator superlattice has immediate relevance to supporting chiral edge conduction and a Kramer’s pair of counter propagating 1D helical edge states. Since the topological quantum Hall effect, characterized by an insulating 2D bulk and a Kramer’s pair of counter propagating 1D helical edge states. The characteristic breakdown field for helical edge conduction splits into two fields with increasing disorder, a field $B_\tau$ for the transition into a quantum Hall insulator (supporting chiral edge conduction) and a smaller field $B_\sigma$, for the transition to bulk conduction in a quasi-massless state. The spatial separation of the inverted bands, typical for broken-gap InAs/GaSb quantum wells, is essential for the magnetic-field induced bulk conduction — there is no such regime in HgTe quantum wells.

*1The work at Princeton and Princeton-led synchrotron-based ARPES measurements is supported by U.S. DOE DE-FG-02-04ER46200.

9:24AM L10.00008 Quantum Confined Sb: An Elemental Topological Insulator*1, SHAYNE CAINRS, JEREMY MASSENGALE, ZHONGE-HUI LIU, JOEL KEAY, CHOMANI GASPE, KAUSHINI WICKRAMASINGHE, TETSUYA MISHIMA, MICHAEL SANTOS, SHEENA MURPHY, Univ of Oklahoma — Sb is a bulk semi-metal which is predicted to undergo a series of quantum phase transitions from a topological semi-metal to a 3D topological insulator (TI) to a 2D TI to a trivial insulator as a function of decreasing film thickness. We report magneto-transport studies on Sb(111) epilayers with thicknesses ranging from 0.7 to 3.2 nm grown via molecular beam epitaxy on nearly lattice-matched GaSb(111) substrates. For thick films the conducting states are metallic. However, we find that a series of quantum phase transitions occurs in the shallowly inverted regime. This system has a charge density of states per spin per atom. This system has a charge carrier density of states per spin per atom. This system has a charge carrier density of states per spin per atom. This system has a charge carrier density of states per spin per atom. This system has a charge carrier density of states per spin per atom. This system has a charge carrier density of states per spin per atom.

*1DMR-1207537

9:36AM L10.00009 Role of Coulomb Interaction in the Bulk Gap of Inverted InAs/GaSb bilayers*1, LINGJIE DU, RUI-RUI DU, Rice Univ, GERARD SULLIVAN, Teledyne Scientific and Imaging — Inverted InAs/GaSb bilayers have been shown to support the quantum spin Hall effect, characterized by an insulating 2D bulk and a Kramer’s pair of counter propagating 1D helical edge states. Since the Fermi energy of electrons and that of holes can be individually turned by gates, the degree of band inversion can be readily controlled in experiments. Here we perform the inplane field magneto-measurement of InAs/GaSb samples, in the two limits of band inversion. In the deeply inverted regime where electron and hole density exceed 10e11/cm2, we found that the bulk gap closes under several Tesla field, consistent with previous results in the same regime (M. J. Yang et al, Phys. Rev. Lett. 78, 4613). On the other hand, in the shallowly inverted regime close to inverted-normal band transition we find that the bulk gap remains open to very high fields (up to 35T). These results suggest that the nature of the bulk gap in InAs/GaSb in the shallowly inverted regime is not well understood. We will discuss the possible role of Coulomb interaction in this regime, where dilute electron-hole gases are unstable against the formation of bilayer excitation.

*1The work in Rice was supported by NSF DMR-1207562 and Welch Foundation.
We study dynamics of vortices in superconductors using the molecular dynamics simulation. Motion of vortices causes a heat generation and also decreases amplitude of the superconducting order parameter on their trail because of quasi-particle relaxation time. We incorporate these effects into the Molecular dynamics methods. In a superconducting corbino-disk, where vortices move along concentric circles, vortex motion is more rapid around the center of the disk than that around the edge. Therefore the heat generation is not uniform and there appears heat transport from the center to the edge. In such case, our simulation shows that vortices move toward the edge of the disk. Also vortices show some dynamical spiral structures depend on the pinning impurity sites and heat resistance between the superconductor and a substrate. We show details of these motions and analyze the effects of the heat transport to the vortex dynamics.

1This work was supported by JSPS KAKENHI Grant Number 26400367.
8:12AM L11.00002 ThermoElectric Measurements of Electronic Diffusivity in Bad Metals1, JIECHENG ZHANG, ELI LEVENSON-FALK, AHARON KAPITULNIK, Stanford University — Many interesting materials, including cuprate superconductors and heavy-fermion systems, exhibit “bad metal” behavior at high temperatures, where the electronic mean free path is shorter than the de Broglie wavelength. Recent theory [1] postulates that conduction in such systems is best described by collective incoherent transport, instead the standard quasiparticle model. This has implications for the temperature dependence of electronic diffusivity in these materials. We present a setup for measuring electronic diffusivity: a laser beam is focused onto a material surface and chopped, creating a periodic, concentrated heat source. The resulting thermoElectric signal is measured at various positions on the same surface with sharp voltage probes. By sweeping temperature in the range 10-450 K, we are able to measure the temperature dependence and anisotropy of the electronic diffusivity of the material. We discuss experimental improvements and measurements of cuprate superconductors.


1This work was funded by the Department of Energy.

8:24AM L11.00003 Heat Transport in non-uniform superconductors, CAROLINE RICHARD, ANTON B. VORONTSOV, Department of Physics, Montana State University, Bozeman, Montana — Thermal transport in superconductors is used as an experimental probe of both quasiparticles states and order parameter structure. Although thermal properties of uniform superconductors have been studied a lot, much less is known about details of the transport in non-uniform phases such as vortex states or the speculative Fulde-Ferrell-Larkin-Ovchinnikov state. Using the quasi-classical Keldysh technique, we theoretically investigate the heat transport in a inhomogeneous superconducting state where the order parameter contains a domain wall. We study the effect of Andreev states, bound to the domain wall, on thermal conductivity, and find the response to be strongly non-local. In linear response, we determine the density of states, impurity self-energy and the effective local temperature gradient required to sustain a stationary heat current through the sample.

8:36AM L11.00004 Heat transport along domain walls and surfaces of superconductors1, ANTON VORONTSOV, CAROLINE RICHARD, Montana State University — We calculate thermal transport in non-uniform states of unconventional superconductors, that appear near pairbreaking surfaces, or due to formation of domain walls in the order parameter. The spectrum of the quasiparticles states in these regions is dominated by the Andreev bound states, including topologically protected modes. We investigate how these states contribute to the heat transport, using non-equilibrium quasiclassical theory in linear response. We report self-consistent calculation of the order parameter, impurity self-energies, density of states and vertex corrections. Particular attention is paid to the non-local nature of the response. We show differences and similarities between domain walls in d-wave materials, and surfaces of multi-component chiral superconducting states. We describe results for Born and unitary impurity scattering limits, and effects of the Zeeman magnetic field on thermal transport.

1Supported by NSF Grants DMR-0954342

8:48AM L11.00005 Vortex relaxation in type-II superconductors following current quenches1, HARSH CHATURVEDI, HIBA ASSI, Virginia Tech, ULRICH DOBRAMYSYL, Mathematical Institute, University of Oxford, UK, MICHEL PLEIMLING, UWE TÄUBER, Virginia Tech — The mixed phase in type-II superconductors is characterized by the presence of mutually repulsive magnetic flux lines that are driven by external currents and pinned by point-like or extended material defects. We represent the disordered vortex system in the London limit by an elastic directed line model, whose relaxation dynamics we investigate numerically by means of Langevin Molecular Dynamics. We specifically study the effects of sudden changes of the driving current on the time evolution of the mean flux line gyration radius and the associated transverse displacement correlation functions. Upon quenching from the moving into the pinned glassy phase, we observe algebraically slow relaxation. The associated two-time height-autocorrelations display broken time translation invariance and can be described by a simple aging scaling form, albeit with non-universal scaling exponents.

1Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-09ER46613.

9:00AM L11.00006 Ordered Pinning Arrays with Tunable Geometry via Thermal Effects1, JUAN TRASTOY, ROZENN BERNARD, JAVIER BRIATICO, JAVIER E. VILLEGAS, Unite Mixte de Physique CNRS/Thales, France, MAXIME MALNOU, NICOLAS BERGAL, JEROME LESUEUR, LPEM, CNRS-ESPCI, France, CHRISTIAN ULYSSE, GIANCARLO FAINI, CNRS, LPN, France — We have used geometrically frustrated pinning arrays to create artificial vortex-ice [1]. The pinning arrays are fabricated via ion irradiation of high-Tc superconducting films. These arrays break time translation invariance and can be described by a simple aging scaling form, albeit with non-universal scaling exponents. Upon quenching from the moving into the pinned glassy phase, we observe algebraically slow relaxation. The associated two-time height-autocorrelations display broken time translation invariance and can be described by a simple aging scaling form, albeit with non-universal scaling exponents.

1Supported by the French ANR MASTHER, the COST Action NanoSC, the Ville de Paris and the Galician Fundacion Barrie

9:12AM L11.00007 Controlling Superconductivity in Thin Film with an External Array of Magnetic Nanorods, WONBAE BANG, K.D.D. RATHNAYAKA, I.F. LYUKSYUTOV, Department of Physics and Astronomy, Texas A&M University, College Station, Texas 77843, USA, W. TEIZER, Department of Physics and Astronomy, Texas A&M University; WPI-Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan, D.G. NAUGLE, Department of Physics and Astronomy, Texas A&M University, College Station, Texas 77843, USA — We have fabricated a novel type of magnet-superconductor hybrid: an ordered array of magnetic nanorods on top of a superconducting film which is electrically insulated from the array. We have studied the transport properties of this magnet-superconductor hybrid including the R(T) and R(H) dependences for temperatures 0.96<T<1.06Tc and magnetic fields H<700 Oe (Tc denotes the critical temperature of the hybrid system). We compare these results with those for a superconducting film on top of alumina template with an array of magnetic nanowires.
9:24AM L11.00008 Effects of heavy ion irradiation on the thermodynamic and transport properties of YBCO1

9:48AM L11.00010 Single vortex pinning and penetration depth in superconducting NdFeAsO$_{1−x}$F$_x$. JESSIE T. ZHANG, Massachusetts Institute of Technology. JEEHOO KIM, MAGDALENA HUEFNER, Harvard University, CUN YE, Tsinghua University, STELLA KIM, PAUL CANFIELD, RUSLAN PROZOROV, Iowa State University, OPHIR M. AUSLÄNDER, Technion - Israel Institute of Technology. JENNIFER E. HOFFMAN, Harvard University — We use a magnetic force microscope (MFM) to investigate single vortex pinning and penetration depth in NdFeAsO$_{1−x}$F$_x$, one of the highest-$T_c$ iron-based superconductors. In fields up to 20 Gaus, we observe a disordered vortex arrangement, implying that the pinning forces are stronger than the vortex-vortex interactions. By manipulating the vortices using the MFM tip, we obtain single vortex depinning forces for vortices in NdFeAsO$_{1−x}$F$_x$. Moreover, our MFM measurements allow the first local and absolute measurement of the superconducting penetration depth in NdFeAsO$_{1−x}$F$_x$ to nanometer scale resolution.

10:00AM L11.00011 Structural and Ground State Vortex Lattice Domains in MgB$_2$2

10:12AM L11.00012 Enhancement of critical current through oxygen irradiation in optimized 2G superconducting coated conductors. KAREN KIHLMSTROM, Argonne National Laboratory, University of Illinois at Chicago, M. LEROUX, U. WELP, W-K. KWOK, A.E. KOSELEV, Argonne National Laboratory, G.W. CRABTREE, Argonne National Laboratory, University of Illinois at Chicago, M.W. RUPICH, S. FLESHER, A.P. MALÖZEMOFF, American Superconductor Corp, A. KAYANI, Western Michigan University, CES COLLABORATION — We demonstrate the strong suppression of the critical current density, $J_c$, of commercial coated conductors (CC) in high magnetic fields using 3 MeV oxygen irradiation. The rapid suppression of $J_c$ of coated conductors in magnetic fields remains a barrier for application of CCs in motors, generators, transformers, solenoids, and MRI systems. Using TRIM simulations, we determined that 3-MeV O-ions produce an essentially uniform defect distribution in bare CC at a rate that is $\sim$ 2500 faster than that achieved with proton irradiation. Irradiating with 3 MeV O-ions to a dose of 1x10$^{13}$ O-ions/cm$^2$ generates a near doubling of the critical current at low temperatures: at 5K, 5T, we enhanced the critical current from 6.4 MA/cm$^2$ to 12.2 MA/cm$^2$. This dose can be achieved in a couple of seconds, thus this irradiation technique could be incorporated into a viable reel-to-reel production process. This work supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. D.O.E., Office of Science, Office of Basic Energy Sciences (K.K., M.L., A.K) and by the D.O.E, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357 (U.W., W.K.).

10:24AM L11.00013 Magnetic Levitation Force Measurement System at Any Low Temperatures From 20K To 300K1

10:36AM L11.00014 Controlling microwave driven vortex avalanches by superconductivity stimulation. ANTONIO LARA, FARKHAD G. ALIEV, Universidad Autonoma de Madrid, Spain, ALEJANDRO V. SILHANEK, Université de Liège, Belgium, VICTOR V. MOSCHCHALOV, Katholieke Universiteit Leuven, Belgium — The response of superconducting devices to electromagnetic radiation is a core concept implemented in diverse applications, ranging from the currently used voltage standard to single photon detectors in astronomy. Surprisingly, a sufficiently high power subgap radiation may stimulate superconductivity itself. Recently we have demonstrated the possibility of stimulating also type II superconductors, in which the radiation may cause nonlinear response of the vortex core [1]. This effect opens the possibility of effective control over vortex avalanches. Here we report on a detailed study of superconductivity enhancement and avalanche control by GHz radiation in type II superconducting Pb films in the presence of vortices. The magnetic field dependence of the vortex related microwave losses in a film with periodic pinning reveals a reduced dissipation of mobile vortices in the stimulated regime due to a reduction of the core size. Results of numerical simulations support the validity of this conclusion. Moreover, we demonstrate that microwave stimulated superconductivity induces a notable increase of microwave depinning power needed to trigger avalanches in the proximity of vortex depinning frequencies. Our findings open new ways to control the vortex dissipation and depinning induced avalanches by using superconductivity stimulation.

1Work supported by Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357.

2This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences under Award DE-FG02-10ER46783.

3This work was supported by TUBTAK--the Scientific and technological research council of Turkey under project of MFGAF - 110T622. This system was applied to the Turkish patent institute with the application number of 2013/13638 on 22/11/2013.
10:48AM L11.00015 Observation of Sinusoidal – Like Regular Voltage Oscillations in Silver Doped YBa2Cu3O7−δ1, ATILGAN ALTINKOK, Giresun University, MURAT OLUTAS, ATILLA KILIC, KIVILCIM KILIC, Abant Izzet Baysal University — The influence of bi-directional square wave (BSW) current was investigated on the evolution of the $V−t$ curves at different periods ($P$), temperatures and external magnetic fields. It was observed that slow transport relaxation measurements result in regular sinusoidal voltage oscillations which were discussed mainly in terms of the dynamic competition between pinning and depinning. The symmetry in the voltage oscillations was attributed to the elastic coupling between the flux lines and the pinning centers along grain boundaries and partly inside the grains. This case was also correlated to the equality between flux entry and exit along the YBCO/Ag sample during regular oscillations. It was shown that the voltage oscillations can be described well by an empirical expression $V(t) ∼ \sin(\omega t + \phi)$. We found that the phase angle $\phi$ generally takes different values for the repetitive oscillations. Fast Fourier Transform analysis of the $V−t$ oscillations showed that the oscillation period is comparable to that ($P$) of the BSW current. This finding suggests a physical mechanism associated with charge density waves (CDWs), and, indeed, the weakly pinned flux line system in YBCO/Ag resembles the general behavior of CDWs. At certain values of $P$, amplitude of BSW current, $H$ and $T$, the YBCO/Ag sample behaves like a double-integrator, since it converts the BSW current to sinusoidal voltage oscillations in time.

Wednesday, March 4, 2015 8:00AM - 11:00AM –
Session L12 DMP GERA FIAP DCOMP: Focus Session: Oxide and Chalcogenide Thermoelectric Materials 007C - Zhifeng Ren, University of Houston

8:00AM L12.00001 Theoretical survey of doped sodium cobaltate and strategies for enhancing the thermoelectric performance1, M. HUSSEIN N. ASSADI, HIROSHI KATAYAMA-YOSHIDA, Osaka University — Doped Na$_x$CoO$_2$ is suitable for highly efficient thermoelectric conversion at $\approx 1000$ K. However, due to complex lattice structure and strong correlation effects, atomistic understanding of dopant’s influence is challenging to resolve experimentally. We examined a wide range of dopants’ electronic structures using density functional method. We found that dopants like Mg, Ba, Sr, Au and Eu always substitute Na for all Na concentrations. In contrast, dopants like Ni, Bi, W, Sb and Sn always substitute Co regardless of Na concentration. Furthermore, there is a third class of dopants like Cu and Y that substitute Na for $x \leq 0.5$, but for higher Na concentrations, they substitute Co. In the case of Mg$_x$Na$_{1-x}$, we could experimentally verify Mg’s local chemical environment using Raman spectroscopy therefore validating the theoretical results. The implication of Na-substituting dopants on thermoelectric performance is the immobilization of Na ions which behave similar to ionic liquid in pristine Na$_x$CoO$_2$. This immobilization reduces the resistivity by improving the mobility of carriers and thus enhancing the thermopower.

1This work was supported by JSPS and Intersect.

8:12AM L12.00002 Anisotropic transport in single-crystal molybdenum bronze, Li$_{0.33}$MoO$_3$. SAEED MOSHEFYEGAN, JOSHUA L. COHN, University of Miami, JOHN J. NEUMEIER, Montana State University — We present transport measurements (resistivity, thermopower, thermal conductivity) on single crystals of the quasi-one-dimensional semiconductor Li$_{0.33}$MoO$_3$ in the temperature range 200-500 K. First synthesized and studied long ago[2] the thermal and thermoelectric properties for this compound have not been previously reported. We find extreme anisotropy in the Seebeck coefficient within the $\alpha−c$ planes, with $S_\alpha − S_\beta \approx 300 \mu$V/K near room temperature. The thermal conductivity at room temperature in the $a−c$ planes was $\sim 1.5−2$ W/mK and 7-8 times smaller along $b^*$. We also report x-ray studies of the out-of-plane ($b^*$) lattice constants indicating a small structural transition at $T \approx 350$ K that coincides with anomalies in the transport properties.


8:24AM L12.00003 Thermoelectric properties of amorphous ZnO-based materials using ab initio methods. ANINDYA ROY, YU-TING CHENG, MICHAEL L. FALK, Johns Hopkins Univ — We use a combination of computational methods - molecular dynamics and density functional theory, to predict thermoelectric properties of amorphous ZnO-based materials. We use BoltzTraP[1] to calculate properties such as Seebeck coefficient and electrical conductivity within semiclassical Boltzmann transport theory, and compare with available experimental results. Additionally, we investigate the change in the thermoelectric parameters caused by alloying amorphous ZnO with tin and other elements. Our preliminary calculations suggest that the thermoelectric performance of amorphous ZnO is on par with the crystalline counterpart. This is encouraging - since amorphous materials are yet to be studied in depth for their potential as thermoelectric materials, and they could see much improvement with sustained effort. Also, while ab initio methods are routinely used to predict properties of crystalline systems, their application in amorphous systems is a less-explored area.


8:36AM L12.00004 Perovskite- and Heusler based materials for thermoelectric converters. ANKE WEIDENKAFF, University of Stuttgart — The broad application of thermoelectric converters in future energy technologies requires the development of active, stable, low cost and sustainable materials. Semiconductors based on perovskite and heusler structures show substantial potential for thermoelectric energy conversion processes [1-3]. Their good performance can be explained based on their suitable band structure, adjusted charge carrier density, mass and mobility, limited phonon transport, electron filtering possibilities, strongly correlated electronic systems, etc. These properties are widely tunable by following theoretical concepts and a deep composition-structure-property understanding to change the composition, structure and size of the crystallites in innovative scalable synthesis procedures. Improved thermoelectric materials are developed, synthesised and tested in diverse high temperature applications to improve the efficiency and energy density of the thermoelectric conversion process. The lecture will provide a summary on the field of advanced perovskite-type ceramics and Heusler compounds gaining importance for a large number of future energy technologies.

9:12AM L12.00005 Thermoelectric properties of Cl-doped In$_2$Pb$_{0.01}$Sn$_{0.03}$Se$_{2.9}$Cl$_x$ polycrystalline compounds. JIN-HEE KIM, MIN JAE. KIM, SUEKYUNG OH, JONG-SOO RHYEE, Kyung Hee Univ - Sawon Campus, SU-DONG PARK, Advanced Materials Group, Korea Electrotechnology Research Institute. We investigated thermoelectric properties of Cl-doped polycrystalline compounds of In$_2$Pb$_{0.01}$Sn$_{0.03}$Se$_{2.9}$Cl$_x$ ($x = 0.02$, $0.04$ and $0.06$). The x-ray diffraction measurement shows gradual change of lattice volume for $x < 0.04$ without any impurity phases indicating systematic change of Cl-doping. The Cl-doping in the compounds has an effect of increasing carrier concentration and effective mass of carrier resulting in the increase of power factor near 700 K than In$_2$Pb$_{0.01}$Sn$_{0.03}$Se$_{2.9}$. Because of the increased electrical conductivity near 700 K, the thermoelectric figure-of-merit $ZT$ is 1.25 at 723 K for $x = 0.04$ Cl-doped compound which is relatively high value as n-type polycrystalline materials.

9:24AM L12.00006 Effects of Ge replacement in GeTe by Ag or Sb on the Seebeck coefficient and carrier concentration modified by local electron imbalance. E.M. LEVIN, A. HOWARD, U.S. DOE Ames Laboratory and Iowa State University, W.E. STRASZHEIM, Iowa State University. Variation in carrier concentration in Ag$_{2-x}$Ge$_{2-x}$Te$_5$ and Sb$_{2-x}$Ge$_{2-x}$Te$_5$ was found for Sb$_2$Ge$_2$Te$_5$ and Ag$_2$Ge$_2$Te$_5$. Interplay between the Seebeck coefficient and electrical resistivity in these alloys results in variation of power factor; the value of 45 mW/cm K° at 300 K and 873 K, respectively, if matched with appropriate p-type legs.

9:36AM L12.00007 Raman Spectroscopy of the Thermoelectric Sr$_{0.6}$Ba$_{3.8}$Nb$_2$O$_6$. MICHAEL PRIMROSE, JEAN TOULOUSE, Physics Department, Lehigh University. JONATHAN BOCK, CLIVE RANDALL, Center for Dielectric Studies, Materials Research Institute, Pennsylvania State University — Strontium Barium Niobate (SBN) has recently been shown by Lee et al. [1] to exhibit high thermoelectric power factor and electrical resistivity of Ag$_2$Ge$_2$Te$_5$ and Sb$_2$Ge$_2$Te$_5$ can be attributed to different electron configurations of valence electrons of Ag (4d$^{10}$5s$^1$) and Sb (5s$^2$5p$^3$) compared to that of Ge (4s$^2$4p$^3$) resulting in local electron imbalances and changing the concentration of charge carriers (holes) generated by Ge vacancies. In contrast, our $^{125}$Te NMR and Seebeck coefficient data for Ag$_2$Sb$_2$Ge$_4$Te$_8$ are similar to those observed for GeTe. This shows that effects from Ag and Sb compensate each other and indicates the existence of [Ag$_x$Sb$_y$] pairs. The effects of Ge replacement in GeTe by Ag, Sb, or [Ag$_x$Sb$_y$] on rhombohedral lattice distortion also have been analyzed. Interplay between the Seebeck coefficient and electrical resistivity in these alloys results in variation of power factor; the value of 45 mW/cm K°, the highest among known tellurides, was found for Sb$_2$Ge$_2$Te$_5$.

9:48AM L12.00008 Bulk oxides: asymmetry between p- and n-type transport properties. ANTOINE MAIGNAN, LABORATOIRE CRISMAT / CNRS / ENSICAEN / UCBN. The thermoelectric power (TEP) of transition metal oxides shows large difference depending on the sign of the charge carriers. In electron-doped oxides, the best TEs in terms of the figure of merit are heavily doped transparent conductors (as doped ZnO). The physics is very similar to that of semiconductors, though the defects chemistry differs: the existence of planar defects created by the dopants (in the conduction band) and the p-doping induced via the formation of oxygen vacancies (in the valence band). In contrast, the best n-types are layered cobaltites (CdI$_2$-type layers with edge-shared Co$_{12}$ octahedra). The Co cations adopt a low spin state. Both electronic correlations and spin entropy have to be considered to explain the S(T) curve for T < 150K, whereas for T > 150K, the spin/orbital configurations and the doping level in the generalized Heikes formula are dominating. This description supported by the results obtained for perovskite ruthenates was recently unvalidated for the quadruple perovskite AC$_2$Ru$_4$O$_{12}$, showing very different S(T) with S saturation at 900K. Their Pauli paramagnetism enlights the role of the spins upon thermopower. Similarly, searching for other n-types, interesting TE properties have been found in Ba$_2$Mn$_2$O$_{12}$; the S(T) evidences a charge/orbital ordering in this manganite ($y_{Mn}=3.7$) coupled to an abrupt change in the unit-cell volume. Ba$_2$Mn$_2$O$_{12}$, although of n-type, exhibits a cst. ($S_{Mn}=-240$ cm$^{-1}$) T-400K, explained by the generalized Heikes formula rather used for p-type. This difference with other n-type oxides is related to the Mn$^{4+}$/Mn$^{3+}$ magnetism and the contribution of e$_g$ orbitals for the transport properties. In this presentation, the richness of the TE properties of metal transition oxides will be emphasized focusing on the important role of the spins.

10:24AM L12.00009 Enhancement of Thermoelectric Performance in n-type PbTe$_{1−y}$Se$_y$ by Cr Doping. EYOBS CHERE, QIAN ZHANG, Univ of Houston. KENNETH MCEANLEY, MIT. MENG LIANG YAO, Boston Collage, FENG CAO, Univ of Houston, CYRIE OPEIL, Boston Collage. We investigated the thermoelectric properties of PbTe$_{1−y}$Se$_y$ with $y = 0.25$, $0.5$, $0.75$, $0.85$, and $1$. We found the peak $ZT$ temperature increased with increasing concentration of Se. A highest $ZT$ of $≈ 0.6$ at room temperature in Te-rich Cr$_{0.015}$Pb$_{0.985}$Te$_{0.75}$Se$_{0.25}$ was obtained due to a lowered thermal conductivity and enhanced power factor resulted from high Seebeck coefficient of about -220 $\mu$V K$^{-1}$ and high Hall mobility $≈ 1120$ cm$^2$ V$^{-1}$ s$^{-1}$ at room temperature. A room temperature $ZT$ of $≈ 0.5$ and peak $ZT$ of $≈ 1$ at about 573 K to 673 K is shown by Se-rich sample Cr$_{0.01}$Pb$_{0.99}$Te$_{0.25}$Se$_{0.75}$. This improvement of the room temperature $ZT$ improved the average $ZT$ over a wide temperature range and could potentially lead to a single leg efficiency of thermoelectric conversion for Te-rich Cr$_{0.015}$Pb$_{0.985}$Te$_{0.75}$Se$_{0.25}$ up to $≈ 11 \%$ and Se-rich Cr$_{0.01}$Pb$_{0.99}$Te$_{0.25}$Se$_{0.75}$ up to $≈ 13 \%$ with cold side and hot side temperature at 300 K and 873 K, respectively, if matched with appropriate p-type legs.

10:36AM L12.00010 Phonon Dispersions of Thermoelectric SnSe$^{1}$. CHEN LI, JIAWANG HONG, ANDREW MAY, JIE MA, TAO HONG, SONGXUE CHI, GEORG EHLERS, OLIVIER DELAIRE, Oak Ridge National Laboratory — SnSe has recently attracted significant interest as a thermoelectric material with very high $ZT$ > 2 along two crystallographic axes. A favorable property of SnSe is its very low thermal conductivity, which is below 1$W/m$ K$^{-1}$ along all axes even at ambient temperature, and decreases with temperature. However, the degree of anisotropy of the thermal conductivity remains somewhat controversial. We present our results of detailed inelastic neutron scattering measurements of the phonon dispersions and their temperature dependence. The results are compared with first-principles calculations to investigate the origin of the low thermal conductivity and its anisotropy.

$^{1}$Funding from the DOE, BES, MSED and as part of the S3TEC EFRC. OD acknowledges the Office of Science Early Career Research Program.
10:48AM L12.00011 Ultrafast investigation of photo-excited carrier-lattice dynamics in PbTe using Fourier-transform inelastic X-ray scattering, MASON JIANG, CRYSTAL BRAY, JESSE CLARK, TOM HENIGHAN, MIKE KOZINA, AARON LINDENBERG, MARIANO TRIGO, PETER ZALDEN, DAVID REIS, PULSE Institute, Stanford University, MATTHIEU CHOLLET, JAMES GLOWNIA, MATTHIAS HOFFMANN, DILING ZHU, LCLS, SLAC National Accelerator Laboratory, OLIVIER DELAIRE, ANDREW MAY, BRIAN SALES, Oak Ridge National Laboratory, STEPHEN FAHY, EAMONN MURRAY, IVANA SAVIC, Tyndall National Institute — We report with fine temporal and momentum resolution non-equilibrium electron-phonon and phonon-phonon dynamics in the widely-used thermoelectric material PbTe. The measurements are made possible by both the intense, ultrafast X-ray pulses of the Linac Coherent Light Source instrument and the recently developed Fourier-transform inelastic X-ray scattering (FT-IXS) technique. We demonstrate experimentally the various effects of impulsive optical photo-excitation on the lattice dynamics of the material as carriers are dramatically redistributed in the system. Specifically, coupled two-phonon states are excited throughout various Brillouin zones and possible plasmon-phonon modes are observed very near zone center. Coupled with calculations from density functional theory (DFT), an analysis of these photo-excited modes yields new insight into the origins of the incipient ferroelectricity and zone center anomalies noted in past measurements on PbTe.

Wednesday, March 4, 2015 8:00AM - 11:00AM — Session L13 DMP: Focus Session: Nanostructured LaAlO$_3$/SrTiO$_3$ Heterostructures 007D - Jeremy Levy, University of Pittsburgh

8:00AM L13.0001 Ultrafast Optical Response of Graphene/LaAlO$_3$/SrTiO$_3$ Nanostructures$^1$, LU CHEN, GIRRIRAJ JNAWALI, MENCHENG HUANG, JEN-FENG HSU, FENG BI, University of Pittsburgh, HYUNGWOO LEE, SANGWOO RYU, CHANG-BEOM EOM, University of Wisconsin-Madison, BRIAN D’URSO, PATRICK IRVIN, JEREMY LEVY, University of Pittsburgh — The exceptional electronic and optical properties of graphene make it promising for tunable plasmonic device applications in the terahertz regime. Plasmons can be induced in graphene by femtosecond laser excitation and its resonance frequency can be tuned over a broad terahertz range by varying the graphene pattern size or gate voltage. Recently, generation, and detection of broadband terahertz (around 10 THz) radiation from 10-nm-scale LaAlO$_3$/SrTiO$_3$ nanostructures created by conductive atomic force microscope (c-AFM) lithography has been demonstrated. This unprecedented control of THz radiation at 10 nm length scales creates a pathway toward hybrid THz functionality in graphene/LaAlO$_3$/SrTiO$_3$ nanostructures. We will discuss efforts to probe graphene plasmonics and its tunability by using this nanoscale THz spectrometer.

8:12AM L13.0002 Probing the nanoelectromechanical properties of LaAlO$_3$/SrTiO$_3$ Sketch-SETs, A. GAUTHIER, F. BI, Department of Physics and Astronomy, University of Pittsburgh, H. LEE, S. RYU, C. B. EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, P. IRVIN, J. LEVY, Department of Physics and Astronomy, University of Pittsburgh — The LaAlO$_3$/SrTiO$_3$ (LAO/STO) interface is reversibly achieved using a locally-tunable metal-insulator transition. This property can be applied to create nanoscale electronic devices such as sketched single-electron transistors (Sketch-SETs) at the LAO/STO interface. A Sketch-SET consists of a quantum dot coupled to source, drain, and gate electrodes. LAO/STO possesses a coupling between lattice distortion and carrier density; mechanical strain applied to the surface can tune the conductance at the interface. Leveraging this property may allow for strain-based control over the electron occupancy of a Sketch-SET. We use a cryogenic scanning probe microscope to create (at room temperature) and measure (at low temperature) the electronic properties of Sketch-SET devices and probe their unique nanoelectromechanical properties.

8:24AM L13.0003 CVD-grown graphene on LaAlO$_3$/SrTiO$_3$: transferring, patterning and c-AFM lithography$^1$, MENGCHENG HUANG, GIRRIRAJ JNAWALI, JEN-FENG HSU, Univ of Pittsburgh, HYUNGWOO LEE, SANGWOO RYU, Univ of Wisconsin-Madison, FENG BI, UNIV of Pittsburgh, FERESHTHE GHAHARI, JAYAKANTH RAVICHANDRAN, PHILIP KIM, Harvard Univ, CHANG-BEOM EOM, Univ of Wisconsin-Madison, BRIAN D’URSO, PATRICK IRVIN, JEREMY LEVY, Univ of Pittsburgh — Interesting properties are anticipated when graphene is integrated with complex-oxide heterostructures. To create these structures, single-layer graphene is grown by chemical vapor deposition and transferred onto LaAlO$_3$/SrTiO$_3$, following a deep UV exposure method, the size and position of the graphene can be patterned to be compatible with the c-AFM lithography technique applied on LaAlO$_3$/SrTiO$_3$. Local control of metal-insulator transition at LaAlO$_3$/SrTiO$_3$ interface is reversibly achieved using the c-AFM lithography technique without observable graphene degradation. The graphene layer can also serve as a top gate to modulate the LaAlO$_3$/SrTiO$_3$ interface conductance.

3We gratefully acknowledge financial support from the following agencies and grants: AFOSR FA9550-12-1-0268 (JL, PRI), AFOSR FA9550-12-1-0342 (CBE), ONR N00014-13-1-0806 (JL, CBE), and NSF DMR-1124131 (JL, CBE), DMR-1104191 (JL) and DMR-1234096 (CBE).

2J. Ju, et al., Nature Nanotech. 6, 630 (2011)


8:36AM L13.0004 High-energy photoemission studies of oxide interfaces$^1$, RALPH CLAESSEN, Physikalisch-Institut und Rontgen Center for Complex Material Systems (RCCM), Universitat Wuerzburg, Germany — The interfaces of complex oxide heterostructures can host novel quantum phases not existing in the bulk of the constituents, with the high-mobility 2D electron system (2DES) in LaAlO$_3$/SrTiO$_3$ (LAO/STO) representing a prominent example. Despite extensive research the origin of the 2DES and its unusual properties — including the supposed coexistence of superconductivity and ferromagnetism — are still a matter of intense debate. Photoelectron spectroscopy, recently extended into the soft (SX-ARPES) and hard (HAXPES) X-ray regime, is a powerful method to provide detailed insight into the electronic structure of these heterostructures and, in particular, of the buried interface. This includes the identification of the orbital character of the 2DES as well as the determination of vital band surface information, such as band alignment, band bending, and even k-resolved band dispersions and Fermi surface topology. Moreover, resonant photoemission at the Ti-L edge reveals the existence of two different species of Ti 3d states, localized and itinerant, which can be distinguished and identified by their different resonance behavior. The role of oxygen vacancies is studied by controlled in-situ oxidation, which allows us to vary the composition from fully stoichiometric to strongly O-deficient. By comparison to free STO surfaces we can thus demonstrate that the metallicity of the heterointerfaces is intrinsic, i.e., it persists even in the absence of O defects. I will discuss our photoemission results on LAO/STO heterostructures in both (100) and (111) orientation as well as on the related system γ-Al$_2$O$_3$/STO(100), which also hosts a 2DES with an even higher mobility. Work in collaboration with J. Mannhart (MPI-FKF, Stuttgart), T. Prbyd (TU Denmark), N. Rijnders (U Twente), S. Saga (U Osaka), M. Giorgoi (BESSY, HZB), W. Drube (DESY Photon Science), V.N. Strocov (Swiss Light Source), J. Denlinger (Advanced Light Source, LBNL), and T.-L. Lee (Diamond Light Source).

$^1$Support by DFG and BMBF is gratefully acknowledged.
we present the investigation of ballistic transport in LaAlO$_3$ of electronic device density is key for any material system to be considered as potential for electronics, which demands ballistic devices at the nanoscale. Here, we gratefully acknowledge financial support from the following agencies and grants: AFOSR (FA9550-12-1-0057 and FA9550-10-1-0524) AFOSR FA9550-12-1-0342 (CBE) and DMR-1234096 (CBE).

Astronomy, University of Pittsburgh, HYUNGWOO LEE, SANGWOO RYU, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Pittsburgh — Weak anti-localization is a macroscopic observation of a quantum transport phenomenon in two-dimensional systems with spin-orbit coupling in which destructive self-interference of carrier trajectories leads to an enhanced conductivity at low magnetic fields. Characterizing spin-orbit coupling at the LaAlO$_3$/SrTiO$_3$ (LAO/STO) interface is important in realizing this system’s potential as a principal host for oxide nanoelectronics. Previously, the spin-orbit coupling at the 2D LAO/STO interface was shown to be gate-tunable. Here, we study a crossover from 2D to 1D regimes using nanowires at the LAO/STO interface using weak anti-localization measurements. Transport measurements were performed on nanowires with widths varying from 200 nm down to 10 nm. A series of magnetoresistance measurements were performed at various backgate voltages to study carrier-density dependence. The results are fit to both 2D and 1D models of a weak anti-localization conductance correction due to Rashba spin-orbit coupling.

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2We gratefully acknowledge financial support from ARO (W911NF-08-1307), AFOSR (FA9550-10-1-0524 and FA9550-12-1-0342), and NSF (DMR-1104191, DMR-1124131 and DMR-1234096).

3We gratefully acknowledge support for this work from ARO (W911NF-08-1307), AFOSR (FA9550-10-1-0524 and FA9550-12-1-0342), and NSF (DMR-1104191, DMR-1124131 and DMR-1234096).

LaAlO$_3$/SrTiO$_3$ nanowires

investigating dimensional crossover of spin-orbit coupling in

LaAlO$_3$/SrTiO$_3$ nanowires


RONGPU ZHOU, MICHELLE TOMCZKYK, GUANGLEI CHENG, SHICHENG LU, MENGCHEN HUANG, PATRICK IRVIN, Univ of Pittsburgh, HYUNGWOO LEE, SANGWOO RYU, CHANG-BEOM EOM, Univ of Wisconsin-Madison, JEREMY LEVY, Univ of Pittsburgh — Scaling of electron device density is key for any material system to be considered as potential for electronics, which demands ballistic devices at the nanoscale. Here we present the investigation of ballistic transport in LaAlO$_3$/SrTiO$_3$ nanowire devices that act as quantum point contacts. In these devices, electron transport shows quantized conductance up to 3rd sub-band energy levels. We also observe odd integer conductance in the units of $e^2/h$ at high magnetic fields, further indicating spin-resolved quantum transport. We analyze the strength of the Zeeman spin-splitting for various sub-bands induced by magnetic field, where 1D sub-bands show a linear Zeeman splitting for out of plane magnetic field. From the transconductance and magnetic field dependence measurements we extract a g-factor for each of these sub-bands. We discuss the various factors related to spin-resolved transport in these devices. Acknowledgements: We gratefully acknowledge financial support from the following agencies and grants: AFOSR (FA9550-10-1-0524 and FA9550-12-1-0268), NSF (DMR-1124131 and DMR-1104191), AFOSR FA9550-12-1-0342 (CBE), and DMR-1234096 (CBE).

Quantized conductance through quantum point contacts in LaAlO$_3$/SrTiO$_3$ nanowires


Quantized conductance through quantum point contacts in LaAlO$_3$/SrTiO$_3$ nanowires

ANIL ANNADI, SHICHENG LU, GUANGLEI CHENG, MICHELLE TOMCZKYK, MENGCHEN HUANG, Department of Physics and Astronomy, University of Pittsburgh, HYUNGWOO LEE, SANGWOO RYU, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — Abstract: Scaling of electronic device density is key for any material system to be considered as potential for electronics, which demands ballistic devices at the nanoscale. Here we present the investigation of ballistic transport in LaAlO$_3$/SrTiO$_3$ nanowire devices that act as quantum point contacts. In these devices, electron transport shows quantized conductance up to 3rd sub-band energy levels. We also observe odd integer conductance in the units of $e^2/h$ at high magnetic fields, further indicating spin-resolved quantum transport. We analyze the strength of the Zeeman spin-splitting for various sub-bands induced by magnetic field, where 1D sub-bands show a linear Zeeman splitting for out of plane magnetic field. From the transconductance and magnetic field dependence measurements we extract a g-factor for each of these sub-bands. We discuss the various factors related to spin-resolved transport in these devices. Acknowledgements: We gratefully acknowledge financial support from the following agencies and grants: AFOSR (FA9550-10-1-0524 and FA9550-12-1-0268), NSF (DMR-1124131 and DMR-1104191), AFOSR FA9550-12-1-0342 (CBE), and DMR-1234096 (CBE).

Analysis of local conductance switching by AFM-writing at the LaAlO$_3$/SrTiO$_3$ interface

MARGHERITA BOSELLI, DANFENG LI, WEI LIU, ALEXANDRE FÉTE, STEFANO GARIGLIO, JEAN-MARC TRISCONE, DQMP, University of Geneva — A two dimensional electron liquid is present at the interface between LaAlO$_3$ and SrTiO$_3$; this system exhibits several interesting physical properties, including tunable superconductivity. In heterostructures with 3 unit cells of LaAlO$_3$, an insulator to metal transition can be induced by the electric field effect. We report here on the use of the atomic force microscopy writing technique developed in the group of J. Levy [1] to locally switch on and off conductivity at the interface. Our results show that a quatz resonator AFM sensor is particularly suitable for this purpose. In this configuration, the measurements can be performed in the dark, strongly reducing photo-doping. Electronic nanostructures are found to be particularly sensitive to the writing procedure and to the ambient humidity. We discuss how these parameters can be optimized to confine electrons in regions down to tens of nanometers. Simulations of the conductance changes upon AFM writing are compared to experiments. The temperature evolution of the conductance shows that nanowires are metallic.


Anisotropic superconducting properties of nanowires at the LaAlO$_3$/SrTiO$_3$ (110) interface

PATRICK IRVIN, MENGCHENG HUANG, ANIL ANNADI, GUANGLEI CHENG, JEREMY LEVY, University of Pittsburgh, KALON GOPINADHAN, THIRUMALAI VENKATESAN, ARIANDO ARIANDO, National University of Singapore — The superconducting properties of nanowires created on anisotropic SrTiO$_3$ (110) surfaces were investigated. Nanowires are created using conductive AFM (c-AFM) lithography at the LaAlO$_3$/SrTiO$_3$ (110) interface along the (001) and (110) crystallographic directions. In these devices we observe anisotropic superconductivity. The upper critical magnetic field along the (001) and (110) directions are found to be markedly different with a superconducting dome that is shifted for the two orientations. These observations can be explained by anisotropic orbital binding of Ti and O atoms or the differences in the spin-orbit coupling along the two different directions.

1We gratefully acknowledge support for this work from NSF (DMR-1124131, DMR-1104191), AFOSR (FA9550-12-1-0057, FA9550-12-1-0268), and CRP-NRF (Tailoring Oxide Electronics).

One-dimensional Quantum Wire Formed at the Boundary Between Two Insulating LaAlO$_3$/SrTiO$_3$ Interfaces

ALON RON, Tel Aviv University, YORAM DAGAN, Tel Aviv Univ — We grow a tiled structure of insulating two dimensional LaAlO$_3$/SrTiO$_3$ interfaces composed of alternating one and three LaAlO$_3$ unit cells. The boundary between two tiles is conducting. At low temperatures this conductance exhibits quantized steps as a function of gate voltage indicative of a one dimensional channel. The step size of half the quantum of conductance is an evidence for absence of spin degeneracy.
10:24AM L13.00011 Metal-insulator transition in nanostructured SrTiO$_3$/LaAlO$_3$\textsuperscript{1} — HOULONG ZHUANG, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, VALENTINO R. COOPER, Materials Science and Technology Division, ORNL, P. GANESH, Center for Nanophase Materials Sciences, ORNL, HAIXUAN XU, Department of Materials Science and Engineering, The University of Tennessee, Knoxville, P. R. C. KENT, Computer Science and Mathematics Division; Center for Nanophase Materials Sciences, ORNL — It is well known that an insulator-to-metal transition occurs at SrTiO$_3$/LaAlO$_3$ epitaxial heterostructures when the number of LaAlO$_3$ layers reaches a critical value of four. With first-principles calculations, we show that instead of requiring the threshold number of layers to trigger metallicity, the so-called 1+2 overlayer heterostructure also exhibits metallic states. Interestingly, we demonstrate that these metallic states form a two-dimensional electron gas at the overlayer heterostructure. We understand that these fascinating phenomena originate from a modified “polar catastrophe” model, where the overlayer heterostructure accumulates an electrostatic potential more rapidly than regular heterostructures, leading to the reduction of number of LAO layers. Using this model, we further show that the thinner 1+1 overlayer heterostructure exhibits a similar 2DEG. Our work provides a novel approach of inducing 2DEGs in oxide heterostructures, which are beneficial for modern electronics applications.

\textsuperscript{1}HZ, PRCK, VRC and PG were sponsored by the LDRD at ORNL for the U.S. DOE and HX by the University of Tennessee JDRD and UT/ORNL-JIAM programs.

10:36AM L13.00012 Nanoscale Electrostatic Confinement at Oxide Interfaces — SRIJIT GOSWAMI, EMRE MULAZIMOGLU, LIEVEN VANDERSYPEN, ANDREA CAVIGLIA, Delft University of Technology — We develop a robust and versatile platform to define nanostructures at oxide interfaces via patterned top gates. Using LaAlO$_3$/SrTiO$_3$ as a model system, we demonstrate controllable confinement of electrons to nanoscale regions in the conducting interface. The excellent gate response, ultra-low leakage currents, and long term stability of these gates allows us to perform a detailed study of devices in a split-gate geometry. Electrical transport through such devices displays a distinct threshold associated with depletion directly below the gates, resulting in the formation of a narrow conducting channel even at room temperature. We examine the effects of cross-talk between the gates, and also show that a combination of top gates and back gate can be used to efficiently modulate charge transport through these nanostructures.

10:48AM L13.00013 Lateral probing of the LaAlO$_3$/SrTiO$_3$ two-dimensional electron liquid\textsuperscript{1} — M.P. STEHNO, A.E.M. SMINK, H. HILGENKAMP, A. BRINKMAN, MESA+ Institute for Nanotechnology, University of Twente, The Netherlands — The 2-dimensional electron liquid (2DEL) at the interface between the insulating oxides lanthanum aluminate and strontium titanate (LAO/STO) has a complex band structure and hosts novel electronic phases with magnetism and superconductivity. Electrical characterization of the 2DEL has focused mainly on magnetotransport in films or confined geometries, and on z-axis tunneling. We contacted the LAO/STO interface laterally and obtained a gate-tunable barrier between the 2DEL and the metallic electrode. Features in the differential conductance spectra are spaced by energies similar to the confinement energy at the oxide interface and may thus yield information on the (sub-) band structure of 2DEL and barrier region.

\textsuperscript{1}This research was supported by the Dutch NWO and FOM foundations.

Wednesday, March 4, 2015 8:00AM - 11:00AM — Session L14 DMP FIAP: Focus Session: Dopants and Defects in Group IV Semiconductors

8:00AM L14.00001 BSE calculations of color center defects in diamond\textsuperscript{1} — S. VIMOLCHALAO, U. of Washington, W.H. LIANG, UC Merced, F.D. VILA, J.J. KAS, J.J. REHR, U. of Washington, F. FARGES, Muséum National d’Histoire Naturelle, Paris — Colored diamonds are both of fundamental and commercial interest. Several recent efforts have focused on determining the origin of their colors. For example, experiments show that the color of blue diamonds is associated with isolated boron impurities\textsuperscript{2}, while nitrogen impurities are responsible for yellow diamonds. It has previously been shown\textsuperscript{3} that theoretical Bethe-Salpeter Equation (BSE) simulations of boron-doped diamond yield a dark-blue diamond in good agreement with that observed. However, the structure of the nitrogen defects is not well understood. Here we present BSE calculations of the optical response of nitrogen-doped diamonds using relaxed 64-atom unit cells. We focus on N$_{Vb}$ defect sites, where $x$ is the number of substitutional nitrogen atoms and $y$ is the number of carbon vacancies. We find that the most likely candidates are the N$_x$V$_y$ and N$_{Vb}$ defects, which show absorption in the 2.5-3.2 eV range, consistent with yellow color. Our results also rule out the N$_{Vb}$ and N$_x$V$_y$ defect types as possible yellow centers.

\textsuperscript{1}Supported by DOE grant DE-FG03-97ER45623.
\textsuperscript{3}F.Farges et al., Europhysics News 43, 20 (2012).

8:12AM L14.00002 Structure and electronic properties of nanodiamond and its fluorination effect, KAZUYUKI TAKAI, KENTA KOGANE, Hosei University, HIDEKAZU TOUHARA, YOSHIIYUKI HATTORI, Sinshu University — Fluorination of nano-sized diamond (ND) is expected not only to stabilize the surface structure, but also to introduce functional groups on the surface, the conduction carriers, and so on. In this study, we evaluate the structure and magnetic properties of ND and fluorinated ND (FND) in order to consider the change in the electronic state and the surface structure by fluorination. Fluorination of ND was carried out by the direct reaction between gaseous fluorine (1 atm) and commercially available detonation diamond at 623 — 873 K. X-ray Diffraction study reveals the structural stability of core part of ND during fluorination. X-ray photoemission spectroscopy exhibits F1s peak at the lower binding energy region than that for physisorbed molecular fluorine, indicating the formation of the chemical bonding between C and F in the sample. The Electron Paramagnetic Resonance results suggest that fluorination induces not only changes in the surface structure but also relaxation of defects in the core part.

8:24AM L14.00003 Determine the number of nitrogen vacancy color centers in the nanodiamond particles with large size difference, JUI-HUNG HSU, National Sun Yat-sen University, LONG-JYUN SU, HUAN-CHENG CHANG, Academia Sinica — The number of emitters in a nano-particle is usually determined by the photon correlation using the Hanbury Brown and Twiss configuration. However, limited to the photon statics, this method is only valid for the small numbers. It would be difficult to measure the number of emitters, if individual nano-particles contain more than several tens or hundreds of emitters. In this contribution, we present a work to quantitatively determine the number of nitrogen-vacancy (NV) centers in the individual nano-diamond (ND) particles. Our previous work (nanotechnology 24, 315702) suggests that the density of NV centers would be significantly decreased while reducing ND particle size from 100 nm to 30 nm. It thus motivates us to measure the number of NV centers of individual ND particles with large size difference. Under saturated the pulse excitation, the emission intensity from individual ND particle is proportional to the number of NV centers and the fluorescence quantum yield, which are able to be determined independently.
8:36AM L14.00004 Designing shallow donors in diamond1
1. JONATHAN MOUSSA, Sandia National Laboratories — The production of n-type semiconducting diamond has been a long-standing experimental challenge. The first-principles simulation of shallow dopants in semiconductors has been a long-standing theoretical challenge. A desirable theoretical goal is to identify impurities that will act as shallow donors in diamond and assess their experimental viability. I will discuss this identification process for the LiN4 donor complex. It builds a scientific argument from several models and computational results in the absence of computational tools that are both trustworthy and computationally tractable for this task. I will compare the theoretical assessment of viability with recent experimental efforts to co-dope diamond with lithium and nitrogen. Finally, I discuss the computational tools needed to facilitate future work on this problem and some preliminary simulations of donors near diamond surfaces.

1Sandia National Laboratories is a multi-program lab managed and operated by Sandia Corp., a wholly owned subsidiary of Lockheed Martin Corp., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:12AM L14.00005 Carbon-antisite vacancy defect in 4H silicon carbide for realizing solid state qubit1
1. ADAM GALI, KRISZTIAN SZASZ, VIKTOR IVADI, Wigler Research Centre for Physics, Hungarian Academy of Sciences, IGOR ABRIKOSOV, Linköping University, MICHEL BOCKSTETDE, University of Erlangen-Nürnberg, ERIK JANZEN, Linköping University — Dopants in solids are promising candidates for implementations of quantum bits for quantum computing. Silicon carbide (SiC) with engineered point defects is considered as very promising material for the next generation devices, with applications ranging from electronics and photonics to quantum computing. Employing density functional theory and many body perturbation theory, we show that the neutral carbon antisite-vacancy pair (CAV) has high spin ground state, and that its spin may be coherently manipulated by optical excitation in n-type 4H SiC. As the positively charged CAV defect in 4H SiC has been recently engineered to act as single photon source [1], our finding brings a hope that optically addressed quantum bits can be realized by the neutral CAV defects in 4H SiC, and provide an additional target for researchers seeking for solid state single color centers for quantum information processes and metrology. The calculated zero-phonon line of the optically excited state is about 1550 nm (0.8 eV) which perfectly fits to the telecom wavelengths, that makes this qubit candidate very promising for integration of quantum optics devices with existing fiber optics technology. [1] S. Castelletto et al., Nature Materials, 13, 151-156 (2014)

9:24AM L14.00006 Determining exact location of Group V dopants below the Si(001):H surface from scanning tunnelling spectroscopy and density functional theory1
1. VERONIKA BRAZDOVA, KITIPHAT SINTHITHARAKOON, PHILIPP STUDER, DAVID R. BOWLER, ADAM RAHNEJAT, NEIL J. CURSON, STEVEN SCHOFIELD, ANDREW J. FISHER, University College London — Group V impurities in silicon provide a way to tailor properties of electronic materials. The magnetically quiet environment that silicon provides for the impurity spins has also led to new applications in coherent quantum devices. In both the ultimate classical devices and in future quantum computers the exact position of the dopants near surfaces and interfaces will determine the functionality: the ability to control and monitor those positions is key in these technologies. We precisely determine the substitutional sites of neutral As dopants that lie between 4.2 A and 15.0 A below the hydrogenated Si(001) surface, using a combination of density functional theory and low-temperature scanning tunnelling microscopy. We describe the interaction of the donor-electron state with the surface.

1Supported by the EPSRC grant COMPASSS

9:36AM L14.00007 Towards bipolar atomic scale dopant devices defined by STM-lithography1
1. ANDREAS FUHRER, SIGRUN KOSTER, NIKOLA PASCHER, IBM Research – Zurich, Säumerstrasse 4, 8803 Rüschlikon — Dopant device fabrication with hydrogen resist lithography has been demonstrated only for n-type dopants. The reason for this is the ease with which phosphorus can be incorporated and activated after gas phase doping with phosphine. Specifically, incorporation on the silicon (001) surface can be achieved at 350°C while keeping the hydrogen resist intact and thus avoiding surface diffusion of the dopants. Here, we present new results on p-type δ-doping of silicon, towards the fabrication of bipolar dopant devices with hydrogen resist lithography. Using diborane as a gas-phase dopant source, Hall bar devices were fabricated to extract hole densities and mobilities in cryogenic magnetooptical transport experiments. Furthermore, the dependence of these parameters on diborane dose and dopant activation temperatures is investigated. We find that gas-phase doping with diborane is compatible with hydrogen resist lithography and dopant structures can be patterned using the STM. However, activation of the boron dopants currently still leads to significant diffusion and therefore blurring of the patterned devices. We will discuss the prospects of further optimising this and present a possible path forward towards bipolar atomic scale device fabrication with the STM.

1Support from EU grants PAMS, SiSpin, SiAM and from Swiss NCCR QST is gratefully acknowledged

9:48AM L14.00008 Suppressed Complete Ionization of Shallow Donors in Germanium1
1. JOSE MENENDEZ, CHI XIU, CHARUTHA SENARATNE, JOHN KOUVETAKIS, Arizona State Univ — For doping levels Nd > 10¹⁷ cm⁻³, an elementary analysis demonstrates that shallow donors should not be completely ionized in germanium at room temperature. The predicted degree of incomplete ionization (I.I.) represents a fundamental limitation in the quest for ultra-low sheet resistances, as required in Ge-based nMOS devices. Unfortunately, the experimental verification of the predictions is made difficult by the possible presence of inactive dopants, which also lead to free carrier concentrations n < Nd. In this work, we prepared n-type Ge films on Ge-buffered Si substrates using novel synthetic approaches that are expected to minimize the presence of inactive dopants. Higher-order germanes (Ge₂H₆ and Ge₃H₁₀) were used as the source of Ge for growth at low temperatures. Phosphorus atoms were furnished via P(MH₂)₃ (M = Ge, Si) compounds in which the P atom is already bonded to three group-IV atoms in a way that is expected to promote substitutional incorporation. Spectroscopic ellipsometry and SIMS were used to determine n and Nd, respectively. The results indicate no observable I.I. Within experimental error, n ≈ Nd in contradiction with the elementary theory. These findings are compatible with the model developed by Altermatt et al. to explain I.I. phenomena in silicon.

1Supported by DOD AFOSR FA9550-12-1-0208 and DOD AFOSR FA9550-13-1-0022

10:00AM L14.00009 Band Structure and Optical Properties of Dilute Ge:C Alloys1
1. CHAD STEPHENSON, WILLIAM O'BRIEN, MENG QI, Department of Electrical Engineering, University of Notre Dame, MICHAEL PENNINGER, WILLIAM SCHNEIDER, Department of Chemical and Biomolecular Engineering, University of Notre Dame, MIIRIAM GILLET-KUNNATH, JAROSLAV ZAJICEK, Department of Chemistry and Biochemistry, University of Notre Dame, MARK WISTEY, Department of Electrical Engineering, University of Notre Dame — The last major missing piece to achieving integrated Si photonics is an efficient light emitter. Dilute Ge:C alloys offer a new route to create efficient lasers directly within conventional CMOS electronics. Although neither Ge nor C emits light, Ge:C is a highly mismatched alloy, similar to GaAsN, in which band anticrossing is expected to create a direct bandgap. We have performed ab initio band structure simulations using hybrid functionals and spin-orbit coupling that show a sharp decrease in bandgap at the direct conduction band valley with C incorporation, turning Ge:C into a direct bandgap semiconductor and even a semi-metal. We report on the optical properties, highlighting the strength of free carrier absorption due to the changes in the band structure. Some of its potential applications include integrated light emitters, modulators, and photodetectors. With the three-band system, Ge:C also has potential for use in upconverting structures. We also report successful incorporation of C in Ge using hybrid gas-solid source molecular beam epitaxy (MBE) using a precursor gas, tetra(germyl)methane (4GeMe), that prevents undesirable C-C bonds and interstitial incorporation.
10:12AM L14.00010 GeSn pin diodes: from pure Ge to direct-gap materials\textsuperscript{1}, JAMES GALLAGHER\textsuperscript{2}, CHARUTHA SENARATNE\textsuperscript{1}, CHI XU\textsuperscript{1}, TOSHIHITO AOYI\textsuperscript{1}, JOHN KOUVETAKIS\textsuperscript{1}, JOSE MENENDEZ\textsuperscript{1}, Arizona State Univ — Complete n−i−p Ge\textsubscript{1−y}Sn\textsubscript{y} diode structures (y=0-0.09) were fabricated on Si substrates with Sn concentrations covering the entire range between pure Ge and direct-gap materials. The structures typically consist of a thick (＞1 \(\mu\)m) \(n+p\) Ge buffer layer grown by Gas Source Molecular Epitaxy using Ge\textsubscript{1−x}H\textsubscript{x} and either P(SiH\textsubscript{4})\textsubscript{3} or P(GeH\textsubscript{3})\textsubscript{3}, followed by a GeSn intrinsic layer (≈500 nm), grown by Chemical Vapor Deposition (CVD) using Ge\textsubscript{3}H\textsubscript{8} and SnD\textsubscript{4}, and a GeSn \(p\)-type top layer (≈200 nm) grown by CVD using Ge\textsubscript{3}H\textsubscript{4}, SnD\textsubscript{4} and B\textsubscript{2}H\textsubscript{6}. Temperature-dependence of the \(I−V\) characteristics of these diodes as well as the forward-bias dependence of their electroluminescence (EL) signal were investigated, making it possible for the first time to extract the compositional dependence of parameters such as band gaps, activation energies, and dark currents. The EL spectra are dominated by direct-gap emission, which shifts from 1.59 nm to 2.30 nm, in agreement with photoluminescence results.

\textsuperscript{1}DOD AFOSR FA9550-12-1-0208 and DOD AFOSR FA9550-13-1-0022

Department of Physics
Department of Chemistry and Biochemistry
Department of Physics
LeRoy Eyring Center for Solid State Science
Department of Chemistry and Biochemistry
Department of Physics

10:24AM L14.00011 Doping and strain dependence of the electronic band structure in Ge and GeSn alloys\textsuperscript{1}, CHI XU, JAMES GALLAGHER, CHARUTHA SENARATNE, CHRISTOPHER BROWN, Arizona State Univ,NALIN FERNANDO, STEFAN ZOLLNER, New Mexico State Univ, JOHN KOUVETAKIS, JOSE MENENDEZ, Arizona State Univ — A systematic study of the effect of dopants and strain on the electronic structure of Ge and GeSn alloys is presented. Samples were grown by UHV-CVD on Ge-buffered Si using Ge\textsubscript{3}H\textsubscript{8} and SnD\textsubscript{4} as the sources of Ge and Sn, and B\textsubscript{2}H\textsubscript{6}/P(GeH\textsubscript{3})\textsubscript{3} as dopants. High-energy critical points in the joint-density of electronic states were studied using spectroscopic ellipsometry, which yields detailed information on the strain and doping dependence of the so-called \(E_1\), \(E_1 + \Delta_1\), \(E_0\) and \(E_2\) transitions. The corresponding dependencies of the lowest direct band gap \(E_0\) and the fundamental indirect band gap \(E_{ind}\) were studied via \(\mu\)-room-T photoluminescence spectroscopy. Of particular interest for this work were the determination of deformation potentials, band gap renormalization effects, Burstein-Moss shifts due to the presence of carriers at band minima, and the dependence of other critical point parameters, such as amplitudes and phase angles, on the doping concentration. The selective blocking of transitions due to high doping makes it possible to investigate the precise \(k\)-space location of critical points. These studies are complemented with detailed band-structure calculations within a full-zone \(k\)-dot-\(p\) approach.

\textsuperscript{1}Supported by AFOSR under DOD AFOSR FA9550-12-1-0208 and DOD AFOSR FA9550-13-1-0022

10:36AM L14.00012 First-principles Study of the NiGe/Ge Schottky Barrier Height under Dopant Segregation\textsuperscript{1}, CHIANG-YUAN LIN, Department of Electronics Engineering and Institute of Electronics, National Chiao Tung University, HAN-CHI LIN, R&D, Taiwan Semiconductor Manufacturing Company — Traditional Si-based MOSFETs are approaching its fundamental scaling limits, and Ge has been comprehensively explored as a potential channel material to replace Si due to its high intrinsic carrier mobility for further performance enhancement. Nevertheless, strong Fermi-level pinning near the valence band edge of Ge leads to high electron Schottky barrier height. Dopant segregation technique has been proposed to achieve shallower junction depth and heavier dopant concentration for NiGe/Ge. However, the role of dopants at the NiGe/Ge interface is not clear. In this study, first-principles calculations are employed to nail down the most stable dopant position and to obtain the physical Schottky barrier height (by HSE06 hybrid functional) of the NiGe/Ge contact. For the conventional n-type dopant such as phosphorous and arsenic, our calculations show that those two elements may be segregated at the interface, while the reduction of the Schottky barrier height is insignificant. This implies that the experimental improvement of the NiGe/n-type Ge junction by dopant are mainly attributed to the increased dopant concentration around the interface.

\textsuperscript{1}The authors acknowledge financial support from the Taiwan Ministry of Science and Technology (under Grant No. MOST 103-2112-M-009-004-).
8:12AM L15.00002 Ellipsometric Study of NbO$_2$ Grown by MBE on LSAT from 77 to 800 K †
T.N. NUNLEY, S. ZOLLNER, NMSU, T. HADAMEK, A.B. POSADAS, A. O’HARA, A.A. DEMKOV, UT Austin — NbO$_2$ is a transition metal oxide that has been of interest for several decades. Like other complex oxides it has a metal-insulator transition provoked by external stimuli such as temperature, pressure, and electric fields. Our study shows the dielectric function of NbO$_2$ grown by molecular beam epitaxy, optical axis in-plane, on (LaAlO$_3$)$_{0.3}$(Sr$_2$TiAlO$_6$)$_{0.7}$ (LSAT) substrates. The ellipsometric angles were measured from 0.76 to 6.52 eV using a UV/VIS variable-angle spectroscopic ellipsometer and from 250 to 1200 cm$^{-1}$ using an FTIR ellipsometer. By using regression analysis we modeled our optical spectra with one model over the entire range from the mid-infrared to the near UV. For the LSAT substrate, we used optical constants from a previous study. A sum of Tauc-Lorentz oscillators describes the dielectric function of the NbO$_2$ film. We have measured the dielectric function of the sample from 77-800 K. This has allowed us to see that the absorption peaks sharpen/broaden with decreasing/increasing temperature. We have also plotted the direct and indirect band gaps as a function of temperature.

8:24AM L15.00003 Lyddane-Sachs-Teller Analysis of Electronic Transitions†
WILLIAM KARSTENS, Saint Michaels College, DAVID Y. SMITH, University of Vermont and Argonne National Laboratory — We have explored the use of the Lyddane-Sachs-Teller (LST) relation for analysis of electronic optical spectra. This relation originated in the theory of IR lattice absorption and, in analogy with the high IR reflectivity of polar crystals, we demonstrate a substantial region of almost-metallic UV reflectivity above the fundamental electronic absorption in selected solids; it is especially pronounced in group IV elements. This electronic Reststrahlen is terminated by a well-defined longitudinal plasmon and may be understood within LST theory. The original LST formulation neglects dissipation; we show it reflects the geometric symmetry of a normalized dispersion curve based on relative frequencies and polarizabilities. If dissipation is included, absorption widths enter only in second order, so the original LST relation applies to optical spectra that can be approximated by the Lorentz model. The Kramers-Kronig based moments formulation of Noh and Sievers [1] holds generally. The normalized curve is specified by a single strength parameter that may be used as an approximate index to characterize optical response. The dielectric response of covalent semiconductors will be discussed as examples of the LST relation and the dependence of energy-loss spectra on electronic properties. [1] T. W. Noh and A. J. Sievers, Phys. Rev. Lett. 63, 1800 (1989).

8:36AM L15.00004 Correlation between heavy-hole and light-hole Mahan Excitons in a two-dimensional electron gas†
J. PAUL, P. DEY, C.E. STEVENS, Dept. of Physics, University of South Florida, Tampa, Florida 33620, USA, T. TOKUMOTO, Dept. of Physics, University of Alabama at Birmingham, Birmingham, Alabama 35294, USA, J.L. RENO, CINT, Sandia National Laboratories, Albuquerque, New Mexico 87185, USA, D.J. HILTON, Dept. of Physics, University of Alabama at Birmingham, Birmingham, Alabama 35294, USA, D. KARAISKAJ, Dept. of Physics, University of South Florida, Tampa, Florida 33620, USA, D. J. HILTON COLLABORATION, J. L. RENO COLLABORATION — We present the coherent two-dimensional Fourier transform (2DFT) spectra of Mahan Excitons associated with the heavy-hole and light-hole resonances observed in a modulation doped GaAs/AlGaAs single quantum well. These resonances are observed to be strongly coupled through many-body interactions. The 2DFT spectra were measured using co-linear, cross-linear, and co-circular polarizations and reveal striking differences. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

8:48AM L15.00005 Optical Properties of LaVO$_3$ and YTiO$_3$\footnote{Supported in part by the US Department of Energy, Office of Science, Office of Nuclear Physics under contract DE-AC02-06CH11357}
JOHN COULTER, EFSTRATIOS MANOUSAKIS, Florida State University & NHMFL — Motivated by recent experimental efforts to fabricate p-n junctions from transition metal oxides (TMOs) and recent theoretical and computational work illustrating that strongly correlated insulators can produce more than one electron-hole pair from a single solar photon through impact ionization, we study the optical properties of LaVO$_3$ and YTiO$_3$ by \textit{ab initio} methods. We apply the Bethe-Salpeter equations (BSE) to calculate the optical properties, starting from quasi-particle energy levels and states found at the level of the GW approximation. We present comparisons of the exciton binding energy to experimental data. We examine the extent to which these materials might be promising for efficient carrier multiplication, as has been shown previously in VO$_2$.

9:00AM L15.00006 FT-IR and Raman Spectroscopic Study of Cobalt Oxides, YANG LI, FAN QIN, WENLAN QIU, Department of Electrical and Computer Engineering, University of Houston, HUI FANG, Department of Physics, Sam Houston State University, VIKTOR G. HADJIEV, Texas Center for Superconductivity and Department of Mechanical Engineering, University of Houston, DMITRI LITVINOV, JIMING BAO, Department of Electrical and Computer Engineering, University of Houston — Fourier transform infrared (FTIR) and Raman spectroscopy are studied on cobalt monoxide (CoO) and cobalt dicobalt oxide (Co$_3$O$_4$) in the presented work. We can experimentally detect the transverse and longitudinal optical modes of Co$_3$O$_4$ using transmittance and diffuse reflectance (DRIFTS) spectra in FTIR, which showed good agreement with theoretical calculation. DRIFTS results also proved that Co$_3$O$_4$ with smaller particle size will lead to an increase in the LO-TO ratio. During the oxidation process from CoO to Co$_3$O$_4$, this ratio is gradually raised. CoO can be identified with a broad band near 500cm$^{-1}$. For the first time, we clearly demonstrate that Co$_3$O$_4$ exhibits only the second order Raman scattering near 1070cm$^{-1}$ at room temperature and ambient pressure (excited by 473nm laser).

9:12AM L15.00007 Infrared magneto-spectroscopy of narrow bandgap metamorphic InAs$_{1-x}$Sb$_x$†
JONATHAN LUDWIG, Florida State University and National High Magnetic Field Laboratory, S. SUCHALKIN, State University of New York at Stony Brook, Y. JIANG, School of Physics, Georgia Institute of Technology, G. KIPSHIDZE, Y. LIN, L. SHTERENGAS, S. LURYI, G. BELENKY, State University of New York at Stony Brook, D. SMIRNOV, National High Magnetic Field Laboratory — Metamorphic InAsSb alloys are a promising narrow gap semiconductor with bandgaps as low as 0.12eV, corresponding to approximately 10um, much smaller eithe InAs or InSb. The effect of bowing on the reduction in the bandgap over its binary counterparts is not completely understood. Here, we report on the systematic low-temperature infrared magneto- absorption study of a series of InAs$_{1-x}$Sb$_x$ layers with varying Sb concentration performed in magnetic fields up to 17.5 T. Several cyclotron resonance series, including interband transitions, are observed. These results allow us to extract and compare the bowing coefficients for the effective mass and bandgap.
Magnetic Field-Induced Direct-Indirect Bandgap Crossover in Al\textsubscript{1-x}Ga\textsubscript{x}As

KIRSTIN ALBERI, ALEKSEJ MIALITSIN, BRIAN FLUEGEL, National Renewable Energy Laboratory, SCOTT CROOKER, National High Magnetic Field Lab, Los Alamos National Laboratory, ANGELO MASCARENHAS, National Renewable Energy Laboratory — Determining the exact alloy composition and energy at which a direct-indirect bandgap crossover occurs in semiconductor alloys is important for engineering optoelectronic materials. However, some amount of error is usually introduced when establishing the crossover from the extrapolation of the direct and indirect bandgap energy trends measured with a discrete set of alloyed samples. We use high magnetic fields up to 58 T to induce the crossover in a single Al\textsubscript{1-x}Ga\textsubscript{x}As sample, thereby allowing us to precisely identify the crossover energy at low temperature \cite{1}. The onset of the crossover is marked by a reduction in the photoluminescence peak energy and the emergence of an asymmetric peak lineshape resulting from the competition between the radiative lifetime and carrier migration times in the indirect regime. Analysis of the lineshape progression through the crossover confirms that the crossover can be classified as an alloy disorder broadened, first order phase transition. \cite{1} K. Alberi, et al, Appl. Phys. Express, 7, 111201 (2014)

Transient Infrared Studies of Carrier Injection Effects on the Reststrahlen Band of SiC

BRYAN SPANN\textsuperscript{3}, RYAN COMPTON\textsuperscript{2}, ADAM DUNKELBERGER\textsuperscript{3}, JAMES LONG, Naval Research Laboratory, PAUL KLEIN, Sotera Defense Solutions Inc., JOSH CADOWELL, JEFF OWRUTSKY, Naval Research Laboratory — Sub-diffraction light confinement has led to advances in imaging, metamaterials, and plasmonics among other fields. A phenomenon that can provide sub-diffraction light is the surface phonon polariton (SPhP). SPhPs couple infrared photons with optical phonons. Because SPhPs are coupled directly to phonons, lifetimes can be longer than that of surface plasmon polaritons (SPPs) whose lifetimes are dominated by electron scattering. SiC is one material that exhibits SPhPs. SIC SPhPs are activated by photons with energies near the Reststrahlen band. In this study we investigate aspects of carrier dynamics by photo-injecting free carriers into the SiC conduction band using a pulsed 355 nm pump laser and probe the resulting dynamics near the Reststrahlen band using a tunable CO\textsubscript{2} laser. Variable pump fluences provided free carrier densities of 1x10\textsuperscript{17} to 1x10\textsuperscript{19}. Probing the excited state dynamics near the Reststrahlen band revealed complex transient behavior resulting in positive and negative changes in transient reflectance depending on the photo-injection level and the probe energy. Numerical simulations were carried out to mimic the initial photo-injection level provided by the transient experiment and resulted in qualitative agreement with the experiment.

Lifetime investigations of recombination in CdTe heterostructures using time-resolved photoluminescence

BOBBY L. HANCOCK, CRAIG H. SWARTZ, MADHAVIE EDIRISOORIYA, ELIZABETH B. LEBLANC, O. NORIEGA, P. A. R. D. JAYATHILAKA, OLANREWAJU S. OGEDEGBE, MARK HOLTZ, THOMAS H. MYERS, Texas State University — Free photocarrier lifetimes are critical parameters in semiconductors used in photovoltaics, such as cadmium telluride (CdTe). However, CdTe is historically plagued by short photocarrier lifetimes due to competing non-radiative recombination attributed to surfaces and interfaces. One consequence of this is an elusive lifetime for the bulk material. We report progress in mitigating the effects of surfaces and interfaces using a CdTe/Mg\textsubscript{1-x}Cd\textsubscript{x}Te double heterostructure grown by molecular beam epitaxy. Photocarrier lifetimes are measured using time-resolved photoluminescence (TRPL). Lifetimes as high as 240 ns are measured at room temperature with barriers having approximately \( \alpha = 35\% \). The results of these studies will be presented along with a discussion of the radiative, surface, and interfacial recombination.

1. U. S. Department of Energy (DEAC36-08GO28308 FPACE II Sub. ZEJ-4-2007-0)

Phonon dispersion relations of Sb\textsubscript{2}S\textsubscript{3} and Bi\textsubscript{2}S\textsubscript{3} using the supercell force-constant method

CHEE KWAN GAN, Institute of High Performance Computing, KUN TING EDDIE CHUA, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, USA, YUN LIU, Institute of High Performance Computing — We present a lattice dynamical study on the orthorhombic antimony telluride sulphide (Sb\textsubscript{2}S\textsubscript{3}) \cite{1} and bismuth sulphide (Bi\textsubscript{2}S\textsubscript{3}) \cite{2} using the supercell force-constant method. We find that the slow decay of the interatomic force constants for these compounds in the Pnma setting critically demand the use of a large supercell of \( 2 \times 4 \times 2 \) that consists of 320 atoms. To enable a practical calculation the space group information is fully utilized where only inequivalent atoms within the primitive cell are displaced for the force calculations. The effect ofBorn effective charges is incorporated into the method. We compare our results with that obtained from the density-functional perturbation theory. We found that smaller supercells could lead to unphysical acoustic phonon softening and lifting of the degeneracies along high symmetry directions. Our results provide a proper guideline for the use of the supercell force-constant method: the supercell size must be carefully be tested along with other parameters such as the kinetic energy cutoff, the Brillouin zone sampling or the self-consistent convergence criteria. \cite{1} Y. Liu, K.T.E. Chua, T.C. Sum, and C.K. Gan, PCCP 16 (2014) 345. \cite{2} Y. Zhao, K.T.E. Chua, C.K. Gan, J. Zhang, B. Peng, Z. Peng, and Q. Xiong, Phys. Rev

Temperature dependent band gaps of GeSiSn alloys grown on Ge buffered Si substrates

NALIN FERNANDO, T.N. NUNLEY, S. ZOLLNER, NMSU, C. XU, J. MENENDEZ, J. KOUVETAKIS, ASU — Band gap engineering of Ge by controlling tensile strain and alloying with Si and Sn has attracted great interest. Ge\textsubscript{1-x}Si\textsubscript{x}Sn\textsubscript{y} ternary alloy with two compositional degrees of freedom allows decoupling lattice constant and electronic structures. Hence it is important to determine the temperature and compositional dependence of optical properties of these materials. The complex pseudodielectric functions of Ge films grown on Si(100) and GeSiSn grown on buffered Ge were measured using spectroscopic ellipsometry in the 0.76-6.6 eV energy range between 77-800 K to investigate the E\textsubscript{1} and E\textsubscript{1} + \Delta\textsubscript{1} critical point (CP) energies. CP energies and related parameters were obtained by analyzing the second-derivative \( d^{2}e/d\omega^{2} \) of the dielectric function. Our experimental results are in good agreement with the theoretics. The predicted E\textsubscript{1} CP energy shift of Ge on Si due to strain generated by thermal expansion mismatch. We will discuss the compositional dependence of the E\textsubscript{1} and E\textsubscript{1} + \Delta\textsubscript{1} CP energies of GeSiSn alloys and effects of temperature on shifting CP energies.

9:48AM L15.00010 Lifetime investigations of recombination in CdTe heterostructures using time-resolved photoluminescence

10:00AM L15.00011 Phonon dispersion relations of Sb\textsubscript{2}S\textsubscript{3} and Bi\textsubscript{2}S\textsubscript{3} using the supercell force-

12AM L15.00012 Temperature dependent band gaps of GeSiSn alloys grown on Ge buffered Si substrates

1This work was supported by the DOE Office of Science under contract DE-AC36-08GO28308. The work at LANL was supported by NSF-DMR-1157490 and the State of Florida.

10:12AM L15.00012 Temperature dependent band gaps of GeSiSn alloys grown on Ge buffered Si substrates

NALIN FERNANDO, T.N. NUNLEY, S. ZOLLNER, NMSU, C. XU, J. MENENDEZ, J. KOUVETAKIS, ASU — Band gap engineering of Ge by controlling tensile strain and alloying with Si and Sn has attracted great interest. Ge\textsubscript{1-x}Si\textsubscript{x}Sn\textsubscript{y} ternary alloy with two compositional degrees of freedom allows decoupling lattice constant and electronic structures. Hence it is important to determine the temperature and compositional dependence of optical properties of these materials. The complex pseudodielectric functions of Ge films grown on Si(100) and GeSiSn grown on buffered Ge were measured using spectroscopic ellipsometry in the 0.76-6.6 eV energy range between 77-800 K to investigate the E\textsubscript{1} and E\textsubscript{1} + \Delta\textsubscript{1} critical point (CP) energies. CP energies and related parameters were obtained by analyzing the second-derivative \( d^{2}e/d\omega^{2} \) of the dielectric function. Our experimental results are in good agreement with the theoretics. The predicted E\textsubscript{1} CP energy shift of Ge on Si due to strain generated by thermal expansion mismatch. We will discuss the compositional dependence of the E\textsubscript{1} and E\textsubscript{1} + \Delta\textsubscript{1} CP energies of GeSiSn alloys and effects of temperature on shifting CP energies.
10:24 AM L15.00013 Optoelectronic properties of Ta$_3$N$_5$: A joint theoretical and experimental study$^1$, JULIANA MORBEC, Institute for Molecular Engineering, University of Chicago, USA, IEVA NARKEVICIUTE, THOMAS JARAMILLO, Department of Chemical Engineering, Stanford University, USA, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago, USA — A joint theoretical and experimental study of the optoelectronic properties of Ta$_3$N$_5$ was conducted by means of ab initio calculations and ellipsometry measurements [1]. Previous experimental work on Ta$_3$N$_5$ has not been conclusive regarding the direct or indirect nature of light absorption. Our work found excellent agreement between the optical spectrum computed using the Bethe-Salpeter equation and the measured one, with two prominent features occurring at 2.1 and 2.5 eV assigned to direct transitions between N and Ta states. The computed optical gap, obtained from the $G^0W_0$ direct photoemission gap, including spin-orbit coupling, electron-phonon interaction, and exciton binding energy, was found to be of excellent agreement with measurements. Our results also showed that Ta$_3$N$_5$ is a highly anisotropic material with heavy holes in several directions, suggesting low hole mobilities, consistent with low measured photocurrents in the Ta$_3$N$_5$ literature. Work is in progress to compute polaronic contributions to the hole and electron mobilities and to investigate the effect of substitutional doping on the electronic structure of Ta$_3$N$_5$.

$^1$Work supported by NSF (NSF Center CHE-1305124 for CCI Solar Fuels). Computing resources provided by NERSC.

10:36 AM L15.00014 Electrically Tunable Hot-Silicon Terahertz Attenuator$^1$, MINJIE WANG, Department of Electrical and Computer Engineering, Rice University, ROBERT VAJTAI, PULICKEL AJAYAN, Department of Materials Science and NanoEngineering, Rice University, JUNICHIRO KONO, Department of Electrical and Computer Engineering, Rice University — We have developed a continuously tunable, broadband terahertz attenuator with a transmission tuning range greater than 10$^3$. Attenuation tuning is achieved electrically, by simply changing the DC voltage applied to a heating wire attached to a bulk silicon wafer, which controls its temperature between room temperature and 550 K, with the corresponding free-carrier density adjusted between 10$^{14}$ cm$^{-3}$ and 10$^{17}$ cm$^{-3}$. This 'hot-silicon'-based terahertz attenuator works most effectively at 450–550 K (corresponding to a DC voltage variation of only 7 V) and completely shields terahertz radiation above 550 K in a frequency range of 0.1-2.5 THz. Both intrinsic and doped silicon wafers were tested and demonstrated to work well as a continuously tunable attenuator, but they exhibited slightly different behaviors before a dramatic transmission drop at 450–550 K: intrinsic silicon wafers showed a monotonic transmission decrease with temperature while doped wafers showed a slight increase in transmission before the drop. All behaviors can be understood quantitatively via the free-carrier Drude model taking into account thermally activated intrinsic carriers.

$^1$This work was supported by the National Science Foundation through Grant No. OISE-0968405.

10:48 AM L15.00015 Photoluminescence measurements of high Sn-content Ge$_{1-x}$Sn$_x$ and Ge$_{1-x-y}$Si$_x$Sn$_y$ grown on Ge-buffered Si, YUNG KEE YEO, THOMAS R. HARRIS$^1$, Department of Engineering Physics, Air Force Institute of Technology, Wright-Patterson AFB, OH 45433, USA, BUGUO WANG, Department of Physics, Wright State University, Dayton, OH 45435, USA, MEE-YI KYU, Department of Physics, Kangwon National University, Chuncheon 200-701, Korea, JOHN KOUVETAKIS, Department of Chemistry and Biochemistry, Arizona State University, Tempe, Arizona 85287, USA — The optical properties of newly developed, high Sn-content Ge$_{1-y}$Sn$_y$ and Ge$_{1-x-y}$Si$_x$Sn$_y$ thin films grown on Ge-buffered Si have been characterized using temperature-dependent and laser power-dependent photoluminescence (PL) measurements. The results show two distinct PL peaks related to both the direct (Γ) and indirect (L) bandgap transitions. Furthermore, the measured separation energy between the direct and indirect bandgap related PL peaks for Ge$_{0.945}$Sn$_{0.055}$ sample is only about 30 meV compared to the value of 140 meV for bulk Ge. This study shows a very encouraging result toward producing Ge- and Si-based direct bandgap semiconductors, whose predicted indirect-to-direct bandgap crossover could be near 6% Sn. Clear competition between the two transitions is also observed as a function of temperature and laser power. Overall, this work represents an extensive PL characterization of Ge$_{1-y}$Sn$_y$ and Ge$_{1-x-y}$Si$_x$Sn$_y$ materials over a wide compositional range and should be useful for the development of next-generation optoelectronic devices.

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Wednesday, March 4, 2015 8:00AM - 11:00AM — Session L16 DMP: Focus Session: van der Waals Bonding in Advanced Materials: Molecular Systems and Interfaces 101AB - Noa Marom, Tulane University

8:00AM L16.00001 Effect of Substrate Chemistry on the Adsorption of Olympicene Radical: A vdW inclusive DFT study$^1$, JERONIMO KARA, University of Central Florida, HANAND YILDIRIM, Purdue University, ABDELKADER KARA, University of Central Florida — We investigate the effects of surface chemistry on the adsorption characteristics of the Olympicene radical on Au and Pt(111) surfaces using vdW inclusive density functional theory (DFT) employing the optimized vdW-DF and vdW-DF2 methods. Adsorption characteristics such as adsorption energy, adsorption geometry, electronic structure, charge transfer, and charge redistribution will be presented. The effect of substrate electronic structure on the nature of bonding will be discussed. Comparison on the nature of bonding will be presented with our previously reported results on the adsorption of Olympicene radical on Cu(111) to provide a more complete picture.

$^1$Work supported by the U.S. Department of Energy Basic Energy Science under Contract No DE-FG02-11ER16243

8:12 AM L16.00002 First Principles Investigation of the C3 Coefficients for Molecular Adsorption on Transition Metal Surfaces$^1$, ABDELKADER KARA, JERONIMO MATOS, University of Central Florida, HANAND YILDIRIM, Purdue University — C6 coefficients are used to investigate the strength of the long-range interactions for weakly interacting dimers as a function of separation distance. These coefficients are useful both as a measure for the accuracy of the various van der Waals (vdW) inclusive methods. In the case of molecule-surface interaction, the C3 coefficient is the counterpart to the C6 coefficient that is used for testing the interaction of dimers. We will present the results of the vdW inclusive density functional theory (DFT) calculations evaluating the C3 coefficients for the adsorption of M/X(110) and X(111), with X: Ag, Au, Cu, Pt, Pd, Ni, Rh and M: Benzene, Thiophene, Selenophene, Pentacene and Olympicene, as described by the PBE exchange-correlation functional and the self-consistent vdW-DF, optimized vdW-DFs and vdW-DF2 functionals.

$^1$work supported by the U.S. Department of Energy Basic Energy Science under Contract No DE-FG02-11ER16243
and the Office of Naval Research grants ONR Award # N00014-08-1-0462 and # N00014-12-1-0527.

1 This work was supported by the DOE; computational resources provided by NERSC.

The authors would like to acknowledge the generous financial support from the Defense Threat Reduction Agency (DTRA) Grant # HDTRA1-13-1-0025, and the Office of Naval Research grants ONR Award # N00014-08-1-0462 and # N00014-12-1-0527.

1 This work was supported by the DOE; computational resources provided by NERSC.

8:24AM L16.00003 Phonon dispersion of acene molecular crystals using van der Waals-corrected density functional theory. FLORIAN ALTVAETER, University of California, Berkeley, TONATIUH RANGEL, Lawrence Berkeley National Laboratory, JEFFREY B. NEATON, University of California, Berkeley, Lawrence Berkeley National Laboratory — Acene molecular crystals are interesting testbeds for the study of phenomena relevant to organic optoelectronics, including charge separation and carrier transport. In such processes, scattering from lattice vibrations is an important dissipation mechanism. Despite their central role in dissipation processes, there are few calculations of phonon spectra in acene crystals. Here, we carry out van der Waals-corrected density functional theory calculations of the ground-state structure and phonon band structure of acene molecular crystals, using neutron diffraction data where applicable. We use a finite-differences method, and compare the performance of several approaches — including standard generalized gradient approximations (GGA) such as PBE, PBE plus pair-wise vdW corrections, and vdW density functionals — to experiments for solid naphthalene and pentacene.

8:36AM L16.00004 Probing Molecule-Molecule Interactions Through Atomic Force Spectroscopy. ANDRAS MAGYARKUTI, Department of Applied Physics and Applied Mathematics, Columbia University, COLIN NUCKOLLS, Department of Chemistry, Columbia University, LATHA VENKATARAMAN, Department of Applied Physics and Applied Mathematics, Columbia University — We investigate the role of molecule-molecule interactions at the single-molecule level using a custom high-resolution atomic force microscope (AFM). We perform break-junction measurements using a gold substrate and gold-coated AFM cantilever on a series of methyl-sulfide terminated alkane chains. We measure, simultaneously, two independent quantities for each junction: force and conductance. This gives us insight into junction elongation and rupture processes. We use conductance as a signature of the junction structure and electronic characteristics and use the measured force to understand its mechanical properties. We find that molecular junctions form with one or two molecules bridging the gap between the cantilever and substrate, with the two-molecule junction having roughly twice the conductance of the one-molecule junction. More importantly, we find that the probability to form a two-molecule junction is higher for alkanes with an odd number of carbon atoms indicating that the van der Waals interactions between the two molecules might be important in forming these junctions. We discuss the implications of these results and compare to those obtained for conjugated molecules.

8:48AM L16.00005 Forces and Dynamics in Aromatic Overlayers on Metal Surfaces. SHAFA T MUBIN, KRISTEN FICHTHORN, Pennsylvania State University — Organic thin films have been the subject of intense research because of their suitability for applications in molecular electronics. The beneficial properties of these films are sensitive to the structure of the film. However, predicting and controlling organic thin-film structures is still a significant challenge. Owing to computational requirements, first-principles calculations cannot probe the link between thin-film deposition conditions and film structure. In this talk, we will discuss a multi-scale approach applied to quantify structures and dynamics of a thin film of benzene on Ag(111). Based on first-principles calculations, we developed a force field to describe the interaction of benzene with Ag(111). We applied this force-field to describe several aspects of this system, including its order-disorder phase transition and its desorption kinetics. Despite the apparent simplicity of this vdW dominated system, it exhibits surprising complexity in binding site preference and in ordering, leading to an interesting interplay between pi-conjugated electrons of benzene and surface-state electrons of Ag(111).

9:00AM L16.00006 Quantifying molecule-surface interactions using AFM-based single-molecule manipulation. F.S. TAUTZ, C. WAGNER, R. TEMIROV, N. FOURNIER, M. GREEN, T. ESAT, P. LEINEN, Forschungszentrum Juelich GmbH, Germany, A. GROETSCH, Federal Institute for Occupational Safety and Health, Dortmund, Germany, V.G. RUIZ, A. TKATCHENKO, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany, C. LI, K. MUELLEN, Max-Planck-Institut fuer Polymerforschung, Mainz, Germany, M. ROHFLING, Universitaet Muenster, Germany — Scanning probe microscopy plays an important role in the investigation of molecular adsorption. Promising is the possibility to probe the molecule-surface interaction while tuning its strength through AFM tip-induced single-molecule manipulation. Here, we outline a strategy to achieve quantitative understanding of such manipulation experiments [1]. The example of qPlus sensor based PTCDA molecule lifting experiments is used to demonstrate how different aspects of the molecule-surface interaction, namely the short-range adsorption potential [2], the asymptotic van der Waals potential [3], local chemical bonds which are the source of the surface corrugation [4], and molecule-molecule interactions [5] can be measured with SPM and interpreted by the help of force-field simulations.

9:12AM L16.00007 Many-Body Dispersion Interactions in Molecular Materials. ROBERT A. DISTASIO JR., Princeton University — In this work, we have developed an efficient method for obtaining an accurate theoretical description of van der Waals (vdW) interactions that includes both long-range Coulomb electrodynamic response screening effects as well as treatment of the many-body vdW energy to infinite order. This method goes beyond the standard C_6/R^6 pairwise additive approximation and can easily be coupled to a wide array of theoretical methods, ranging from classical force fields to higher-level quantum chemical calculations. To demonstrate the increasingly important role played by many-body vdW interactions in large, structurally complex molecular systems, we use this method to investigate several pertinent molecular properties, such as binding energies/affinities in gas-phase molecular dimers and supramolecular complexes, relative conformational energetics in small polypeptides, and thermodynamic stabilities among competing molecular crystal polymorphs.

9:48AM L16.00008 Predicting Elastic Properties of β-HMX from First-principles Calculations. QING PENG, ROBERT A. DISTASIO, FLORIAN ALTVAETER, University of California, Berkeley, TONATIUH RANGEL, Lawrence Berkeley National Laboratory, JEFFREY B. NEATON, University of California, Berkeley, Lawrence Berkeley National Laboratory — We investigate the performance of the van der Waals (vdW) functions in predicting the elastic constants of the β-polymorph of cycloctetramethylene tetranitramine (HMX) energetic molecular crystal using density functional theory (DFT) calculations. We confirm that the accuracy of the elastic constants is significantly improved using the vdW corrections with environment dependent C_6 together with PBE and revised PBE exchange-correlation functionals. The elastic constants obtained using PBE-D3(0) calculations yield the most accurate mechanical response of β-HMX, with respect to the experimental stress-strain data. The PBEsol without vdW corrections can also predict the elastic constants well. Our results suggest that PBE-D3 calculations are reliable in predicting the elastic constants of this material.
10:00AM L16.00009 Quantitative bond energetics in atomic-scale junctions with significant van der Waals character, LATHA VENKATARAMAN, Columbia Univ, SRIHARSHA ARADHYA1, Columbia University, Applied Physics, MARK HYBERTSEN, CFN, Brookhaven National Labs. — A direct measurement of the potential energy surface that characterizes individual chemical bonds in complex materials has fundamental significance for many disciplines. Here, we demonstrate that the energy profile for metallic single-atom contacts and single-molecule junctions can be mapped by fitting ambient atomic force microscope measurements carried out in the near-equilibrium regime to a physical, but simple, functional form.[1] In particular we are able to extract bond energies for metal-molecule link bonds in cases where the interaction has significant contribution from nonspecific interactions attributed to van der Waals (vdW) interactions at short length scale in addition to specific donor-acceptor bonds.[2] Our approach significantly expands the quantitative information extracted from these measurements, allowing direct comparisons to density functional theory (DFT) calculations instead of relying on trends in bond rupture forces alone. [1] S.V. Aradhya, A. Nielsen, M.S. Hybertsen, L. Venkataraman, ACS Nano 8, 7522–7530 (2014) [2] S.V. Aradhya, M. Frei, M.S. Hybertsen, L. Venkataraman, Nature Materials, 11, 872-876, (2012)

1Currently at Cornell University

10:12AM L16.00010 Charge transfer from first principles: self-consistent GW applied to donor-acceptor systems , VIKTOR ATALLA, Fritz Haber Institute, Berlin, FABIO CARUSO, University of Oxford, ANGEL RUBIO, Universidad del Pais Vasco, San Sebastián, Spain, MATTHIAS SCHEFFLER, Fritz Haber Institute, Berlin, PATRICK RINKE, Aalto University, Helsinki, Finland — Charge transfer in donor-acceptor systems (DAS) is determined by the relative alignment between the frontier orbitals of the donor and the acceptor. Semi-local approximations to density functional theory (DFT) may give a qualitatively wrong level alignment in DAS, leading to unphysical fractional electron transfer in weakly bound donor-acceptor pairs. GW calculations based on first-order perturbation theory (G0W0) correct the level alignment, but leave unaffected the electron density. We demonstrate that self-consistent GW (scGW) provides an ideal framework for the description of charge transfer in DAS. Moreover, scGW seamlessly accounts for many-body correlations and van der Waals interactions. As in G0W0, the scGW level alignment is in agreement with experimental reference data. However in scGW, also the electron density is treated at the GW level and, therefore, it is consistent with the level alignment between donor and acceptor leading to a qualitatively correct description of charge-transfer properties.

10:24AM L16.00011 Van der Waals Interactions in Aspirin , ANTHONY REILLY, Cambridge Crystallographic Data Centre, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG — The ability of molecules to yield multiple solid forms, or polymorphs, has significance for diverse applications ranging from drug design and food chemistry to nonlinear optics and hydrogen storage. In particular, aspirin has been used and studied for over a century, but has only recently been shown to have an additional polymorphic form, known as form II. Since the two observed solid forms of aspirin are degenerate in terms of lattice energy, kinetic effects have been suggested to determine the metastability of the less abundant form II. Here, first-principles calculations provide an alternative explanation based on free-energy differences at room temperature. The explicit consideration of many-body van der Waals interactions in the free energy demonstrates that the stability of the most abundant form of aspirin is due to a subtle coupling between collective electronic fluctuations and quantized lattice vibrations. In addition, a systematic analysis of the elastic properties of the two forms of aspirin rules out mechanical instability of form II as making it metastable [A. M. Reilly and A. Tkatchenko, Phys. Rev. Lett. 113, 055701 (2014).]

10:36AM L16.00012 Determination of Surface-Substrate Adsorption Energy using the Exchange-Hole Dipole Moment , MATTHEW CHRISTIAN, Univ of California - Merced, ALBERTO OTERO DE LA ROZA, National Institute for Nanotechnology, ERIN JOHNSON, Univ of California - Merced — Calculated surface-substrate binding energies are usually underestimated because conventional density functionals do not include dispersion, which is necessary to capture the van der Waals interactions that lead to weak physisorption. The exchange-hole dipole moment (XDM) model is a non-empirical density-functional approach to model dispersion. Adsorption energies for several aromatic molecules and nucleobases on noble metal surfaces were calculated using B86bPBE-XDM. In this talk, I compare the calculated adsorption energies with experiment and present implications for future applications to modeling surface interactions.


10:48AM L16.00013 Van der Waals Dispersion Interactions and Excited States of Oligoacene Molecular Crystals , TONATIUVIANGELGORDILLO, SAHARSHARIFZADEH, Molecular Foundry, LBNL, KRISTIAN BERLAND, Chalmers University of Technology, Sweden, FLORIAN ALTVATER, Molecular Foundry, LBNL; UC-Berkeley, KYUHO LEE, Molecular Foundry, LBNL, PER HYLDGAARD, Chalmers University of Technology, Sweden, LEEDORONEN, Weizmann Institute of Science, Israel, JEFFREY B. NEATON, Molecular Foundry, LBNL; UC-Berkeley — Molecular crystals are a prototypical class of van der Waals (vdWs)-bound organic materials with novel excited state properties relevant for photovoltaics applications. Predicting the structure and excited state properties of oligoacene crystals presents a challenge for standard density functional theory (DFT), as standard functionals do not have long-range dispersion, and DFT does not yield excited-state properties. In this work, we use a combination of vdW-corrected DFT both pair-wise correction methods and correlation functionals and many-body perturbation theory to study the geometry and excited states of oligoacene crystals. We find that vdWs methods can predict lattice constants up to 1% of the experimental measurements. Low lying excited states computed with MBPT compare well with experiments, and are found to be quite sensitive to geometry. Our study reveals the importance of vdWs dispersion interactions to the determination of excited states; moreover, our work suggests routes for predictive calculations, in which both structures and excited states are calculated entirely from first-principles.

3We thank DOE for external funds, and NERSC for computational resources.

Wednesday, March 4, 2015 8:00AM - 11:00AM — Session L17 DCMP: Graphene: Optical Properties 102AB - Hua Chen, University of Texas at Austin
8:00AM L17.00001 Graphene in Ultrafast and Ultrastrong Laser Pulses1. HAMED KOOCHEK KELARDEH, VADYM APALIKOV, MARK STOCKMAN, Georgia State Univ — We have shown that graphene subjected to an ultrafast (near-single-oscillation pulse) and strong (F ~ 1-3 V/Å) pulse exhibits fundamental behavior dramatically different from both insulators and metals. In such an ultrafast and ultrastrong field, the electron dynamics is coherent, in contrast to relatively long pulses (τ > 100 fs) where the electron’s dephasing becomes important leading to incoherent dynamics. Electron transfer from the valence band (VB) to the conduction band (CB) is deeply irreversible i.e., non-adiabatic, in which the residual CB population (after pulse ends) is close to the maximum one. The residual CB population as a function of wave vector is nonuniform with a few strongly localized spots near the Dirac points, at which the CB population is almost 100%. Furthermore, it is shown the direction of charge transfer depends on the pulse amplitude. Namely, at small pulse amplitude, <1V/Å, the charge is transferred in the direction of the pulse maximum (positive transferred charge), while at large amplitude, >1 V/Å, it is in opposite direction of the pulse maximum (negative transferred charge). Consequently, in terms of charge transport, graphene at small pulse intensities behaves as a dielectric while at large intensities acts as a metal. These femtosecond currents and charge transfer in graphene may provide fundamental basis for detection and calibration of ultrashort intense laser pulses and are promising for petahertz information processing.

3This work was supported by U.S. Office of Naval Research No.N00014-13-1-0649 and NSF Grant No.ECCS-1308473.

8:12AM L17.00002 Giant mid-infrared Kerr enhancement from films on SiC1. ALOK MUKHERJEE, M. MURAT ARIK, State Univ of NY - Buffalo, CHASE T. ELLIS, Electronics Science & Technology Division Code 6800, U.S. Naval Research Laboratory, Washington, DC, USA., PAYAM TAHERI, ANDREAS V. STIER, MYOUNG HWAN KIM, HAO ZENG, JOHN CERNE, State Univ of NY - Buffalo, JOSEPH G. TISCHLER, EVAN R. GLASER, RACHEL L. MYERS WARD, JOSEPH L. TEDDSCO, CHARLES R. EDDY JR, D. KURT GASKILL, Electronics Science & Technology Division Code 6800, U.S. Naval Research Laboratory, Washington, DC, USA., YU LIU, SHUNCHONG WANG, GANG WANG, Institute of Physics, Chinese Academy of Sciences, China — We report an enhancement of over an order of magnitude in the complex Kerr angle at photon energies near 121 meV in a variety of films on SiC substrates. The change in the reflected polarization in the presence of an out-of-plane magnetic field (polar magneto-optical Kerr effect, PMOKE) is measured in films ranging from graphene on SiC, aluminum doped SiC and iron oxide deposition on SiC. We model the PMOKE signal using multilayer analysis and find that the main contributor to this enhancement is the index of SiC becoming unity near 121 meV, at the edge of the Reststrahlen band of SiC. This result not only increases our sensitivity to PMOKE in a wide range of materials but also suggests that choice of substrate plays an important role in enhancing Kerr signal. This work is supported by NSF-DMR1006078.

3This work is supported by NSF-DMR1006078.

8:24AM L17.00003 Graphene thermal transport studies via radio-frequency, cross-correlated Johnson noise thermometry. JESSE CROSSNO, XIAOMENG LIU, KE WANG, ACHIM HARZHEIM, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, THOMAS OHKI, KIN CHUNG FONG, Raytheon BBN Technologies, PHILIP KIM, Harvard University — The electronic temperature of a dissipative, mesoscale device can be determined and monitoring the Johnson noise power emitted over a wide frequency range. Using radiometry techniques, we have developed a high-frequency, wide bandwidth, cross-correlation Johnson noise thermometer operating from room temperature to cryogenic levels that is compatible with strong magnetic fields. Precisions ranging from 2 to 25 mK are demonstrated over the temperature range of 3 to 300 K with 1 second of integration time. This non-invasive thermometer has enabled us to perform sensitive electronic thermal transport studies in boron nitride encapsulated monolayer graphene over two orders of magnitude in temperature. This versatile technique also enables precision Fano factor measurements as well as studies of correlated noise phenomena, such as those found in layered Van der Waals heterostructures.

8:36AM L17.00004 Valley polarized transport through irradiated graphene. ARIJIT KUNDU, HERB FERTIG, BABAK SERAYDJEH, Indiana Univ - Bloomington — Graphene under the application of circularly polarized light can go through Floquet topological transitions between various topological phases. With a drive protocol that breaks the valley symmetry, such transitions can occur at different points in the drive parameter space for different valleys. This may lead to valley polarized transport. We apply this concept to propose geometries for valleytronics devices like valves and transistors, which we theoretically analyze.

8:48AM L17.00005 Interaction of Dirac Fermion excitons and biexciton-exciton cascade in graphene quantum dots. ISIL OZFIDAN, University of Ottawa, MAREK KORKUSINSKI, National Research Council Canada, PAWEL HAWRY-LAK, University of Ottawa — We present a microscopic theory of interacting Dirac quasi-electrons and quasi-holes confined in graphene quantum dots. The single particle states of quantum dots are described using a tight binding model and screened direct, exchange, and scattering Coulomb matrix elements are computed using Slater pₓ orbitals. The many-body ground and excited states are expanded in a finite number of electron-hole pair excitations from the Hartree-Fock ground state and computed using exact diagonalization techniques. The resulting exciton and bi-exciton spectrum reflects the degeneracy of the top of the valence and bottom of the conduction band characteristic of graphene quantum dots with C3 symmetry. We study the interaction of multi-electron and hole complexes as a function of quantum dot size, shape and strength of Coulomb interactions. We identify two degenerate bright exciton (X) states and hole complexes as a function of quantum dot size, shape and strength of Coulomb interactions. We identify two degenerate bright exciton (X) and hole complexes as a function of quantum dot size, shape and strength of Coulomb interactions. We next calculate the exciton to bi-exciton transitions and hole complexes as a function of quantum dot size, shape and strength of Coulomb interactions. We identify two degenerate bright exciton (X) and hole complexes as a function of quantum dot size, shape and strength of Coulomb interactions. We next calculate the exciton to bi-exciton transitions and hole complexes as a function of quantum dot size, shape and strength of Coulomb interactions.

9:00AM L17.00006 Optical limiting and nonlinear optical properties of gold-decorated graphene nanocomposites. RAMAKRISHNA PODILA, Clemson University, PRABIN PRADHAN, MURALIKRISHNA MOLLI, Sri Sathyai Sai Institute of Higher Learning, DARSHASH KANIVIYOR, Indian Institute of Technology Madras (IITM), SAI MUTHUKUMAR V. S. SIVA SANKARA SAI, Sri Sathyai Sai Institute of Higher Learning, S. RAMAPRABHU, Indian Institute of Technology Madras (IITM), APPARAO RAO, Clemson University, DEPARTMENT OF PHYSICS, SRI SATHYA SAI INSTITUTE OF HIGHER LEARNING TEAM, ALTERNATIVE ENERGY AND NANOTECHNOLOGY LABORATORY (AENL), INDIAN INSTITUTE OF TECHNOLOGY MADRAS TEAM, DEPARTMENT OF PHYSICS AND ASTRONOMY, CLEMSON NANOMATERIALS CENTER, CLEMSON UNIVERSITY TEAM — Although metal nanoparticle-decorated nanomaterials exhibit excellent optical limiting (OL) performance at a relatively higher fluence (>9 J/cm²), there is a dearth of OL materials for protecting low damage threshold (<1 J/cm²) photonic devices. The rehybridization of some metal d-orbitals and graphene p-orbitals often leads to undesirable changes in graphene’s electronic structure, which adversely affects OL. Here, we demonstrate that d-orbitals of Au nanoparticles exhibit little or no rehybridization with graphene, and result in an enhanced OL behavior even at a low fluence of ~0.4 J/cm² due to the excellent photo-absorption of Au combined with rapid carrier thermalization by graphene.
9:12AM L17.00007 Background-Free Ultrafast Pump-Probe Transmission Spectroscopy of Graphene. JOSEPH R. MURPHY, Department of Physics, University at Buffalo, State University of New York, TIANMU ZHANG, TIM THOMAY, ALEXANDER N. CAVALIERI, Department of Electrical Engineering, University at Buffalo, State University of New York, SAIMA HUSAINI, ROBERT G. BEDFORD, Sensors Directorate, Air Force Research Laboratory, Wright-Patterson Air Force Base — Graphene and graphene-related materials exhibit properties of interest for optical applications. Time-resolved pump-probe spectroscopy has been proven an effective tool to measure the time scales of carrier dynamics of materials with adequate absorption. Ultrafast measurements are challenging to conduct due to graphene’s low absorption of 2.3% per layer and time scales of the carrier dynamics in the sub-picosecond range. To perform these experiments, laser pulses with a duration of 200 fs from the 800 nm beam from an amplified Ti:sapphire laser system with a repetition rate of 250 kHz were used with energy densities as low as 4 μJ/cm². The difficulty of the detection of the low absorption in this single-color experiment is further exacerbated by the need to distinguish the signal in the probe beam from the noise present in the two beams used. We present the results from a background-free technique used in our ultrafast pump-probe measurements; these results reveal the presence of electronic processes with time scales on the order of 500 to 700 fs in multilayer graphene. This background-free technique uses optical chopping to modulate the pump and probe beams at different frequencies and we have found that this method significantly improves the signal to noise ratio.

9:24AM L17.00008 Photocurrent Generation in the Fractional Quantum Hall Regime of Graphene. SANFENG WU, Department of Physics, University of Washington, LEI WANG, Department of Electrical Engineering, Columbia University, YOU LAI, National High Magnetic Field Laboratory, GRANT AIVAZIAN, HELIN CAO, Department of Physics, University of Washington, CORY DEAN, Department of Physics, Columbia University, JAMES HONE, Department of Mechanical Engineering, Columbia University, ZHIQIANG LI, National High Magnetic Field Laboratory, XIAODONG XU, Department of Physics, University of Washington — Significant understanding toward fractional quantum Hall effects has been made through probing the quantum transport of carriers at the Fermi surface. However, little is known about the non-equilibrium behavior of the carriers that are excited above the Fermi Sea. In this talk, we will discuss the transport phenomena of photo-excited carriers in the quantum Hall regime of graphene. By probing the photocurrent generation through the edge channels of a graphene field effect transistor under high magnetic field and low temperature, we observe chiral edge transport of photo-excited carriers. The observed photocurrent can directly resolve both integer and fractional quantum Hall states. Our measurements may provide a new experimental approach to uncover the rich and exotic physics related to fractional quantum Hall effects.

9:36AM L17.00009 Study of photocurrent response in bilayer graphene. LONG JU, University of California, Berkeley, LEI WANG, JAMES HONE, Columbia University, FENG WANG, University of California, Berkeley — Bilayer graphene is a unique system where the electronic band structure can be controlled by external electric field. The transition between semimetal to semiconductor with a bandgap up to 250 meV can be achieved by applying voltages on top and bottom gates. In this talk I’ll show our photocurrent measurement in dual-gated bilayer graphene devices. Different mechanisms of photocurrent generation will be discussed. I’ll also talk about its implications for potential opto-electronic applications of bilayer graphene.

9:48AM L17.00010 Photoresponse in Graphene Boron Nitride Vertical Heterostructures. TROND ANDERSEN, GIONG MA, CHUN-HUNG LUI, Massachusetts Inst of Tech-MIT, NITYAN NAIR, University of California, Berkeley, NATHANIEL GABOR, University of California, Riverside, ANDREA YOUNG, WENJING FANG, Massachusetts Inst of Tech-MIT, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute of Materials Science, Japan, JING KONG, NUH GEDIK, PABLO JARILLO-HERRERO, Massachusetts Inst of Tech-MIT — Combining two-dimensional materials into vertical heterostructures reveals diverse, intriguing phenomena and provides a novel way of engineering materials with desired electronic properties. Placing graphene on hexagonal boron nitride (hBN) has given particularly interesting results, including enhanced mobility, opening of a band gap, and highly controllable photo-induced doping. We explore the photoresponse of vertical graphene-hBN-graphene heterostructures in a high electronic temperature regime where thermonic emission dominates. Near the charge neutral point, we observe a pronounced conductance peak, which we attribute to a cooling bottleneck that appears at low carrier density, thus suggesting hot carrier enhanced thermonic emission. To further investigate the mechanism by which current is generated, we conduct two-pulse correlation measurements and study the temporal dynamics of the system. We observe a positive correlation, implying that the hot carriers thermalize before crossing the hBN barrier. Finally, we propose an advanced, modified two-temperature model, which allows for numerical simulations that are consistent with our measurements.

10:00AM L17.00011 Scanning photocurrent microscopy in Graphene mediated by photo-Nernst effect. ZAIYAO FEI, HELIN CAO, GRANT AIVAZIAN, Department of Physics, University of Washington, JASON ROSS, Department of Materials Science and Engineering, University of Washington, DAVID COBDEN, Department of Physics, University of Washington, XIAODONG XU, Department of Physics, Department of Material Science and Engineering, University of Washington — We have performed scanning photocurrent microscopy on monolayer graphene devices in a perpendicular magnetic field of up to 7 T. At zero field we observe photocurrent generated only near the contacts, but for a finite magnetic field an additional edge magnetophotocurrent contribution appears far from the contacts which is odd in magnetic field. The edge photocurrent also has opposite polarities for opposite edges. At low field this contribution can be well explained by the photo-Nernst effect combined with the nonlocal current generation mechanism described by Son and Levitov (ref. Phys. Rev. B 90, 075415, 2014). The effect persists to room temperature. At higher fields Landau quantization effects are seen along with oscillations of the magneto-photocurrent. The theory remains inadequate to explain all the features in this regime.

10:12AM L17.00012 Altshuler-Aronov-Spivak Oscillation in Graphene Antidot lattice. YAGI, RYOJI SAKAKIBARA, JUNPEI ONISHI, ADSM, Hiroshima University, YAGI LAB. TEAM — We have observed the Altshuler-Aronov-Spivac (AAS) oscillation in triangular antidot lattice of single layer graphene. Low temperature magnetoresistance exhibited h/2e periodic oscillations near zero magnetic field, negative magnetoresistance, and h/e periodic (AB-type) oscillations at higher magnetic fields. Phase of the AAS oscillation was the same as those for conventional 2D electrons with negligible spin orbit interaction, showing that inter-valley scattering averaged the Berry phase effect which results in anti-localization. (Yagi et al. J. Phys. Soc. Jpn. 81, 064707 (2012).)

10:24AM L17.00013 Low-gate-biased edge-state manipulation for tunable spin-polarized current source in zigzag graphene ribbon. LI CHANG, CHON-SAAR CHU, Department of Electrophysics, National Chiao-Tung University — In this work, we investigate the spin transport through a region with inhomogeneous edge-potential generated by split gates in a zigzag graphene ribbon (ZGNR). The split gates (each covers the lower and upper edges of the ribbon) actively modify the coupling between the pair of edge states and electrically generate the tunable edge-sate gap (ESG). With a homogeneous exchange field in the whole background, the ESGs of opposite spins are separated. We utilize these separated gaps to realize the tunable spin-polarized current source. Specifically, the split gates are placed in the middle segment of the ZGNR and we numerically study the spin transport through the potential region. With the exchange field strength of 5 meV and the on-site energy uncertainty within ±4 meV, we still get nearly 100% spin polarized current.
**10:36AM L17.00014 Temperature-dependent Transport Properties of CVD grown Graphene with Pd Functionalization**, BOCHEN ZHONG, Department of Physics and Astronomy, University of South Carolina, AHSAN UDDIN, AMOL SINGH, Department of Electrical Engineering, University of South Carolina, GOUTAM KOLEY, Department of Electrical and Computer Engineering, Clemson University, RICHARD WEBB, Department of Physics and Astronomy, University of South Carolina — We have investigated the temperature dependence of carrier density and mobility of CVD grown graphene before and after 2nm Pd deposition by Hall effect measurement. In our samples, Hall mobility increases as temperature increases, indicating that Coulomb scattering is the most important scattering mechanism. The Pd functionalization layer scattering limited carrier mobility is modeled as a function of temperature, and a least-square fit is done. Furthermore, Hall mobility of the Pd-functionalized graphene enhances significantly after exposure to H2 and the dominant scattering mechanism switches to thermal excited substrate optical phonon scattering.

**10:48AM L17.00015 Toward High Performance Graphene-based Solar Cells: Spectroscopic Study on Doped Graphene**, JAN-KAI CHANG, Department of Physics, Caltech; Graduate Institute of Photonics and Optoelectronics, National Taiwan University, CHEN-CHIH HSU, WEI-HSIANG LIN, Department of Physics, Caltech, CHIH-I WU, Graduate Institute of Photonics and Optoelectronics, National Taiwan University, NAI-CHANG YEH, Department of Physics, Caltech — We have investigated the temperature dependence of graphene-based devices: Spectroscopic study on doped graphene. The proposed facile strategy led to a tunable work function from 3.25 eV to 5.10 eV, enabling graphene anode and cathode for solar cell devices. Both hybrid and organic photovoltaics using graphene electrodes have been carried out with a series of optimization based on spectroscopic characterizations. Since aging of doped graphene is crucial to the lifetime of graphene-based solar cells, the doping-induced electronic state variation with time has been investigated via X-ray and ultra-violet photoemission spectroscopy analysis to gain insight in its electronic properties and stability. The doping effect developed in graphene has also been studied via Raman spectroscopy, including time evolution of the Raman D, G and 2D bands under normal and humid conditions for up to 30 days. This systematic investigation of aging effect provides better understanding and helps optimize the stacking of doped graphene films for achieving high performance graphene-based devices.

Wednesday, March 4, 2015 8:00AM - 11:00AM

**Session L18 DPOLY FIAP GSOFT: Invited Session: Industry Day: Dynamics and Non-Equilibrium Processes of Colloids and Filled Polymer Blends** Mission Room 103A - Valeriy Ginzburg, Dow Chemical

**8:00AM L18.00001 Structure-Property Relationships of Architectural Coatings by Neutron Methods**, ALAN NAKATANI, The Dow Chemical Company — Architectural coatings formulations are multi-component mixtures containing latex polymer binder, pigment, rheology modifiers, surfactants, and colorants. In order to achieve the desired flow properties for these formulations, measures of the underlying structure of the components as a function of shear rate and the impact of formulation variables on the structure is necessary. We have conducted detailed measurements to understand the evolution under shear of microstructure and larger scale mesoscale in model architectural coatings formulations by small angle neutron scattering (SANS) and ultra small angle neutron scattering (USANS), respectively. The SANS results show an adsorbed layer of rheology modifier molecules exist on the surface of the latex particles. However, the additional hydrodynamic volume occupied by the adsorbed surface layer is insufficient to account for the observed viscosity by standard hard sphere suspension models (Krieger-Dougherty). The USANS results show the presence of latex aggregates, which are fractal in nature. These fractal aggregates are the primary structures responsible for coatings formulation viscosity. Based on these results, a new model for the viscosity of coatings formulations has been developed, which is capable of reproducing the observed viscosity behavior.

**8:36AM L18.00002 Thermal Imaging Processes of Polymer Nanocomposite Coatings**, JEFFREY METH, CR&I, DuPont Co. — Laser induced thermal imaging (LITI) is a process whereby infrared radiation impinging on a coating on a donor film transfers onto an adjacent film to produce a pattern. This talk describes how LITI patterning can print color filters for liquid crystal displays, and details the physical processes that are responsible for transferring the nanocomposite coating in a coherent manner that does not degrade its optical properties. Unique features of this process involve heating rates of 10^7 K/s, and cooling rates of 10^4 K/s, which implies that not all of the relaxation modes of the polymer are accessed during the imaging process. On the microscale, the polymer flow is forced by devolatilization of solvents, followed by deformation akin to the constrained blister test, and then fracture caused by differential thermal expansion. The unique combination of disparate physical processes demonstrates the gamut of physics that contribute to advanced material processing in an industrial setting.

**9:12AM L18.00003 Dynamics of Polyelectrolyte Chains within Layer-by-Layer Assemblies**, SVETLANA SUKHISHVILI, Department of Chemistry, Chemical Biology and Biomedical Engineering, Stevens Institute of Technology, Hoboken 07030 — Layer-by-layer (LbL) assembly of charged polymers/nanoparticles finds diverse industrial applications ranging from NIR reflective heat-reduction to multi-stage drug delivery. Internal layering of film components lies at the heart of their performance. I will discuss experiments aimed to unravel relationships between center-of-mass diffusion of polyelectrolyte (PE) chains within LbL films, PE molecular characteristics, environmental conditions (salt concentration), and film structure. Upon film annealing in salt solutions, chain diffusion is highly anisotropic (as probed by fluorescence recovery after photobleaching and neutron reflectometry), and is strongly coupled with film structure. For layered LbL films, PE diffusion in the direction parallel to the substrate reveals quasi-Rouse scaling with molecular weight (D ~ M^−1), even for long chains, suggesting that chains disentangle upon adsorption. Finally, I will discuss quantitative aspects of salt-induced PE chain diffusion in directions parallel and perpendicular to the substrate, and their consequences for persistent layering within LbL films.

**9:48AM L18.00004 Field responsive shear thickening fluids for personal protective equipment and MMOD shielding for spacecraft and astronauts**, NORMAN WAGNER, University of Delaware / STF Technologies LLC — Shear thickening fluids (STFs) are novel, field responsive materials and have been shown to provide enhanced ballistic and puncture resistance when integrated into nanocomposites. In this talk, I will review the basic principles of shear thickening in colloidal dispersions by introducing new, recent results describing the unique material functions of the shear thickened state and how these material functions relate to those observed in simulation and experiments, as well as models for these material functions and their dependence on particle concentration. Next, performance data for STF-Armor(TM) nanocomposites (STF intercalated with aramid and other textiles) in puncture, ballistic and hypervelocity impact experiments, as well as energy absorbing impact experiments, will be shown and related back to the material properties of the STF fluids. Finally, advances in product development to achieve suitable puncture resistance for novel applications such as puncture resistant surgical gloves (STF Technologies LLC) will be presented along with challenges for the future product development.

1 This work was supported by the National Science Foundation under Award DMR-0964747.

2 Support from NSF STTR # IIP-1346269 and NASA NNX11AQ28A is gratefully acknowledged.
WEISS, Pennsylvania State Univ — No abstract available.

JOSEPH BEAMAN, University of Texas at Austin — Starting in the
Monitoring applies to industrial gas turbines for stationary land power.

AZAR ALIZADEH

maintaining their structural integrity and providing wireless power, sensor interrogation, and real-time diagnostics. We detail this approach as it specifically

networks must be robust to environmental factors, including: corrosion, EMI/RFI, and thermal/mechanical variations. In this talk, we describe the use of

be supplied to a sensor network via single or multiple data concentrators in an architecture that ensures reliable/secure interconnectivity. In addition, such

in-the-loop control. In closed or proprietary systems, such as in aerospace vehicles and life safety or security building systems; wireless signals and power must

a means for globally optimizing systems of systems by providing both real time PHM (prognostics, diagnostics, and health monitoring), as well as expanded

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Integrated Building Systems

presented.

that were used in the past and those that are used today to create manufactured parts. Finally, a discussion of new methods and future directions of AM is

and improvements in quality over time. The emphasis will be on Additive Manufacturing processes that are being considered for direct manufacturing, which

out of a commercial need for rapid prototyping. This market has a different requirement for process and quality control than traditional manufacturing. The

processes. This presentation gives a brief history of Additive Manufacturing and gives an assessment for these technologies. These technologies initially grew

of a commercial need for rapid prototyping. This market has a different requirement for process and quality control than traditional manufacturing. The

relatively poor process control of the existing commercial Additive Manufacturing equipment is a vestige of this history. This presentation discusses this history

and improvements in quality over time. The emphasis will be on Additive Manufacturing processes that are being considered for direct manufacturing, which

is a different market than the 3D Printing “Makerbot” market. Topics discussed include past and present machine sensors, materials, and operational methods

that were used in the past and those that are used today to create manufactured parts. Finally, a discussion of new methods and future directions of AM is

presented.

9:12AM L19.00003 3D Printing, Additive Manufacturing, and Solid Freeform Fabrication:
The Technologies of the Past, Present and Future . JOSEPH BEAMAN, University of Texas at Austin — Starting in the
late 1980’s, several new technologies were created that have the potential to revolutionize manufacturing. These technologies are, for the most part, additive
processes that build up parts layer by layer. In addition, the processes that are being touted for hard-core manufacturing are primarily laser or e-beam based
processes. This presentation gives a brief history of Additive Manufacturing and gives an assessment for these technologies. These technologies initially grew
out of a commercial need for rapid prototyping. This market has a different requirement for process and quality control than traditional manufacturing. The
relatively poor process control of the existing commercial Additive Manufacturing equipment is a vestige of this history. This presentation discusses this history
and improvements in quality over time. The emphasis will be on Additive Manufacturing processes that are being considered for direct manufacturing, which
is a different market than the 3D Printing “Makerbot” market. Topics discussed include past and present machine sensors, materials, and operational methods
that were used in the past and those that are used today to create manufactured parts. Finally, a discussion of new methods and future directions of AM is
presented.

9:48AM L19.00004 Additive Manufacturing Enabled Ubiquitous Sensing in Aerospace and
Integrated Building Systems1 . JOSEPH MANTESE, United Technologies Research Center — Ubiquitous sensing is rapidly emerging as
a means for globally optimizing systems of systems by providing both real time PHM (prognostics, diagnostics, and health monitoring), as well as expanded
in-the-loop control. In closed or proprietary systems, such as in aerospace vehicles and life safety or security building systems; wireless signals and power must
be supplied to a sensor network via single or multiple data concentrators in an architecture that ensures reliable/secure interconnectivity. In addition, such
networks must be robust to environmental factors, including: corrosion, EMI/RFI, and thermal/mechanical variations. In this talk, we describe the use of
additive manufacturing processes guided by physics based models for seamlessly embedding a sensor suite into aerospace and building system components; while
maintaining their structural integrity and providing wireless power, sensor interrogation, and real-time diagnostics. We detail this approach as it specifically
applies to industrial gas turbines for stationary land power.

1This work is supported through a grant from the National Energy Technology Laboratory (NETL), a division of the Department of Energy

10:24AM L19.00005 Manufacturing of Wearable Sensors for Human Health and Performance
Monitoring . AZAR ALIZADEH2, GE Global Research — Continuous monitoring of physiological and biological parameters is expected to improve
performance and medical outcomes by assessing overall health status and alerting for life-saving interventions. Continuous monitoring of these parameters
requires wearable devices with an appropriate form factor (lightweight, comfortable, low energy consuming and even single-use) to avoid disrupting daily
activities thus ensuring operation relevance and user acceptance. Many previous efforts to implement remote and wearable sensors have suffered from high
cost and poor performance, as well as low clinical and end-use acceptance. New manufacturing and system level design approaches are needed to make the
performance and clinical benefits of these sensors possible while satisfying challenging economic, regulatory, clinical, and user-acceptance criteria. In this talk we
will review several recent design and manufacturing efforts aimed at designing and building prototype wearable sensors. We will discuss unique opportunities and
challenges provided by additive manufacturing, including 3D printing, to drive innovation through new designs, faster prototyping and manufacturing, distributed
networks, and new ecosystems. We will also show alternative hybrid self-assembly based integration techniques for low cost large scale manufacturing of single
use wearable devices.

2Coauthors: Prabhjot Singh and Jeffrey Ashe

Wednesday, March 4, 2015 8:00AM - 11:00AM –
Session L20 DAMOP: Invited Session: Novel Probes for New Physics in AMO Systems Ballroom
B - Bryce Gadway, University of Illinois at Urbana-Champaign

8:00AM L20.00001 Interferometric probes of many-body localization , EUGENE DEMLER, Harvard Univ —
No abstract available.

8:36AM L20.00002 Quantum distillation and confinement of vacancies in a doublon sea . DAVID
WEISS, Pennsylvania State Univ — No abstract available.
9:12AM L20.00003 Probing Quantum Magnetism in 2D with an Array of Hundreds of Trapped Ions\(^1\). JOHN BOLLINGER, NIST, Boulder CO 80305 — Quantum simulations using AMO systems promise a new way to experimentally study emergent quantum phenomena, but few systems have demonstrated the capability to control ensembles in which quantum effects cannot be directly computed. The 2D array of 100s of \(^{9}\)Be\(^+\) ions in a Penning trap, crystallized in a triangular lattice when laser cooled, is a promising platform for intractable quantum simulations using the \(^{9}\)Be\(^+\) valence electron spin as a qubit \([1]\). Spin-dependent forces are employed to modify the strong Coulomb interaction of the ions, mimicking a quantum magnetic interaction. The range of the magnetic interaction can be tuned from infinite to a dipole-dipole like coupling. Combining the application of the spin-dependent force with a transverse magnetic field should lead to the development of quantum correlations between the spins, which can be measured through optical readout of the spin state, both globally and with site-resolved imaging. In this way, trapped atomic ions can be used to probe novel and intractable aspects of quantum magnetism, including the effects of long-range interactions and simulations of quantum non-equilibrium phenomena \([2]\). In addition to a general overview, I will discuss recent work from a new Penning trap set-up at NIST.


\(1\) In collaboration with Joseph Britton, Brian Sawyer, and Justin Bohnet

9:48AM L20.00004 Quantum atom optics with BEC: Fisher information for entangled non-Gaussian many particle states, MARKUS OBERTHALER, Kirchhoff Institute for Physics, Heidelberg University, 69120 Heidelberg/Germany — Our results build on the successful generation of spin squeezed states utilizing the quantum dynamics in an interacting two component Bose gas. The initial state is close to an unstable fixed point of the underlying classical system and thus the dynamics leads to squeezing for the initial time (harmonic regime) but generates non-Gaussian states for longer times. With this new method we generate 6dB spin squeezed states on a short time scale. The novel way of squeezing generation also allows the exploration of over-squeezed states i.e. transient non-Gaussian states towards the generation of cat states. We will report on our results preparing and characterizing these transient non-Gaussian states. They reveal variances which are larger than the classical shot noise limit thus suppression of fluctuations cannot be employed as an entanglement witness. We therefore developed a novel method for detecting the presence of entanglement by extracting from the experimentally detected distribution functions a bound of the Fisher information present in the system. With that we confirm that the entanglement is still present although the states are not spin squeezed. Furthermore interferometry beyond classical limits with these novel states is demonstrated by employing maximum likelihood estimation of the interferometric phase. We will also present a general approach which allows the upscaling of squeezed states to large atom numbers by employing the concept – divide and conquer. We explicitly demonstrate 5dB squeezing for more than 13000 particles. We use this resource and combined this with swapping the squeezing to magnetically sensitive states for demonstration of quantum enhanced magnetometry with high spatial resolution.

10:24AM L20.00005 SU(N) orbital magnetism and synthetic dimensions with two-electron fermions, LEONARDO FALLANI, LENS / Florence — I will report on recent experiments performed at LENS with ultracold 173Yb Fermi gases. These two-electron atoms offer a range of new opportunities for quantum simulation with ultracold gases, since they grant the access to two stable degrees of freedom—nuclear spin and electronic state—that can be manipulated independently and coherently. By controlling the electronic state via an ultranarrow clock transition, we have obtained the first demonstration of fast, coherent spin-exchange oscillations between fermionic atoms trapped in two different long-lived electronic orbitals [1]. This result paves the way to the observation of exotic quantum magnetism and of paradigmatic condensed-matter effects in a fermonic system exhibiting SU(N)-invariant interactions. Finally, I will present the results of a very recent experiment, where we have used Raman transitions between different 173Yb nuclear spin states to synthesize an effective lattice dynamics in a finite-sized “extra dimension.” By using this innovative approach, we have realized synthetic magnetic fields for effectively-charged fermions and we have demonstrated the emergence of chiral edge states propagating along the edges of the system, thus providing a direct evidence of a prominent feature of quantum Hall physics in condensed-matter systems [2].


Wednesday, March 4, 2015 8:00AM - 11:00AM –

8:00AM L21.00001 Design and performance of a cryogenic scanning tunneling microscope in high magnetic field for 2D layered materials study\(^1\). TIEN-MING CHUANG, FEI-FANG CHUNG, SYU-YOU GUAN, SHAN-AN YU, CHE-AN LIU, CHIA-SHENG HSU, CHIH-CHUAN SU, Institute of Physics, Academia Sinica, Nankang, Taipei 11529, Taiwan, RAMAN SANKAR, FANG-CHENG CHOU, Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan — We will describe the design and performance of a cryogenic scanning tunneling microscope (STM) system in a high magnetic field. A Pan-type STM is mounted on a homemade low vibration 4He pot refrigerator, which can be operated in continuous flow mode at \(T \sim 1.6\)K and in a magnetic field of up to 9 Tesla. A cleavage device at \(T=4.2\)K stage is used to cleave the 2D layered materials before inserting into STM as well as functioning as the radiation shield. The liquid helium boil rate of 4.6 liters per day is achieved due to our careful design, which allows the measurement at base temperature up to 10 days. We will demonstrate its capability of measuring atomically registered energy resolved spectroscopic maps in both real space and momentum space by our recent results on Rashba BiTeI.

\(1\)This work is supported by Ministry of Science and Technology, Taiwan and Kenda Foundation, Taiwan.

8:12AM L21.00002 ABSTRACT WITHDRAWN –
8:24AM L21.00003 Quantum Interference between Energy Absorption Processes of Molecular Exciton and Interface Plasmons on Luminescence Induced by Scanning Tunneling Microscopy

KUNIKIYUKI MIWA, HIROSHI IMADA, RIKEN, MANORI SAKAUE, HIDEAKI KASAI, Graduate School of Engineering, Osaka University, YOUSOO KIM, RIKEN — Luminescence induced by the tunneling current of a scanning tunneling microscope (STM) from molecule-covered metal surfaces is attributed to radiative decays of molecules and interface plasmons localized near the tip-substrate gap region. Since the dynamics of molecule and interface plasmons strongly influence each other, the interplay between these dynamics gives rise to peculiar phenomena originating from quantum many-body effects. In this study, we develop the effective model of the system and investigate the luminescence properties using the nonequilibrium Green’s function method. The results show that, in addition to the dynamic spectrum of molecular, energy reabsorption by interface plasmons have a critical role in determining the luminescence spectral profile of interface plasmons. The additional peak structure arises owing to the interference between these energy absorption processes. Origin of prominent peak and dip structures observed in recent experiments are identified by the developed theory. The details of the interference effects on the luminescence properties will be discussed.

1 This work was supported by JSPS KAKENHI Grant Number 26886013.

8:36AM L21.00004 Image Distortions of Molecules in Atomic Force Microscopy with Carbon Monoxide Terminated Tips

NIKOLAJ MOLL, LEO GROSS, BRUNO SCHULER, ALESSANDRO CURIONI, GERHARD MEYER, IBM Research - Zurich — Using functionalized tips, the atomic resolution of a single organic molecule can be achieved by atomic force microscopy (AFM) operating in the regime of short-ranged repulsive Pauli forces while the van-der-Waals and electrostatic interactions only add a diffuse attractive background. The underlying mechanisms of image distortions with CO-terminated tips are identified and studied in detail. Parts of a molecule appear different in size, which primarily originates from the charge density. Further, tilting of the CO at the tip, induced by van der Waals forces, enlarges the apparent size of parts of the molecule by up to 50%. Moreover, the CO tilting in response to local Pauli repulsion causes a significant sharpening of the molecule bonds in AFM imaging. With these image distortions it is possible to distinguish different bond orders of individual carbon-carbon bonds in organic molecules by AFM.


8:48AM L21.00005 Three-Dimensional Imaging of Complex Molecular Electronic States via Atomic Manipulation Reconstruction

ERIC CHATTERJEE, DOMINIK RASTAWICKI, ALEX CONTRYMAN, YAN SUN, DYLAN RUETER, HARI MANOHARAN, Stanford Univ — We describe a method based on STM atomic manipulation for experimentally capturing the complete three-dimensional electronic structure of complex molecules. Using techniques we have recently developed for assembling molecular graphene and related materials, we vary specific site potentials, intersite hopping amplitudes, and Fermi energy in 2D nanostructures which when wrapped into a 3D container represent a new probe molecule. Here we present the design methods and analyses of a number of such molecules, focusing on those containing rotational symmetry. We show how various types of fullerenes, of interest due to their electronic and vibrational properties, can be unwrapped on a 2D surface, reprogrammed, and rewrapped to 3D. Examples of the unwrapping methods include cutting selected bonds in order to sever adjacent faces or sites. Analysis of the local density of states for 2D correspondents to fullerenes yields the presence of peaks at the highest occupied molecular orbital and lowest unoccupied molecular orbital, with an energy gap between these levels. The replication of these properties of fullerenes in 2D space serves as evidence of the significant potential of STM assembly and spectroscopy in studying the applicability of exotic 3D molecules in electronics.

9:00AM L21.00006 Gauge Fields and Topological Confinement in Synthetic Nanomaterials Assembled via Atomic Manipulation

DOMINIK RASTAWICKI, ERIC CHATTERJEE, YAN SUN, ALEX CONTRYMAN, DYLAN RUETER, HARI MANOHARAN, Stanford Univ — The assembly of molecular graphene and related nanostructures demonstrated that atomic manipulation can be used to build functional quantum nanomaterials site by site and bond by bond. This level of precise control lets one tune the potential of each site, the hopping strength of each bond, and—by adjusting lattice size—the Fermi energy and relative interaction strength inside and between sites. Here we present examples of new molecular materials assembled and characterized by STM/STS exploiting these techniques. We show that lattices with varying site potential across six sites of a unit cell show signatures of non-abelian gauge fields. We will contrast observed behavior with conventional abelian gauge fields built into the same structures. We will also show that boundaries between patterned mass domains can induce topological edge states and topological charge confinement. We will also discuss the engineering of flat bands into more complex materials, and show effects of the resulting quenching of kinetic energy.


FABIAN DONAT NATTERER, NIST, Center for Nanoscale Science and Technology — In graphene, phonons are important agents for a wide range of phenomena; they mediate relaxation rates for hot carriers, they lead to van-Hove singularities, and they induce a renormalization of the Fermi velocity due to electron-phonon coupling and many-body interactions [1]. The previous observations of phonons [2-4] by inelastic electron tunneling spectroscopy (IETS) have been expandable in terms of detail and resolution due to weak signals and other spectral features which inhibit a clear distinction between phonons and miscellaneous excitations. We find that utilizing a back gated graphene device, where the graphene charge carrier density can be varied in magnitude and sign, allows all the critical point graphene phonons with large density of states to be sampled by IETS with the scanning tunneling microscope, and in good agreement with density functional calculations. In addition, a strong overtone excitation at 360 meV is observed. Quite surprisingly, we observe all the graphene excitations are resonantly enhanced when the charge carrier type is switched, indicating that this amplification occurs whenever the inelastic transition allows a change in the graphene chirality. The chiral enhancement is observed to follow a linear trend with energy and reaches almost an order of magnitude for the highest transition. Our averaging technique suppresses charge carrier dependent excitations, while it improves the signal for inelastic transitions. This approach can be employed as a guide in advanced studies that are relying on gate tunable graphene devices, such as for the detection of spin, vibrational, or rotational excitations in adsorbates.


9:48AM L21.00008 Probing the Hydrogen Bond Strength at Single Bond Limit1, JING GUO, International Center for Quantum Materials, School of Physics, Peking University, JING-TAO LU, School of Physics, Huazhong University of Science and Technology, JI CHEN, JINBO PENG, XUANGZHI MENG, ZIHANG WANG, International Center for Quantum Materials, School of Physics, Peking University, XIN-ZHE LI, School of Physics, Peking University; Collaborative Innovation Center of Quantum Matter, Beijing, ENGE WANG, YING JIAOQING, International Center for Quantum Materials, School of Physics, Peking University; Collaborative Innovation Center of Quantum Matter, Beijing — Many extraordinary physical, chemical and biological properties of water are determined by hydrogen-bonding interaction between the water molecules. So far, the routine way to determine the hydrogen-bonding strength of water is probing the frequency shift of O—H stretching mode using various spectroscopic techniques, which all suffer from the difficulty of spectral assignment and the broadening of vibrational signals due to the lack of spatial resolution. In this talk, we show the ability to probe the hydrogen-bonding strength of interfacial water at single bond limit using resonantly enhanced inelastic electron tunneling spectroscopy (IETS) with a scanning tunneling microscope (STM). The conventional IET signals of water molecules are extremely weak and far beyond the experimental detection limit due to the negligible molecular density of states (DOS) around the Fermi level. This difficulty can be surmounted by turning on the tip-water coupling, which shifts and broadens the frontier molecular orbitals of water to the proximity of Fermi level, resulting in a resonantly enhanced IET process.

1International Center for Quantum Materials, School of Physics, Peking University


10:12AM L21.00010 Elemental Fingerprinting of Materials with Sensitivity at the Atomic Limit1, MARVIN CUMMINGS, NOZOMI SHIRATO, Argonne Natl Lab, HEATH KERSELL, YANG LI, Ohio U., BENJAMIN STRIPE, DANIEL ROSEN-MANN, Argonne Natl Lab, SAW-WAI HLA, Argonne Natl Lab — Variants of scanning probe microscopes have proven tremendously valuable for extracting detailed information about the nature of a sample’s surface (atomic, electronic, magnetic), however it has proven difficult to yield chemical information utilizing scanning probe techniques alone. At Argonne National Laboratory’s Advanced Photon Source, a new in-situ high-resolution microscopy technique, the synchrotron x-ray scanning tunneling microscopy (SXSTM), utilizes x-rays as a chemical, electronic and magnetic probe and the nanofabricated tips of a scanning tunneling microscope as the chemical detector to take full advantage of the sub-nm spatial resolutions that STM provides. Utilizing the new SXSTM technique, chemical fingerprinting of individual nickel clusters on a Cu(111) surface has been demonstrated with a 2 nm lateral resolution and a sensitivity confined to the first atomic surface layer. In addition, the photoionization cross-section from a single nm-scale Ni cluster has been successfully measured. SXSTM could be proved to be a powerful new surface characterization technique, enabling exciting areas of opportunity and discovery in the chemical and materials sciences.

1This work was funded by the Office of Science Early Career Research Program through the Division of Scientific User Facilities, Office of Basic Energy Sciences, U.S. Department of Energy, through Grant SC07005.

10:24AM L21.00011 Direct elemental and magnetic contrast of magnetic thin films and nanoparticles measured by synchrotron X-ray scanning tunneling microscopy and spectroscopy, ANDREW D’IULLO, Argonne National Laboratory, IL 60439, USA, N. SHIRATO, M. CUMMINGS, Argonne National Laboratory, Lemont, IL 60439, USA, H. KERSELL, Ohio University, Athens, OH 45701, USA, S.-W. HLA, V. ROSE, Argonne National Laboratory, IL 60439, USA — Synchrotron X-ray scanning tunneling microscopy (SX-STM) combines two of the most robust characterization instruments of materials science in a single setting and it can provide elemental fingerprinting of materials down to the atomic limits [1]. Here, we show that the SX-STM can also be useful for the magnetic measurements with elemental specificity by combining tunneling microscopy and spectroscopy with the X-ray magnetic circular dichroism (XMCD) technique. The experiments are performed in the Advanced Photon Source beam line 4-ID-C using a custom-built SX-STM system. During the experiment, the circularly polarized synchrotron light is projected onto iron nanoclusters adsorbed on a cobalt thin film on Cu(111) surface, and the resulting photo-current is collected by a nano-fabricated SX-STM tip. The photocurrent intensity clearly reveals major and minority spin states when measured at L2 and L3 edges of the magnetic materials.


10:36AM L21.00012 Schottky Barrier mapping of the W/Si diode using ballistic electron emission microscopy, CHRISTOPHER DURCAN, ROBERT BALSANO, NICHOLAS PIENIAZEK, College of Nanoscale Science and Engineering, State University of New York at Albany, VINCENT LABELLA, Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute — The Schottky barrier of the W(001)/Si(001) diode was investigated and spatially mapped at the nanoscale using ballistic electron emission microscopy (BEEM) and ballistic hole emission microscopy (BHEM). The miscibility of tungsten and silicon creates a thin silicide upon deposition with transmission electron microscopy (TEM) and Rutherford backscattering spectrometry (RBS) showing the changes in the silicide over several weeks. Using standard current voltage measurements there is no change in the charge transport across the diode during this time period. However, BEEM measurements do show dramatic changes to the transport of ballistic electrons over time with nanoscale resolution. Time dependent Schottky barrier maps are generated over a 1 µm x 1 µm area and provide valuable insight to the barrier height homogeneity, defect formation, and interfacial effects occurring in the diode.

10:48AM L21.00013 Obtaining reliable friction data at the nanoscale by tuning AFM parameters1, SUNG HYUN KIM, SUENNIE KIM, Hanyang University — Carefully devised experimental study of friction at the nanoscale in dry system is desired for proper mathematical modeling or for quantitative research. Experimentally, contact mode atomic force microscope (AFM) which is able to perform lateral force microscopy (LFM) can be used for acquiring frictional data. To obtain reliable LFM information, we have investigated the effect of scanning parameters, especially gain and scanning rate, on the LFM measurements. Depending on the parameters selected, the relative ratio of the friction force obtained from graphene to that of SiO2 varies greatly from about 1 to 0.1. We will discuss, here, firstly how to understand this behavior and secondly the parameter-optimization procedure for the LFM imaging, which is different from the height imaging, eventually to aid quantitative LFM studies.

1This research was supported by Basic Science Research Program through NRF of Korea funded by the ministry of Education(2014R1A1A2056555).
8:00AM L22.00001 New Phases Stabilized by Anisotropic Impurity in $^{3}$He , A.M. ZIMMERMAN, J.I.A. LI, Northwestern University, J. POLLANEN, California Institute of Technology, C.A. COLLETT, W.P. HALPERIN, Northwestern University — We have introduced anisotropic impurity into superfluid $^{3}$He using well-characterized silica aerogel samples negatively strained by mechanical compression along the cylinder axis by $\approx 10\%$, $20\%$, and $30\%$. Using NMR measurements, we determined the temperature-magnetic field phase diagrams for these amounts of strain. In previous work it was found that in the presence of negative strain of $\approx 20\%$ the superfluid A-phase is only stable above a critical magnetic field, $H_{c}^{A}$. We have found that $H_{c}^{A}$ increases linearly with strain. By comparing the measured NMR longitudinal resonance frequency to results from unstrained isotropic aerogel, we have determined that in the presence of negative strain the B-phase evolves into a new anisotropic phase. This new anisotropic phase is more stable than the A-phase for fields below $H_{c}^{A}$. This work was supported by the National Science Foundation, DMR-1103625.


8:12AM L22.00002 Puddles of Helium on graphite surfaces , USHNISH RAY, NORMAN TUBMAN, University of Illinois at Urbana-Champaign — The ground state of $^{3}$He in 2D has long been theoretically suspected to be in a non-binding gaseous state. Recent experiments with ultra low density $^{3}$He adsorbed on Grafoil have shown, however, that below a critical density ($0.6 - 0.9\ nm^{-2}$) this 2D system becomes a self bound liquid. Subsequent numerical studies with an idealized graphite potential indicate that such a state is forbidden, but can possibly form on other alkali substrates. A key aspect not taken into consideration in such studies are the details of the anisotropic graphite potential. Our studies with finite temperature Path-Integral Monte-Carlo and ground state Diffusion Monte-Carlo techniques that use the full anisotropic graphite potential, on the other hand, reveals an alternate picture. We find that although the effective mass induced by the graphite surface is not enough to induce a macroscopic liquid, the system can still form ultra low density liquid puddles composed of a few $^{3}$He atoms. This picture is in agreement with experimental findings and illuminates a novel phase of Helium on graphite surfaces


8:24AM L22.00003 Confinement effect on Anderson-Higgs modes in superfluid $^{3}$He-B , T. MIZUSHIMA, Osaka University, J.A. SAULS, Northwestern Univ — Superfluid $^{3}$He is a prototype to observe the spectrum of Anderson-Higgs (AH) modes associated with spontaneous symmetry breaking. In bulk superfluid $^{3}$He, AH modes have been observed experimentally through attenuation of zero sound, propagation of transverse sound and its acoustic Faraday rotation. Starting from a Lagrangian formulation, we examine the AH modes of $^{3}$He-B confined in a restricted geometry. For bulk $^{3}$He-B this formalism leads to the well known spectrum of bosonic collectives modes of the bulk B-phase labelled by the quantum numbers for total angular momentum, $J = 0, 1, 2, ...$, the projection along an axis, $J_{z} = -J, ... , J$, and the parity under particle-hole conversion, $K = \pm 1$. For the equilibrium phases of $^{3}$He confinement induces pair breaking and leads to symmetry breaking, giving rise to a rich topological phase diagram. In terms of the bosonic excitations, we find that confinement induces symmetry breaking and leads to mixing of modes with different $J$, as well as to level splittings of the AH modes that are otherwise degenerate in bulk $^{3}$He-B. We find a new spectrum of Bosonic modes is generated that are bound to the surface of superfluid $^{3}$He in a restricted geometry. We also report on the coupling of the AH modes to ultra-sound.

8:36AM L22.00004 Topological quantum phases of helium-4 confined to nanoporous materials , LODE POLLET, LMU Munich, Germany, ANATOLY KUKLOV, College of Staten Island, City University of New York, New York — The ground state of $^{4}$He confined in a system with the topology of cylinder can display properties of solid, superfluid, and liquid crystal. This phase, which we call a compactified supersolid (CSS), originates from wrapping the basal planes of the bulk hcp solid into concentric cylindrical shells, with several central shells exhibiting superfluidity along the axial direction. Its main feature is the presence of a topological defect which can be viewed as a disclination with Frank index $\pi$. For the equilibrium phases of $^{4}$He confinement induces pair breaking and leads to symmetry breaking, giving rise to a rich topological phase diagram. In terms of the bosonic excitations, we find that confinement induces symmetry breaking and leads to mixing of modes with different $J$, as well as to level splittings of the AH modes that are otherwise degenerate in bulk $^{3}$He-B. We find a new spectrum of Bosonic modes is generated that are bound to the surface of superfluid $^{3}$He in a restricted geometry. We also report on the coupling of the AH modes to ultra-sound.

8:48AM L22.00005 $^{3}$He Condensation and Dissolution at Layer Completion in $^{3}$He-$^{4}$He Mixtures Adsorbed on Carbon Nanotubes , GARY WILLIAMS, EMIN MENACHEKIAN, JOHN ABRAHAM, BOB CHEN, VITO IAIA, ANDREW LI, SERGEY SUSHCHIKH, UCLA — The condensation and then dissolution of $^{3}$He has been observed at layer completion in $^{3}$He-$^{4}$He mixtures adsorbed on multiwall carbon nanotubes. With an initial fill of 3.5 layers of $^{3}$He, the addition of $^{3}$He in five steps of 0.07 layers uniformly reduces $T_{K}/c^{2}$, showing that the $^{3}$He is uniformly distributed. With the final 0.35 layer of $^{3}$He still present, additional $^{4}$He is then added at low temperature (225 mK). An abrupt transition is observed in the third sound signal very near the total-thickness 4.0 layer completion, where the Q factor suddenly drops by two orders of magnitude and the sound speed becomes constant. With the addition of another 0.1 layer of $^{4}$He the sound speed starts to decrease again and the Q climbs back to its initial value. We postulate that this behavior marks the formation of condensed $^{3}$He “islands” induced by the layer completion, and then the $^{3}$He dissolves back to uniform coverage past that point.

9:00AM L22.00006 Dissipative neutral mass flow and quantum phase slips in one dimension , ADRIAN DEL MAESTRO, Univ of Vermont — Motivated by experimental progress towards confining bosonic quantum fluids inside nanoscale constrictions, we have determined how quantum phase fluctuations of the superfluid order parameter modify neutral mass transport through a one dimensional channel open to vacuum. In the one dimensional limit, dissipation occurs in the guise of phase slips which may be nucleated due to the presence of impurity scattering, disorder, or a periodic potential. By combining equilibrium quantum Monte Carlo simulations with non-equilibrium calculations in the framework of Luttinger liquid theory, we have computed the relationship between the applied pressure and resistive mass flow for a one dimensional quantum fluid of neutral bosons. Understanding the temperature dependence of the resulting nonlinear pressure-flow behavior may be essential for the interpretation of quasi-1D superfluid flow experiments on helium-4.

This work was supported by the University of Alberta, Faculty of Science; the Natural Sciences and Engineering Research Council, Canada; the Canada Foundation for Innovation; Alberta Innovates Technology Futures; and the Alfred P. Sloan Foundation.

9:24AM L22.00008 Pressure driven flows of superfluid helium-4 through a single nanopipe. ANGEL VELASCO, ZUZANNA SIWY, PETER TABOREK, University of California, Irvine — We have measured flow rates of helium-4 through a single etched nanopore of 31 nm diameter with a mass spectrometer. Flow rates were measured as a function of pressure at constant temperature and at saturated vapor pressures along the coexistence curve between 0.5 K and 3.5 K. Due to the constraint of the mass spectrometer the low pressure side was maintained at P=0 creating an intrinsic superfluid/vapor interface which forms inside the pipe and at its exit. We observed two flow regimes at low temperatures with velocities in the range of 6 and 11 m/s consistent with Feynman’s vortex critical velocity and a thermal vortex nucleation model respectively. The velocity in a laminar, viscous flow is proportional to the pressure drop while in superfluid flows to zeroth order the velocity is independent of the pressure. A first order correction shows a linear dependence on the pressure with the slope continuously varying from a positive to a negative value near the lambda point. We have also measured flow rates in the normal state and found rates in exact agreement with conventional viscous theory that incorporates the Laplace pressure and a zero slip length[1]. Supported by NSF DMR-0907495. [1] Velasco et al. Appl. Phys. Lett. 105, 2014

9:36AM L22.00009 A titanium transition-edge sensor for the in-situ detection of individual He3* excimers in superfluid helium 1. FAUSTIN CARTER, SCOTT HERTEL, CATHERINE MATULIS, MICHAEL ROCKS, DANIEL MCKINSEY, DANIEL PROBER, Yale University — Incident radiation can excite superfluid helium into a diatomic He3* excimer, which decays through the emission of a 15 eV photon. Such excimers have been used as tracers to measure the superfluid’s quantum turbulence, thanks in part to the long half-life of the He3* triplet state (~13 seconds). However, the efficient detection of single or a few excimers remains a challenge. We present a detector capable of in-situ detection of the He3* excimers either directly (the excimer collides with the detector), or by collecting the 15 eV photon emission upon decay. This detector is based on a titanium superconducting transition-edge sensor (TES), with an energy resolution of 1.5 eV fwhm, coupled to an aluminum absorber. The TES is designed to operate from 20-300 mK in a dilution refrigerator. We will discuss operating characteristics of the detector and present preliminary data for detection of individual excimers.

3We acknowledge support from YINQE, NSF MRSEC DMR-1119826, and NSF DMR-1007974.

9:48AM L22.0010 Interaction of Ions, Atoms and Small Molecules with Quantized Vortex Lines in Superfluid 4He1. JUSSI ELORANTA, DAVID MATTEO, Chemistry Dept., Calif. State University Northridge, GARY WILLIAMS, UCLA — The interaction of a number of impurities (H2, Ag, Cu, Ag2, Cu2, Li, He3+, He4+, He5 (5S), He3 (5S1/2)) with quantized rectilinear vortex lines in superfluid 4He is calculated using density functional methods at 0 K. The technique yields the impurity radius as well as the vortex line core parameter. The core parameter at 0 K (0.74 Å) obtained either directly from the vortex line geometry or from the trapping potential fitting is smaller than previously suggested but is compatible with a re-analysis of the Rayfield-Reif experiment. All of the impurities have significant binding energies to the vortex lines below 1 K where the thermally assisted escape process becomes very inefficient. Even at higher temperatures the trapping times, especially for larger clusters, are sufficiently long that the observed metal nanowire assembly in superfluid helium can take place at vortex lines. The binding energy of the electron bubble is predicted to decrease as a function of both temperature and pressure, which allows adjusting the trap depth for either permanent trapping or thermally assisted escape. A new scheme for determining the trapping of impurities on vortex lines by optical absorption spectroscopy is outlined and demonstrated for He3*.

1Work supported by the NSF, grants CHE-1262306 and DMR-1205734, and the Interdisciplinary Research Institute for the Sciences

10:00AM L22.00011 Shapes of Swiftly Spinning Superfluid He Nanodroplets. CHARLES BERNANDO, R 1: We acknowledge support from NSF grant: DMR 1209291

10:12AM L22.00012 Helium-3 Confined to a 1.08 Micron Deep Cavity1, NIKOLAY ZHELEV, ABHILASH SEBASTI, Cornell University, LEV LEVITIN, BEN YAGER, ANDREW CASEY, JOHN SAUNDERS, Royal Holloway University London, JEEVAK PARPIA, Cornell University — We describe measurements of superfluid Helium-3 confined to a high-aspect ratio cavity within the head of a high quality factor torsion pendulum. The 1.08 μm deep, rotationally symmetric cavity (11 mm diameter) is defined into a 14 mm diameter silicon disk. The silicon disk is anodically bonded to a matching octagonal glass piece to complete the torsion head. The thickness of 1 mm for both the glass and the silicon ensures minimal distortion of the cavity up to a few bars of pressure. We observe that the normal fluid component stays coupled to the smooth walls of the cavity down to the lowest measured temperatures. By tracking the torsion pendulum frequency and quality factor, we can identify a well defined superfluid transition in the fluid within the pendulum head. We plan to map out the phase diagram for the highly confined Helium-3 at low pressures and observe whether a “stripe phase” is realized in the vicinity of the transition between the A and B superfluid phases.1

A.B. Vorontsov and J.A. Sauls, PRL 98, 045301.
10:24AM L22.00013 The Fermionic spectrum, phase transition and domain walls of confined 3He-A film

HAO WU, J. A. SAULS, Northwestern University — The edge states of a 3He film are Weyl Fermions propagating on the edge in a direction determined by the chirality of the bulk phase. Under lateral confinement, the wave functions for counter-propagating Weyl Fermions on opposing edges overlap. We show that the edge states hybridize and form a band, and the continuum states exhibit band gaps. We report self-consistent calculations of the reduction in the spontaneous edge mass currents due to hybridization as a function of lateral confinement, $D$. Strong lateral confinement leads to a sequence of quantum phase transitions. The phase undergoes a transition to a pair density wave (PDW) phase with broken translational symmetry at $D_{c1} \approx 13\xi_0$, and a transition to a polar state at $D_{c2} \approx 9\xi_0$. The PDW phase for $D < D_{c1}$ is periodic array of chiral domains separated by domain walls with currents that conflict with the direction of edge currents. We report self-consistent calculations of the PDW phase near $D_{c2}$ that resolves the competition in energy between edge states and Fermions bound to the domain wall. The resulting pattern of circulating currents also resolves the apparent violation of current conserved $\xi_0$.

1Supported by NSF Grant DMR-1106315.
2Y. Tsutsumi, J. Low Temp. Phys. 175, 2014

10:36AM L22.00014 A Variable Path Length Cell for Transverse Acoustic Studies of Superfluid 3He

C.A. COLLETT, M.D. NGUYEN, J.I.A. LI, A.M. ZIMMERMAN, W.P. HALPERIN, Northwestern University, Evanston, IL 60208, USA, J.P. DAVIS, University of Alberta, Edmonton, AB, Canada T6G 2R3 — Transverse sound has recently emerged as an effective probe of the order parameter of superfluid 3He. It has allowed for the study of quantum fluids. Our study in 3He-B showed that the temperature dependence of the damping in this device was consistent with a damping model derived from thermal quasi-particles and demonstrated its potential as a sensitive quasi-particle flux detector. It is natural to conceive a scheme to build angle-resolved or space-momentum resolved 3He quasi-particle detectors in the form of array of resonators. This type of detectors could play an important role in revealing detailed structure of excitations or visualizing vortices in quantum fluids. A prototype detector is composed of 4 x 4 or 6 x 6 array of comb-drive resonators with strategically dispersed resonance frequencies. In this paper, We will discuss the working principle and design of the detector array.


10:48AM L22.00015 Micromachined Angle Resolved 3He Quasi-particle Detector1, YOONSEOK LEE, C.S. BARQUIST, P. ZHENG, W.G. JIANG, Department of Physics, University of Florida, Gainesville, FL, T.R. SCHUMANN, Y.K. YOON, Department of Electrical and Computer Engineering, University of Florida, Gainesville, FL — Micromachined comb-drive mechanical resonators have been developed for the study of quantum fluids. Our study in 3He-B showed that the temperature dependence of the damping in this device was consistent with a damping model derived from thermal quasi-particles and demonstrated its potential as a sensitive quasi-particle flux detector. It is natural to conceive a scheme to build angle-resolved or space-momentum resolved 3He quasi-particle detectors in the form of array of resonators. This type of detectors could play an important role in revealing detailed structure of excitations or visualizing vortices in quantum fluids. A prototype detector is composed of 4 x 4 or 6 x 6 array of comb-drive resonators with strategically dispersed resonance frequencies. In this paper, We will discuss the working principle and design of the detector array.

1This work is partially supported by NSF DMR-1205891 (YL).

Wednesday, March 4, 2015 8:00AM - 10:36AM –
Session L23 DCMP DCOMP: Matter at Extreme Conditions II 202B - Zsolt Jenei, Lawrence Livermore National Laboratory

8:00AM L23.00001 First Principles Simulations of P-V-T Unreacted Equation of State of LLM-1051, RIAD MANAA, I-FENG KUO, LAURENCE FRIED, Lawrence Livermore National Laboratory — Equations of states (EOS) of unreacted energetic materials extending to high-pressure and temperatures regimes are of particular interest since they provide fundamental information about the associated thermodynamic properties of these materials at extreme conditions. Very often, experimental and computational studies focus only on determining a pressure-volume relationship at ambient to moderate temperatures. Adding elevated temperature data to construct a P-V-T EOS is highly desirable to extend the range of materials properties. Atomic scale molecular dynamics simulations are particularly suited for such a construct since EOSs are the manifestation of the underlying atomic interactions. In this work, we report dispersion-corrected density functional theoretical calculations of unreacted equation of state (EOS) of the energetic material 2,6-diamino-3,5-dinitropyrazine-1-oxide (LLM-105). We performed large-scale constant-volume and temperature molecular dynamics simulations for pressures ranging from ambient to 35 GPa, and temperatures ranging from 300 K to 1000 K. These calculations allowed us to construct an unreacted P-V-T EOS and obtain bulk modulus for each P-V isotherm. We also report the thermal expansion coefficient of LLM-105 in the temperature range of this study.

1This work performed under the auspices of the U.S. Department of Energy Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

8:12AM L23.00002 Ultrafast Shocked Single Crystal PETN and Beta-HMX: Shock Hugoniot Measurements to Guide the Development of Continuum Models1, JOSEPH ZAUG, MICHAEL ARMSTRONG, JONATHAN CROWHURST, LOUIS FERRANTI, RYAN AUSTIN, LAURENCE FRIED, Lawrence Livermore National Laboratory — We report results derived from a 372 ps drive duration yielded anisotropic elastic wave response in single crystal beta-HMX ((110) and (010) impact planes). Here we provide results using a >2x drive duration to extend measurements into the plastic or bulk wave regime. We compare our ultrafast time domain interferometry (TDI) results with previous gun platform results. These 10 ps time scale resolution TDI measurements guide the development of a continuum model to study pore collapse and energy localization in shock-compressed crystals of beta-HMX.

1This work was performed under the auspices of the U.S. Department of Energy jointly by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
8:24AM L23.00003 Dynamic response of matter heated by ultrafast laser pulses¹. ELISEO GAMBOA, LUKE FLETCHER, SEBASTIAN GOÈDE, ULF ZASTRAU, HAE-JA LEE, ERIC GALTIER, WILL SCHUMAKER, ROHINI MISHRA, PHILIPP SPERLING, MAXENCE GAUTHIER, ALESSANDRA RAVASIO, MICHAEL MACDONALD, SIEGFRIED GLENZER, SLAC National Accelerator Laboratory — The material properties of the light elements at extreme conditions are of utmost importance to a diverse set of fields, from astrophysics and cosmology to research into controlled nuclear fusion energy production. These high-energy density states, defined as solid density plasmas with $T > 10$ eV, may be produced in the laboratory by irradiation of materials with high-energy or high-power lasers. Characterizing these material conditions using optical means is challenging because the plasma is above critical density and the experimental conditions are maintained over only very brief timescales. We present a preliminary analysis of x-ray scattering data from ultrafast, isochorically-heated hydrogen and carbon in experiments conducted at the Matter in Extreme Conditions endstation at the Linac Coherent Light Source (LCLS) x-ray free electron laser, SLAC National Accelerator Laboratory. By observing the collective and non-collective x-ray scattering of the LCLS beam at multiple pump-probe delays, we infer the time-history of the electron and ion temperatures and thus the equilibration rate.

1This work was performed at the Matter at Extreme Conditions (MEC) instrument of LCLS, supported by the DOE Office of Science, Fusion Energy Science under contract No. SF00515. This work was supported by DOE Office of Science, Fusion Energy Science under F

8:36AM L23.00004 Micron-scale Reactive Atomic Simulation of Void Collapse and Hotspot Growth in PETN¹. Tzu-Ray Shan, Ryan Wixom, Aidan Thompson, Sandia National Laboratories, SANDIA NATIONAL LABORATORIES TEAM — Material defects and other heterogeneities such as dislocations, micro-porosity, and grain boundaries play key roles in the shock-induced initiation of detonation in energetic materials. We performed non-equilibrium molecular dynamics simulations to explore the effect of nanoscale voids on hotspot growth and initiation in micron-scale pentahexitrol tetranitrate (PETN) crystals under weak shock loading (Up = 1.25 km/s; Us = 4.5 km/s). We used the ReaxFF potential implemented in LAMMPS. We built a pseudo-2D PETN crystal with dimensions 0.3 μm × 0.22 μm × 1.3 nm containing a 20 nm cylindrical void. Once the initial shockwave traversed the entire sample, the shock-front absorbing boundary condition was applied, allowing the simulation to continue for ~0.5 nanoseconds. Results show an exponentially increasing hotspot growth rate. The hotspot morphology is initially symmetric about the void axis, but strong asymmetry develops at later times, due to strong coupling between exothermic chemistry, temperature, and divergent secondary shockwaves emanating from the collapsing void.

1Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s NNSA under contract DE-AC04-94AL85000.

8:48AM L23.00005 Post-stishovite transition in hydrous aluminum SiO$_2$¹. RENATA WENTZCOVITCH, Department of Chemical Engineering and Materials Science, U of Minnesota, Twin Cities, KOICHIRO UMEMOTO, Department of Earth Sciences, U of Minnesota, Twin Cities, MN, USA and Earth and Life Sciences Institute, Tokyo-Tech, Tokyo, Japan, KATSUYUKI KAWAMURA, Department of Sustainable Resource Science, Okayama University, Okayama, Japan, KEI HIROSE, Earth and Life Sciences Institute, Tokyo-Tech, Tokyo, Japan — Incorporation of aluminum and some water into SiO$_2$ significantly reduces the post-stishovite transition pressure in SiO$_2$. This behavior suggests that the ferroelastic post-stishovite transition in subducted Earth’s crust could be the source of seismic anomalies with low shear velocities observed in the mid to upper lower mantle. Using ab initio static calculations and molecular dynamics with inter-atomic potentials, we show that hydrogen bonds play a crucial role in lowering the transition pressure. A cooperative redistribution of hydrogen atoms is the main mechanism responsible for the transition pressure reduction in hydrous aluminium stishovite. The effect is enhanced by increasing the water content and suggests a relationship between the depth of these seismic anomalies and degree of hydration of stishovite in the subducted crust.

1Research supported by NSF/EAR.

9:00AM L23.00006 The Dilemma of the High-Spin Persistence Into the Mbar Range of Some Ferric-Metal Oxides¹. MOSHE P. PARTENAK, GREGORY KH. ROZENBERG, ERAN GREENBERG, WEIMING XU, MARK NIKOLAEVSKY, Tel Aviv University, School of Physics & Astronomy — The fate of the strongly correlated $d-d$ Mott-Hubbard (MH) insulators at extreme conditions of pressure is determined by two main reactions: (i) correlation breakdown due to broadening leading to bands overlap of the empty-filled band resulting in metallization consequently loss of magnetic moment and, (ii) spin crossover due to the augmented crystal-field (10Dq ~ r$^{-5}$) which in the case of the Fe$^{3+}$ - oxides results in $S=5/2 > S=1/2$ transition. The experimental observation of these high pressure phenomena using Diamond-Anvils-Cells and the experimental methods of resistance and $^{57}$Fe Mössbauer effect at varying (P,T) and Synchrotron XRD at RT. This presentation will focus on the recent discovered cases of some Fe$^{3+}$ M/O where the high-spin state prevails into the Mbar region; showing no signs of correlation breakdown. The persistence of correlated, HS states to such pressures cannot be explained. This will be preceded by a short introduction to the experimental methods and cases of pressure-induced spin-crossover or MH transitions.

1Supported in parts by the ISF #789/10 grant.

9:12AM L23.00007 Semi-empirical equations of state for NaCl¹. MICHEL SANTOS, University of Sao Paulo, RENATA WENTZCOVITCH, University of Minnesota — Despite diamond anvil cell experiments having reached pressures of hundreds of GPa, measuring high pressures is still a challenge. One of the strategies adopted in high pressure measurements is to measure the lattice spacing, via x-ray diffraction, of a calibrant pressurizer. This behavior suggests that the ferroelastic post-stishovite transition in subducted Earth’s crust could be the source of seismic anomalies with low shear velocities observed in the mid to upper lower mantle.

¹Research supported by NSF/EAR and CAPES of Brazil.

9:24AM L23.00008 Phase stability and elasticity of CaSiO$_3$ perovskite, FAWEI ZHENG, Department of Chemical Engineering and Materials Science, U of MN -Twin cities, MN, USA, TAO SUN. Key Laboratory of Computational Geodynamics, University of the Chinese Academy of Sciences, Beijing, China, RENATA WENTZCOVITCH, Department of Chemical Engineering and Materials Science, and Minnesota Supercomputing Institute, U of MN -Twin cities, MN, USA — CaSiO$_3$ perovskite (CaPv) is the third most abundant mineral in the Earth’s lower mantle and is a major component of mid-ocean ridge basalt (MORB). This perovskite is stable only at high pressures, it is highly anharmonic, and undergoes a tetragonal to cubic transition at conditions that are still debated. We have used a recently developed hybrid method combining ab initio molecular dynamics with vibrational normal mode analysis to compute its free energy, thermal equation of state, and phase boundary at relevant geophysical conditions. These results are essential for understanding several aspects of mantle convection.
The idea that fossil fuel emissions might cause global warming was first proposed nearly a century ago. In the 1980s, nearly all experts recognized that civilization faced a monumental challenge. By around 2000 the major likely impacts were well understood. Now the task was to pin down the specific risks in each of the many different regions, ecosystems, and human systems. Meanwhile actual impacts began to appear, such as changes in species ranges and unprecedented deadly heat waves. Two common energetic materials, PETN and RDX, were studied wherein we have found unique emission peaks in the frequency range of 0-10THz that arise from select carrier frequencies.

1Research supported by NSF/EAR and NSF/CAREER

10:00AM L23.00011 Thermoelasticity of Al$^{3+}$- and Fe$^{3+}$-bearing bridgemanite$^1$, JUAN VALENCIA-CARDONA, GAURAV SHUKLA, University of Minnesota Twin cities, MATTEO COCCOCIIONI, Ecole Polytechnique Federale de Lausanne, Switzerland, RENATA WENTZCOVITCH, University of Minnesota Twin cities — We present LDA+U calculations of high temperature elastic properties of (Mg$_{1-x}$Fe$_{x}$$^{3+}$)SiO$_3$, bridgemanite ($0 \leq x \leq 0.125$), the most abundant constituent of Earth’s lower mantle. Calculations of aggregate elastic moduli and acoustic velocities for the Mg-end member ($x=0$) are in excellent agreement with the latest high pressure and high temperature experimental measurements. In the iron bearing system, we particularly focus on the change in thermoelastic parameters across the state change that occurs in ferrous iron above ~30 GPa, often attributed to a high-spin (HS) to intermediate spin (IS) crossover but explained by calculations as a lateral displacement of substitutional iron in the bridgemanite cage. We show that the measured effect on the equation of state of this change in the state of iron can be explained by the lateral displacement of substitutional iron, not by the HS to IS crossover. Calculated elastic properties of (Mg$_{0.475}$Fe$_{0.525}$)SiO$_3$ along an adiabatic mantle geotherm, somewhat overestimate longitudinal velocities but produce densities and shear velocities consistent with Preliminary Reference Earth Model data throughout most of the lower mantle.

1Research supported by NSF/EAR and NSF/CAREER

10:12AM L23.00012 Molecular modeling of high-pressure ramp waves in tantalum, J. MATTHEW D. LANE, HOJUN LIM, Sandia National Laboratories, JUSTIN L. BROWN, Sandia National Labs — Ramp wave compression experiments of bcc metals under extreme conditions have produced differing measurements of material strength response. These variations are often attributed to differing experimental techniques, and varying material factors such as microstructure, and strain-rate. We present non-equilibrium molecular dynamics simulations of tantalum for single crystal and two polycrystalline nanostructures out to 250 GPa, over strain states ranging from 10$^{10}$ to 10$^{11}$ 1/s. Results will be compared to recent Z-machine strength experiments, meso-scale crystal plasticity models and continuum-scale polycrystalline model. Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

10:24AM L23.00013 Singly Bonded Layered Polymeric Nitrogen (LP-N)$^1$, CHOONG-SHIK YOO, DANE TOMASINO, MINSEOB KIM, Washington State Univ, JESSE SMITH, HPCAT/APS, Geophysical Laboratory — We report the discovery of novel nitrogen phase synthesized using laser-heated diamond anvil cells at pressures well above the stability field of cg-N. This new phase is characterized by its singly bonded, layered polymeric (LP) structure similar to the predicted Pba2 and two colossal Raman bands, arising from two groups of highly polarized nitrogen atoms in the bulk and surface of the layer, respectively. The present result also provides a new constraint for the nitrogen phase diagram, highlighting an unusual symmetry breaking of the layered polymeric structure.

1The work has been supported by the NSF-DMR (Grant No. 1203834) and DTRA (HDTRA1-12-01-0020).

Wednesday, March 4, 2015 8:00AM - 11:00AM — Session L24 FHP FPS: Invited Session: Pais Prize Session: Physics at the Intersection of History, Technology and Society 203AB - Catherine Westfall, Michigan State University

8:00AM L24.00001 Abraham Pais Prize Lecture: Understanding the Impacts of Global Warming: a History, SPENCER WEART, American Institute of Physics — The idea that fossil fuel emissions might cause global warming was first proposed around the end of the 19th century, and for the following half century it sounded like a good thing. In the 1950s, confirmation that warming really might be coming leading to more varied speculations. Scientists could only state possible problems in vague terms. First on the list were sea-level rise and a threat to food supplies. New ideas were added through the 1960s and 1970s, ranging from the degradation of natural ecosystems to threats to human health. Experts in fields from forestry to economics, even national security, pitched in to assess a variety of possible consequences. It turned out to be impossible to make solid predictions, given the differences from one region to another and the ways human society itself might try to adapt to the changes. In the 1990s, lengthy technical studies abandoned specific predictions of impacts to address “vulnerabilities” under different likely “scenarios.” Researchers also began to explore the risks and consequences of extreme weather events like droughts and floods. By around 2000 the major likely impacts were well understood. Now the task was to pin down the specific risks in each of the many different regions, ecosystems, and human systems. Meanwhile actual impacts began to appear, such as changes in species ranges and unprecedented deadly heat waves. Nearly all experts now understood that civilization faced a monumental challenge.
8:36AM L24.00002 Burnt by the Sun: Jack Kilby and the ’70s Solar Boom . CYRUS MODY, Rice University — Much has been written, by both scientists and historians, about the contributions of Jack Kilby (co-winner of the 2000 Nobel Prize in Physics) to the invention of the integrated circuit and semiconductor microelectronics more generally. The story goes that Kilby conceived of the integrated circuit in 1958 during his first weeks working for Texas Instruments. Considerably less well known, however, is that Kilby took a leave of absence from TI in 1970 to become a consultant and independent inventor. The projects Kilby chose to pursue — from teaching machines to electronic checkwriters to offering advice to the military — offer insights into how establishment scientists and engineers thought about science’s role in solving America’s social and economic problems in the dreary 1970s. I focus in particular on Project Illinois, a residential solar energy system that Kilby and two colleagues proposed in the wake of the OPEC embargo, and which Texas Instruments developed almost to the point of large-scale manufacturing. The cancelation of Project Illinois in 1983 — which precipitated Kilby’s final resignation from TI and retreat from active research — tells us a great deal about the frustrations of doing “socially relevant” science and engineering in the 1970s, and possibly also today.

9:12AM L24.00003 Optimistic Dangers: Views of Radium Therapy During the American Radium Craze , AIMEE SLAUGHTER, Los Alamos Historical Society — 1903 marked the beginning of intense and widespread popular interest in and curiosity about the newly-discovered element radium. This American radium craze was marked by an outpouring of media attention. Radium captured the public’s attention because of its strange properties, which could not be fully explained by scientists: it remained warmer than its surroundings, it glowed in the dark, and it emitted energy from an unknown internal source. The radioactivity emitted by radium also had marked effects on the body. In this talk I will focus on views of these physiological effects of radium during the height of the American radium craze, 1903–1907. Physicists experimented with radium as a therapy, and newspapers reported on radium treatments of ailments ranging from acne to whooping cough. When applied to superficial cancers, radium seemed to melt the tumor away, to be replaced by healthy tissue. Newspapers were quick to report that radium had cured cancer. At the same time, radium was also understood to be a dangerous substance: newspapers discussed the possibility of weaponizing its internal stores of energy, patients were often burned in the course of treatment, and it was speculated that radium in large amounts might blind, maim, or kill someone exposed to it. These dangers were well known but were never mentioned in the uniformly optimistic reports on the potentials of radium therapy. The modern expectation that beneficial applications of science may have a hidden darker side was not part of American culture at the beginning of the twentieth century. The early radium clinic was a unique site where non-scientists physically experienced a new scientific discovery, an element that was both familiar and unknown. At the height of the radium craze, the dangers of radium were optimistically set aside as physicians and physicists were tamed the new element.

9:48AM L24.00004 To Rule the Waves: Cable Telegraphy and the Making of “Maxwell’s Equations” , BRUCE HUNT, University of Texas — How and why did Maxwell’s theory of the electromagnetic field come to be cast into the now familiar form of four vector equations? In particular, how and why was this done not by James Clerk Maxwell himself, but by Oliver Heaviside in a series of articles published in a London electrical trade journal in 1885, several years after Maxwell’s death? The answer, I will argue, lies in the demands and opportunities presented by the global network of submarine telegraph cables, one of the characteristic technologies of the Victorian British Empire. Heaviside, himself a former telegrapher, was steeped in the problems confronting cable telegraphy, particularly the distortion or “retardation” that signals suffered in passing along a cable. It was Heaviside’s search for an effective tool with which to tackle such problems that led him to take up Maxwell’s theory and then to recast it into the four “Maxwell’s equations.”

10:24AM L24.00005 The Social Appropriation of Quantum Language and Imagery , ROBERT CREASE, Stony Brook University — Planck introduced ‘quantum’ as a technical term in 1900 in connection with studies of the emission and absorption of light. Following the development of quantum mechanics in 1925-1927, quantum terminology and imagery – including ‘quantum leap,’ ‘Heisenberg’s Uncertainty Principle,’ and ‘complementarity’ – began appearing in ever-widening cultural spheres, including journalism, literature, philosophy, television, and coffee cups and t-shirts. Later, these terms and images were joined by others, including ‘Schroedinger’s Cat’ and ‘parallel worlds.’ As a result, numerous quantum terms and images have become popular and powerful metaphors in the public imagination. Each of these terms and images followed a different trajectory in moving from their original scientific context into popular culture. This talk explores the trajectories and popular meanings of these terms, as well as their uses and misuses.

Wednesday, March 4, 2015 8:00AM - 10:48AM — Session L25 DCMP: Superconductivity: Miscellaneous Experiments 203B - Eric Palm, High Magnetic Field Laboratory

8:00AM L25.00001 Studying Superconductivity and Magnetism in Y₀₃Co₇ with a Tunnel Diode Resonator Circuit , R.T. GORDON, Western Illinois University, M.D. VANNETTE, Saginaw Valley State University, J. STRYCHALSKA, T. KLIMCZUK, Gdansk University of Technology, R.J. CAVA, Princeton University, R. PROZOROV, Ames Laboratory and Iowa State University — I will discuss recent tunnel diode resonator (TDR) circuit measurements on a single crystal of the material Y₀₃Co₇. This material displays a superconducting transition at Τ_c = 2.5 K and an unusual magnetic state at temperatures just above this transition, up to 8 K. The exact nature of this magnetic state is a point of contention. Following the development of quantum mechanics in 1925-1927, quantum terminology and imagery – including ‘quantum leap,’ ‘Heisenberg’s Uncertainty Principle,’ and ‘complementarity’ – began appearing in ever-widening cultural spheres, including journalism, literature, philosophy, television, and coffee cups and t-shirts. Later, these terms and images were joined by others, including ‘Schroedinger’s Cat’ and ‘parallel worlds.’ As a result, numerous quantum terms and images have become popular and powerful metaphors in the public imagination. Each of these terms and images followed a different trajectory in moving from their original scientific context into popular culture. This talk explores the trajectories and popular meanings of these terms, as well as their uses and misuses.

8:12AM L25.00002 Polaronic high-temperature superconductivity in optimally doped bismuthate Ba₁₋ₓKₓBiO₃ , NICHOLAS DERIMOW, JACOB LABRY, ARMOND KHODAGULIAN, Department of Physics & Astronomy, California State University, Los Angeles, JUN WANG, Department of Physics, Faculty of Science, Ningbo University, Ningbo, P. R. China, GUO-MENG ZHAO, Department of Physics & Astronomy, California State University, Los Angeles — Magnetic measurements have been carried out in the superconducting and normal states of the optimally doped nonmagnetic bismuthate superconductor Ba₁₋ₓKₓBiO₃. The magnetic data along with previous µSR, resistivity, and tunneling data consistently show that there is a large polaronic enhancement in the density of states and effective electron-phonon coupling constant. The first-principle calculation within the density-functional theory indicates a small electron-phonon coupling constant of about 0.3-0.4, which can only lead to about 1 K superconductivity within the conventional phonon-mediated mechanism. Remarkably, the polaronic effect increases the electron-phonon coupling constant to about 1.4, which is large enough to lead to 32 K superconductivity. The present work thus uncovers the mystery of high-temperature superconductivity in bismuthate superconductors, which will also provide important insight into the pairing mechanism of other high-temperature superconductors.

²Derimow acknowledges NIH Grant R25 GM 061331-13.
8:24AM L25.00003 Search for electron-phonon coupling in superconducting BKBO  D. PARSHALL, NIST Center for Neutron Research, Gaithersburg MD 20899, J.L. NIEDZIELA, Oak Ridge National Laboratory, Oak Ridge TN 37831, S. BARILO, Institute of Solid State and Semiconductor Physics, Minsk, 220072, Belarus, J.W. LYNN, NIST Center for Neutron Research, Gaithersburg MD 20899 — Ba0.6K0.4BiO3 is a superconductor with a Tc = 30 K. While generally regarded as a BCS superconductor, previous work searching along the high-symmetry directions did not find characteristic signatures of electron-phonon coupling near the energy gap of ~9 meV. Making use of the new Multizon Phonon Refinement technique, we are able to examine the phonon spectrum at all symmetry points and look for signatures of electron-phonon coupling.

8:36AM L25.00004 Pressure effects on static and dynamic spin properties in CrAs1  M. MATSUDA, M. B. STONE, Quantum Condensed Matter Division, Oak Ridge National Laboratory, J.-G. CHENG, W. WU, F. LIN, J. L. LUO, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, K. MATSUBAYASHI, Y. UWATOKO, Institute for Solid State Physics, University of Tokyo, Japan — CrAs is an antiferromagnetic metal, which shows a helical spin structure accompanied by an abrupt lattice expansion at T\textsubscript{N} ~ 260 K in ambient pressure. With applying pressure, this material shows superconductivity with a maximum transition temperature of ~2 K. Since Cr has the spin degree of freedom, elucidating the magnetic contribution to the superconductivity is crucial to understand the pairing mechanism. Our neutron diffraction studies have revealed that the static magnetic order as well as the structural anomaly is suppressed with applying external pressure. Chemical pressure effect was also studied by substituting As by P, which is found to be almost the same as the external pressure. We also plan to show the magnetic excitations in undoped and P-doped CrAs measured by inelastic neutron scattering experiments, which will give useful information on a coupling between the magnetism and the superconductivity.

8:48AM L25.00005 Chemical doping and pressure effects on the noncentrosymmetric superconductors ZrRe\textsubscript{6} and BiPd1  MOJAMMEL ALAM KHAN, DAVID P. YOUNG, AHMAD US SALEHEEN, AMAR KARKI, DANA BROWNE, P.W. ADAMS, TAPAS SAMANTA, Louisiana State University — Polycrystalline samples of ZrRe\textsubscript{6} doped with Ti, W and Os and BiPd doped with Te and Ni were made using arc melting and RF - induction furnaces. Variation of the superconducting transition temperature with different types of doping was observed. Small suppression of T\textsubscript{c} was observed for both hole and electron doping in ZrRe\textsubscript{6} samples. Suppression in T\textsubscript{c} was also observed for BiPd. The effect of hydrostatic pressure on T\textsubscript{c} was determined for both compounds. Effect of Re depreciation on T\textsubscript{c} for ZrRe\textsubscript{6} were observed by synthesizing samples, ZrRe\textsubscript{5.95} ~ 5.85. In addition, small diameter wires (0.0005" ~ 0.004") of BiPd were synthesized for critical current density measurements. The critical temperature of the wires was found to be slightly higher (~4.07 K) than that reported for bulk samples (~3.78 K).

9:00AM L25.00006 Giant Two-Phonon Raman Signal from NbC Coherent Precipitates in Niobium  JOHN ZASADZINSKI, CHAOYUE CAO, Illinois Institute of Technology, RUNZHE TAO, ROBERT KLIB, University of Illinois Chicago, LANCE COOLEY, Fermi National Accelerator Laboratory — High purity Nb, subjected to the processing steps used in SRF cavity fabrication, has been shown to reveal nanoscale NbC precipitates near the surface that are coherent with the host Nb matrix. Raman backscattering from such regions reveal spectra similar to the earlier work on bulk NbC but with a strongly enhanced two-phonon signal. The unprecedented strength and sharpness of the two phonon response has allowed a direct comparison to \textit{ab initio} calculations of the phonon dispersion curves of NbC under uniform compression where it is shown directly that the two phonon signal originates in the regions of strong electron-phonon renormalization. The strong two phonon signal may indicate an enhancement of the electron phonon spectral function, α\textsuperscript{2}F(ω).

9:12AM L25.00007 Experimental demonstration of superconducting critical temperature increase in electromagnetic metamaterials1  VERA SMOLYANINOVA, BRADLEY YOST, KATHRYN ZANDER, THOMAS GRESSOCK, Towson University, MICHAEL O'SOFSKY, HEUNGOOSO KIM, NRL, SHANTA SAHA, RICHARD GREENE, IGOR SMOLYANINOV, University of Maryland — A recent proposal that the metamaterial approach to dielectric response engineering may increase the critical temperature of a composite superconductor-dielectric metamaterial has been tested in experiments with compressed mixtures of tin and barium titanate nanoparticles of varying composition. An increase of the critical temperature of the order of 0.15 K compared to bulk tin has been observed for 40% volume fraction of barium titanate nanoparticles. Similar results were also obtained with compressed mixtures of tin and strontium titanate nanoparticles.

9:24AM L25.00008 Magneto-transport near a quantum critical point  IAN HAYES, NICHOLAS BREZNAY, University of California Berkeley, ARKADY SHEKHTER, ROSS MCDONALD, National High Magnetic Field Lab, Los Alamos, JAMES ANALYTIS, University of California Berkeley — The physics of quantum critical phase transitions connects to some of the most difficult problems in condensed matter physics, including metal-insulator transitions, frustrated magnetism and high temperature superconductivity. Near a quantum critical point (QCP) a new kind of metal emerges, whose thermodynamic and transport properties do not fit into the unified phenomenology with which we understand conventional metals — the Landau Fermi liquid (FL) theory - characterized by a low temperature limiting T-linear specific heat and a T\textsuperscript{2} resistivity [1]. Studying the evolution of the T\textsuperscript{2} dependence of these observables as a function of a control parameter leads to the identification both of the presence and the nature of the quantum phase transition in candidate systems. In this study we measure the transport properties of basp, at T < T\textsubscript{c} by suppressing superconductivity with high magnetic fields. At sufficiently low temperatures, the resistivity of all compositions (x ≥ 0.31) crosses over from a linear to a quadratic temperature dependence, consistent with a low temperature FL ground state. As compositions with optimal T\textsubscript{c} are approached from the overdoped side, this cross-over becomes steeper, consistent with models of quantum criticality where the effective Fermi temperature T\textsubscript{F} goes to zero.

1This work was supported in part by NSF grant DMR-1104676 at Towson and AFOSR grant FA9550-09-1-0603 at Maryland.

1NSF DMR No.1306392

9:36AM L25.00009 Low-temperature STM Measurements of Granular Pb films\textsuperscript{1}, S.A. MOORE, J. FEDOR, Department of Physics, Temple University, Philadelphia, PA 19122, J. CURTIS, G. KARAPETROV, Department of Physics, Drexel University, Philadelphia, PA 19104, I. BEŁBORODOV, Department of Physics, California State University Northridge, Northridge, CA 91330, M. IAVARONE, Department of Physics, Temple University, Philadelphia, PA 19122 — Using low-temperature scanning tunneling microscopy and spectroscopy (LT-STM/STS) we have investigated the electronic properties of granular Pb films grown on HOPG at low temperature. Films grown under these conditions form a two-dimensional array of disconnected grains with a similar distribution of sizes. Local spectroscopic measurements as a function of field and temperature reveal a grain size dependent competition between the repulsive electron-electron interaction and the attractive superconducting pairing interaction. Our results show the presence of an increased depletion of states around the Fermi energy for all grain sizes, with a complete suppression of the superconducting state below a critical grain size. We compare these results to those found on 9ML and 100ML continuous films also grown on HOPG, where the superconducting state completely dominates the electronic properties.

\textsuperscript{1}Work at Temple University was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0004556.

9:48AM L25.00010 Paramagnetic Meissner effect in electrochemically doped Indium-Tin Oxide films, ALI ALIEV, Alan G. MacDiarmid NanoTech Institute, University of Texas at Dallas, Richardson, TX, 75083 — Transparent conductive indium tin oxide (ITO) thin films, electrochemically intercalated with alkali (Li\textsuperscript{+}, Na\textsuperscript{+}, K\textsuperscript{+}, Rb\textsuperscript{+}, Cs\textsuperscript{+}), alkali earth (Mg\textsuperscript{2+}, Ca\textsuperscript{2+}), or complex NH\textsubscript{4}\textsuperscript{+} ions show tunable superconducting transition with dome shape behavior of $T_c$ versus electron density around the maximum at 5 K. The zero resistance transition in superconducting state is accompanied with paramagnetic Meissner response to the applied external magnetic field, i.e. the increase of magnetization in field cooling regime. We provide extensive evidences of flux trapping using dc SQUID, ac susceptibility and transport measurements. In particular, we present evidence that the paramagnetic response results from the lower $T_c$ on the center of disk samples than on the edges leading to the trapping of magnetic flux in the center, and that change of $T_c$ profile to opposite removes the paramagnetic response. The flux trapped state is metastable. An alteration of external magnetic field destroys the giant vortex.

10:00AM L25.00011 Novel fabrication process for all-MgB\textsubscript{2} Josephson junctions and circuits\textsuperscript{1}, THOMAS MELBOURNE, ELIAS GALAN, XIAOXING XI, KE CHEN, Temple University — A novel process for fabricating high-quality MgB\textsubscript{2}/Mo/MgB\textsubscript{2} Josephson junctions and circuits is reported. A 100 nm-thick bottom electrode of MgB\textsubscript{2} was grown on SiC (0001) substrate by hybrid physical-chemical vapor deposition (HPCVD) and then coated by a 1 – 5 nm-thick MgO junction barrier layer and a 20 nm-thick TiO\textsubscript{2} protection layer. After the bottom MgB\textsubscript{2} layer was patterned an 80 nm-thick MgO etch-stop layer was then deposited on the sample with a pattern created by photo- or e-beam lithography and lift-off, followed by reactive ion etching in SF\textsubscript{6} to form TiO\textsubscript{2} from the Josephson junction areas. Finally, a 100 nm-thick MgB\textsubscript{2} serving as both the top electrode and wiring layer was deposited and patterned by photolithography and ion mill. The advantage over previously reported process is that this process combines the MgB\textsubscript{2} top electrode and the wiring layer, which simplifies fabrication and allows for an additional layer of MgB\textsubscript{2} to be dedicated to a ground plane in circuits. Characteristics of all-MgB\textsubscript{2} Josephson junctions fabricated by this process are shown.

\textsuperscript{1}This work is supported by the U.S Office of Naval Research under grant N00014130052.

10:12AM L25.00012 Electrical transport property of nano carbon superconductors, YUKI MATSUDA, Department of Physics, Tohoku Univ, SATOSHI HEGURI, WPI-AIMR, Tohoku Univ, YOICHI TANABE, Department of Physics, Tohoku Univ, KATSUHIRO NAKAGAWA, WPI-AIMR, Tohoku Univ, MARUKO KOBAYASHI, Kitami Institute of Technology, Asahidai, Kitami, Japan, KAZUYUKI OKAJIMA, Department of Physics, Tohoku Univ, TATSUO TOMITA, Department of Electrical Engineering, Tohoku Univ, YUKI HAYABUSA, Department of Physics, Tohoku Univ — Using low-temperature scanning tunneling microscopy and spectroscopy (LT-STM/STS) we have investigated the electronic properties of granular Pb films grown on HOPG at low temperature. Films grown under these conditions form a two-dimensional array of disconnected grains with a similar distribution of sizes. Local spectroscopic measurements as a function of field and temperature reveal a grain size dependent competition between the repulsive electron-electron interaction and the attractive superconducting pairing interaction. Our results show the presence of an increased depletion of states around the Fermi energy for all grain sizes, with a complete suppression of the superconducting state below a critical grain size. We compare these results to those found on 9ML and 100ML continuous films also grown on HOPG, where the superconducting state completely dominates the electronic properties.

10:24AM L25.00013 Confinement of superconducting fluctuations due to emergent electronic inhomogeneities in ultrathin films, CLÉMENCE CARBILLET, Sorbonne Universités, UPMC, UMR 7588, Institut des Nanosciences de Paris, F-75005, Paris, France, SERGIO CAPRARA, MARCO GRILLI, Department of Physics, University of Rome “La Sapienza,” Piazzale A. Moro 5, I-00185 Rome, Italy, CHRISTOPHE BRUN, TRISTAN CREN, FRANCOIS DEBONTRIDDER, Sorbonne Universités, UPMC, UMR 7588, Institut des Nanosciences de Paris, F-75005, Paris, France, BAPTISTE VIGNOLLE, CNRS/INCM, 143 Avenue de Rangueil, 31400 Toulouse, France, KONSTANTIN ILIN, MICHAEL SIEGLER, Institute of Micro- and Nano-electronic Systems, Karlsruhe Institute of Technology, Hertzstrasse 16, D-76187 Karlsruhe, Germany, DIMITRI RODITCHEV, BRIGITTE LERIDON, LPEM-CNRS/ESPCI-ParisTech/UPMC/PSL, 10 rue Vauquelin, 75005 Paris, France — The question of homogeneity, granularity, or glassiness of materials on the verge of a superconductor/insulator transition is fundamental and hotly debated. Here, by combining macroscopic and nano-scale studies of superconducting ultrathin NbN films, we reveal some nanoscopic electronic inhomogeneity that emerges when the film thickness is reduced. While thicker films display a purely two-dimensional behavior in electrical transport measurements, we demonstrate a seemingly zero-dimensional regime in the superconducting thermal fluctuations for the thinner samples. This regime corresponds to a longer survival and anomalous local diffusion of the Cooper pair fluctuations. Remarkably, the typical length scale, 20-40 nm, extracted from the fluctuation conductivity coincides with the correlation length of the electronic inhomogeneities directly revealed by local scanning tunneling spectroscopy.

10:36AM L25.00014 Hall coefficient of ultrathin niobium in Si/Nb/Si trilayers, MARTA Z. CIEPLAK, I. ZAYTSEVA, O. ABAL’OSHEV, P. DLUZEWSKI, W. PASZKOWICZ, Institute of Physics, PAS, Warsaw, Poland, L.Y. ZHU, C.L. CHIEN, Johns Hopkins University, M. KONCZYKOWSKI, Ecole Polytechnique, Palaiseau, France — We study the structural and magnetotransport properties of ultrathin Nb layers in Si/Nb/Si trilayers, grown by magnetron sputtering at room temperature. The thickness of Nb, d, is in the range from 1.1 nm to 50 nm, with a fixed Si thickness of 10 nm. With decreasing d the superconductivity is suppressed for d < 1.2 nm, and the structure of the Nb layers evolves, from polycrystalline at d > 6 nm, to amorphous at d < 3.3 nm. The Hall coefficient, positive in thick Nb layers, initially increases with decreasing d, but starts to diminish at d < 6 nm, and eventually changes sign into negative at d < 2 nm. In the thinnest Nb layers the dependence of the Hall voltage on magnetic field becomes non-linear at lower temperatures, indicating that two types of carriers contribute to transport. The influence of boundary scattering on the relaxation rate of carriers, and band broadening in the amorphous films, may be responsible for this effect. We discuss the correlation between the superconductivity suppression and the appearance of the electron contribution to the conductance, observed in the present films; we also compare our results to the properties of other previously studied ultrathin Nb films.

\textsuperscript{2}Supported by: Polish NSC Grant No. 2011/01/B/ST3/00462, NSF Grant No. DMR 1262253, French-Polish Program PICS 2012; partially performed in laboratories co-financed by the ERDF Projects POIG.02.01-04-032/08 and POIG.02.01-00-005/09.
8:00AM L26.00001 Exciton Dynamics in Quantum Dot Films and Interfaces1, WILLIAM TISDALE, Massachusetts Inst of Tech-MIT — Colloidal quantum dots (QD) are a promising material platform for solution-processable optoelectronics, devices such as solar cells, light-emitting diodes, thermoemodules, and flexible electronics. Central to the operation of these devices is the formation, transport, and conversion of free charges and excitons. In the first part of the talk, I will present a comprehensive study of exciton diffusion in inhomogeneously broadened QD assemblies, including spectrally-resolved transient photoluminescence spectroscopy, transient photoluminescence quenching, time-resolved optical imaging, and kinetic Monte Carlo simulations. In the second part of the talk, I will show how nanoscale dielectric screening phenomena in atomically thin semiconductors such as MoS_2 can lead to counterintuitive energy transfer behavior from QD donors.

8:36AM L26.00002 Ligand Chemistry and the Low-Frequency Vibrations of Semiconductor Nanocrystals2. ANNA JOLENE MORK, WILLIAM TISDALE, Massachusetts Institute of Technology — A variety of phonon-mediated processes can lead to counterintuitive energy transfer behavior from QD donors.

8:48AM L26.00003 Evolution of “waterproof” photoluminescent complexes of rare earth ions in crowded environment1. MICHAEL BLADES, Lehigh University, TETYANA IGNAITOVA, UC Irvine, JUAN DUQUE, STEPHEN DOORN, Los Alamos National Lab, IVAN BIAGGIO, SLAVA V. ROTKIN, Lehigh University — Understanding behavior of rare-earth ions (REI) in crowded environments is crucial for several nano- and bio-technological applications. Evolution of REI photoluminescence in small compartments inside a silica hydrogel, mimic to a soft matter bio-environment, has been studied and explained within a solvation model. The model uncovered the origin of high rare earth photoluminescence efficiency to be the formation of REI complexes, surrounded by sodium deoxycholate molecules. Comparative study of these REI-deoxycholate complexes in bulk water solution and those enclosed inside the hydrogel revealed a strong correlation between an up to 5 times longer photoluminescence lifetime of REIs and appearance of the deoxycholate ordered phase, further confirmed by dynamics of REI solvation shells, REI diffusion experiments and morphological characterization of microstructure of the hydrogel.

9:00AM L26.00004 Nanointerfaces in InAs-SnxS6 nanocrystal-ligand networks: atomistic and electronic structure from first principles1. EMILIO SCALISE, STEFAN WIPPERMANN, Max-Planck-Institute for Iron Research, GIULIA GALLI, University of Chicago — Semiconducting nanocomposites – consisting of nanocrystals (NCs) embedded in a host matrix – offer exciting prospects for solar energy conversion, light emission and electronic applications. Recent advances in wet chemical techniques allow for the synthesis of NCs, their assembly into superlatices and embedding into a host matrix using only inexpensive solution processing. However, the atomicistic details of such composites are poorly understood, due to the complexity of the synthesis conditions and the unavailability of robust experimental techniques to probe nanointerfaces at the microscopic level. Here we present a density functional theory investigation of the interaction of SnSx ligands with InAs NCs. Employing a grand canonical approach, we considered a multitude of structures possibly realized at the NC-ligand interface, such as surface termination, reconstructions, passivation, substitution of subsurface atoms, ligand dissociation, NC core-shell formation and the adsorption of the ligands on NCs with different structures. This study provides guidance about the experimental conditions which lead to specific structural motifs and highlights the impact of structural details on the composite’s electronic properties.

9:12AM L26.00005 Defect Chemistry of Nanocarbon. YUHUANG WANG, University of Maryland — Defects can rule the properties of a crystal. This effect is particularly intriguing in atom-thick materials such as single-walled carbon nanotubes and graphene, where electrons, excitons, phonons, and spin may strongly couple at the defects due to reduced dimensionality. In this talk, we will discuss our recent progress in fundamental understanding and molecular control of sp3 defects in sp2 carbon lattices, and their applications. An sp3 defect (tetrahedral bonding, diamond-like) is created by covalently attaching a functional group to the sp2 carbon lattice (trigonal planar, honeycomb-like) of a carbon nanotube or graphene. The beauty of this type of defect is its well-defined structure and chemical tunability at the molecular level. Our experimental results have unraveled a series of intriguing and surprising roles of defects. Specific examples will be given to illustrate how defects may be used to drive reaction propagation on sp2 carbon lattices, brighten carbon nanotube photoluminescence, and create selective chemical sensors.

9:48AM L26.00006 Localized Excitons in Carbon Nanotubes. LYUDMYLA ADAMSKA, STEPHEN K. DOORN, SERGEI TRETIAK, Los Alamos National Lab — It has been historically known that unintentional defects in carbon nanotubes (CNTs) may fully quench the fluorescence. However, some dopants may enhance the fluorescence by one order of magnitude thus turning the CNTs, which are excellent light absorbors, in good emitters. We have correlated the experimentally observed photoluminescence spectra to the electronic structure simulations. Our experiment reveals multiple sharp asymmetric emission peaks at energies 50-300 meV red-shifted from that of the lowest bright exciton peak. Our simulations suggest an association of these peaks with deep trap states tied to different specific chemical adducts. While the wave functions of excitons in undoped CNTs are delocalized, those of the deep-trap states are strongly localized and pinned to the dopants. These findings are consistent with the experimental observation of asymmetric broadening of the deep trap emission peaks, which can result from scattering of acoustic phonons on localized excitons. Our work lays the foundation to utilize doping as a generalized route for wave function engineering and direct control of carrier dynamics in SWCNTs toward enhanced light emission properties for photonic applications.
10:00AM L26.00007 Understanding the effect of surface defects on sp2 carbon and HOPG . ANDREW KOZBIAL, VAHID VAHDAT, HAITAO LIU, LEI LI, Univ of Pittsburgh, DEPARTMENT OF CHEMICAL & PETROLEUM ENGINEERING TEAM, DEPARTMENT OF CHEMISTRY TEAM — Basal planes of graphite are traditionally believed to be inert and electrochemical activity of graphitic materials was thought to occur at high energy defect sites, i.e., step edges. However, recent studies have shown the basal surface of graphite to be highly active and these results have significant implication on design of graphitic electrodes along with numerous other graphite, graphene, and carbon nanotube-based products. The mildly hydrophobic surface of fresh graphite subsequently adsorbs airborne contaminants causing the surface to transition towards hydrophobic behavior. A missing link between electrochemical activity and wettability requires elucidation of basal plane behavior and answering whether defect density on a graphite surface affects wettability. We have quantified defect density on various grades of highly ordered pyrolytic graphite (HOPG) through AFM imaging and contrasted wettability results to describe the effect of defect sites on wettability and surface contamination.

10:12AM L26.00008 Calculating exciton downconversion rates in Coulombically coupled chromophores , CRAIG CHAPMAN, GEORGE SCHATZ, Northwestern University — Exciton downconversion is a second order energy transfer process that splits a high energy exciton in a donor chromophore into multiple lower energy excitons in acceptor chromophores. Downconversion has been seen in a variety of materials including rare-earth doped glassy matrices, organic crystals, and semiconductor nanocrystals, and has the potential to efficiently convert a single high energy photon into a broad distribution of lower energy excitons. A comprehensive mechanistic understanding of the energy conversion process will allow for the rational engineering of materials that can control the flow of energy in a guided fashion. To this end we formulate and implement a method for calculating multi-chromophore Förster-like exciton transfer rates using transition charges obtained from time-dependent density functional theory.

10:24AM L26.00009 Raman spectroscopy of electric-field-tuned molecule-semiconductor interface1 , ALEXEY ZAYAK, FLOYD HILTY, ANDREW KUHLMAN, Bowling Green State University — In the search for methods of studying chemical properties of surfaces and atomic-scale heterogeneous interfaces, Raman scattering promises significant potential for measuring physical and chemical properties that vary on the scale of a few chemical bonds, reporting not only about a particular chemical species, but also about the immediate chemical environment. In this work we use first-principles (DFT) computations to investigate the chemical modification of Raman spectra of organic species after being chemically absorbed on semiconductor surfaces. We examine the binding of a trans-1,2-twot(4-pyridyl) ethylene molecule to the PbSe semiconductor surface and show that we can control the degree of the interfacial chemical coupling by means of an external electric field, and at the same time, observe the induced changes in Raman spectra. In the process of applying electric bias, we observed a crossover between two regimes of the interfacial electron-vibron coupling: with vibration-induced charge transfer, and without it.

We acknowledge BGSU for financial support and TACC and OSC for computing time.

Wednesday, March 4, 2015 8:00AM - 10:36AM — Session L27 DCP: Focus Session: Solvation of Ions and Electrons I 204B - Mary T. Rodgers, Wayne State University

8:00AM L27.00001 Comprehensive thermochromoscopy for the hydration of copper ions . PETER ARMENTROUT, University of Utah — Cross sections for the threshold collision-induced dissociation (TCID) of Cu2+(H2O)n+, where n = 8 – 10, and of CuOH+(H2O)n+, where n = 1 – 4, are measured using a guided ion beam tandem mass spectrometer. In both cases, the primary dissociation pathway is found to be loss of a single water molecule followed by the sequential loss of additional water molecules. In the Cu2+ complexes, charge separation to form CuOH+(H2O)2 and H+(H2O)7 is also observed and CuOH+(H2O) competitively loses both H2O and OH. The data are analyzed using a statistical model after accounting for internal and kinetic energy distributions, multiple collisions, and kinetic shifts to obtain 0 K bond dissociation energies (BDEs). In addition, BDEs for the loss of OH from CuOH+(H2O)n, where n = 0 – 4 are derived using the experimental BDEs for dissociation of CuOH+(H2O)n and literature values for Cu+(H2O)n. Experimental BDEs are compared to theoretical BDEs determined at several levels of theory with reasonable agreement. Structural information regarding complexes of CuOH+(H2O)n+, where n = 2 – 9, are also obtained using infrared photodissociation spectroscopy (IRPD) in the OH stretching region and comparison to theoretical spectra. The IRPD spectra of all complexes where n ≥ 3 are consistent with structures generally having a coordination number (CN) of 4 although CuOH+(H2O)7 exhibits bands characteristic of both CN = 4 and CN = 5 isomers.
Nano Lett. [1] V. K. Voora, and K. D. Jordan, systems. The model potentials are used to study nonvalence correlation-bound anion states of large water clusters as well as “superatomic” states of fullerene to characterize nonvalence correlation-bound anion states of a variety of systems including C

Following the completion of the molecule or cluster being dominated by long-range correlation effects. Failure of conventional Hartree-Fock reference based approaches for treating these noncovalent interactions, as electrostatic interactions can be adjusted by introducing different monovalent cations and hydrogen bonding interactions can be adjusted by varying the level of hydration. IRPD spectra with isotopic (H/D) analysis helped unravel the overlapping N-H and O-H stretching modes, a major challenge of earlier studies. Thermodynamic analysis using relative Gibbs free energies, for energy ordering, together with spectral analysis provided unambiguous assignment of spectral features and structural configurations. A systematic hydration model with an in-depth account of noncovalent interactions is presented.

8:48AM L27.00003 Hydration Structures and Thermodynamic Properties of Cationized Biologically Relevant Molecules, M+(Indole)(H2O)n, (M = Na, K; n = 3-6). HAOCHEN KE, JAMES LISY, Univ of Illinois - Urbana — The balance between various noncovalent interactions plays a key role in determining the hydration structures and thermodynamic properties of biologically relevant molecules in biological mediums. Such properties of biologically relevant molecules are closely related to their often unique biological functionalities. The indole moiety is a basic functional group of many important neurotransmitters and hormones and has been used as tractable model for more complex biomolecules. The cationized indole water cluster is a perfect system for the quantitative and systematic study of the competition and cooperation of noncovalent interactions, as electrostatic interactions can be adjusted by introducing different monovalent cations and hydrogen bonding interactions can be adjusted by varying the level of hydration. IRPD spectra with isotopic (H/D) analysis helped unravel the overlapping N-H and O-H stretching modes, a major challenge of earlier studies. Thermodynamic analysis using relative Gibbs free energies, for energy ordering, together with spectral analysis provided unambiguous assignment of spectral features and structural configurations. A systematic hydration model with an in-depth account of noncovalent interactions is presented.

8:48AM L27.00003 Hydration Structures and Thermodynamic Properties of Cationized Biologically Relevant Molecules, M+(Indole)(H2O)n, (M = Na, K; n = 3-6). HAOCHEN KE, JAMES LISY, Univ of Illinois - Urbana — The balance between various noncovalent interactions plays a key role in determining the hydration structures and thermodynamic properties of biologically relevant molecules in biological mediums. Such properties of biologically relevant molecules are closely related to their often unique biological functionalities. The indole moiety is a basic functional group of many important neurotransmitters and hormones and has been used as tractable model for more complex biomolecules. The cationized indole water cluster is a perfect system for the quantitative and systematic study of the competition and cooperation of noncovalent interactions, as electrostatic interactions can be adjusted by introducing different monovalent cations and hydrogen bonding interactions can be adjusted by varying the level of hydration. IRPD spectra with isotopic (H/D) analysis helped unravel the overlapping N-H and O-H stretching modes, a major challenge of earlier studies. Thermodynamic analysis using relative Gibbs free energies, for energy ordering, together with spectral analysis provided unambiguous assignment of spectral features and structural configurations. A systematic hydration model with an in-depth account of noncovalent interactions is presented.

9:00AM L27.00004 How big is the hydrated electron? Thermodynamics of electron solvation and its partial molar volume. DAVID BARTELS, Notre Dame Radiation Laboratory — Several models for the hydrated electron solvation structure have been proposed, which all can do a reasonable job of reproducing the room temperature optical spectrum. As Larsen, Glover and Schwartz [1] demonstrated, tweaking the electron-water pseudopotential can completely change the structure from a cavity to a non-cavity geometry. Deciding between the competing models then requires comparison with other observables. The resonance Raman spectrum and the temperature dependence of the optical spectrum can be cited as evidence in favor of a non-cavity structure [2]. In the present work we will re-examine the thermodynamics of hydration [3]. In particular, we will present new experimental and simulation results for the partial molar volume, which can bear directly on the cavity vs. non-cavity controversy.


9:36AM L27.00005 Theoretical studies of nonvalence correlation-bound anions. VAMSEE VOORA, KENNETH JORDAN, University of Pittsburgh — Nonvalence correlation-bound anion states have been investigated using state-of-the-art ab initio methodologies as well as by model potential approaches. In nonvalence correlation-bound anion states the excess electron occupies a very extended orbital with the binding to the molecule or cluster being dominated by long-range correlation effects. Failure of conventional Hartree-Fock reference based approaches for treating these anionic states is discussed. Ab initio approaches that go beyond Hartree-Fock orbitals, such as Green’s function, and equation-of-motion methods are used to characterize nonvalence correlation-bound anion states of a variety of systems including C60 and C60F6. Edge-bound nonvalence correlation-bound anionic states are established for polycyclic aromatics. Accurate one-electron model potential approaches, parametrized using the results of ab initio calculations, are described. The model potentials are used to study nonvalence correlation-bound anion states of large water clusters as well as "superatomic" states of fullerene systems.

[2] Travel support through New Investigator Travel Award from Division of Chemical Physics (APS) and NSF grant CHE-1111235 are greatly acknowledged.
[3] Presently at University of California, Irvine
10:24AM L27.00007 Mapping the UV Photophysics of Platinum Metal Complexes Bound to Nucleobases\(^1\), ANANYA SEN, CAROLINE DESSENT, University of York — We report the first UV laser spectroscopic study of isolated gas-phase complexes of Platinum metal complexes bound to a nucleobase as model systems for exploring at the molecular level the key photophysical processes involved in photodynamic therapy. Spectra of the Pt\(^{IV}\) (CN)\(_2^−\) • Uracil and Pt\(^{II}\) (CN)\(_2^−\) • Uracil complexes were acquired across the 220–320 nm range using mass-selective photodepletion and photofragment action spectroscopy. The spectra of both complexes reveal prominent UV absorption bands that we assign primarily to excitation of the Uracil \(\pi - \pi^*\) localized chromophore. Distinctive UV photofragments are observed for the complexes, with Pt\(^{IV}\) (CN)\(_2^−\) • Uracil photooxidation resulting in complex fission, while Pt\(^{II}\) (CN)\(_2^−\) • Uracil photooxidation initiates a nucleobase proton-transfer reaction across 4.4–5.2 eV and electron detachment above 5.2 eV. The observed photofragments are consistent with ultrafast decay of a Uracil localized excited state back to the electronic ground state followed by intramolecular vibrational relaxation and ergodic complex fragmentation. In addition, we present recent results to explore how the photophysics of the Platinum complex-nucleobase clusters evolves as a function of nucleobase. Results are presented for Pt\(^{II}\) (CN)\(_2^−\) • Uracil complexed to Cytosine, Thymine and Adenine, reveal distinctive decay dynamics which we attribute to the intrinsic decay dynamics of the nucleobase.

\(^1\)JPC. Lett. 2014, 5, 3281 to 3285 and PCCP 2014, 16, 15490 to 15500

Wednesday, March 4, 2015 8:00AM - 11:00AM –
Session L28 GMAG DMP: Focus Session: Spin Liquids I

8:00AM L28.00001 Thermodynamic properties of magnetic strings on a square lattice\(^1\), LUCAS MOL, DENIS DA MATA OLIVEIRA, Departamento de Física, Universidade Federal de Minas Gerais, MICHAEL BACHMANN, The University of Georgia — In the last years, spin ice systems have increasingly attracted attention by the scientific community, mainly due to the appearance of collective excitations that behave as magnetic monopole like particles. In these systems, geometrical frustration induces the appearance of degenerated ground states characterized by a local energy minimization rule, the ice rule. Violations of this rule were shown to behave like magnetic monopoles connected by a string of dipoles that carries the magnetic flux from one monopole to the other. In order to obtain a deeper knowledge about the behavior of these excitations we study the thermodynamics of a kind of magnetic polymer formed by a chain of magnetic dipoles in a square lattice. This system is expected to capture the main properties of monopole-string excitations in the artificial square spin ice. It has been found recently that in this geometry the monopoles are confined, but the effective string tension is reduced by entropic effects. To obtain the thermodynamic properties of the strings we have exactly enumerated all possible string configurations of a given length and used standard statistical mechanics analysis to calculate thermodynamic quantities. We show that the low-temperature behavior is governed by strings that satisfy ice rules.

\(^1\)Financial support from FAPEMIG and CNPq (Brazilian agencies) are gratefully acknowledged.

8:12AM L28.00002 Dimer liquid state in the quantum dimer-pentamer model on the square lattice, OWEN MYERS, University of Vermont, C.M. HERDMAN, University of Waterloo — We study the ground state of the quantum dimer-pentamer model (QDPM) on the square lattice. This model is a generalization of the square lattice quantum dimer model (QDM) as its configuration space comprises fully-packed hard-core dimer coverings as well as configurations containing pentamers, where four dimers touch a vertex. Thus in the QDPM, the fully-packed, hard-core constraint of the QDM is relaxed such that the local dimer number at each vertex is fixed modulo 3; correspondingly, the local U(1) gauge symmetry of the QDM Hilbert space is reduced to a local Z\(_3\) gauge symmetry in the QDPM. We construct a local Hamiltonian for which the Rokhsar-Kivelson (RK) state (the equal superposition of all configurations in a topological sector) is the exact ground state and has a 9-fold topological degeneracy on the torus. Using Monte Carlo calculations, we find no spontaneous symmetry breaking in the RK wavefunction and that its dimer-dimer correlation function decays exponentially. Additionally, we discuss the possibility of \(Z_3\) topological order in the ground state of the QDPM.

8:24AM L28.00003 Breakdown of antiferromagnetism and the Coulomb phase for RVB states on anisotropic three-dimensional lattices, K.S.D. BEACH, University of Mississippi — Nearest-neighbor (NN) resonating-valence-bond (RVB) wave functions often serve as prototype ground states for various frustrated models in two dimensions because of their lack of long-range magnetic correlations. In three dimensions, these states are generally not featureless, and their tendency is toward antiferromagnetic order. On the cubic and diamond lattices, for example, the NN RVB state exhibits both antiferromagnetism and power law dimer correlations characteristic of the “Coulomb phase” (in analogy with classical hardcore dimer models). The introduction of strong spatial anisotropy, however, leads to the destruction of these long-range and algebraic correlations, leaving behind an apparent short-range spin liquid state. We characterize the critical exponents at the phase boundaries for wave functions built from products of SU(2) singlets as well as their SU(N) generalizations and discuss attempts to construct a field theory that describes the transitions.

8:36AM L28.00004 Topological defects in quantum spin-nematics, YUTAKA AKAGI, HIROAKI T. UEDA, NIC SHANNON, Okinawa Institute of Science and Technology — Topological defects play an important role in the theory of nematic phases in liquid crystals. However, relatively little is known about their role in quantum spin nematic phases which have no long-range dipole order and break only spin-rotational symmetry [1-3]. Here, we consider the topological defects in these nontrivial states. The model is the spin-1 bilinear biquadratic model on the triangular lattice [4-6]. We classify the defects by homotopy theory and numerical optimization approach, simulated annealing. We also discuss new type defects at particular point, which has global SU(3) symmetry.

8:48AM L28.00005 Singlet-triplet excitations and long range entanglement in the spin-orbital liquid candidate FeSc$_2$S$_4$\(^1\). N. J. LAURITA, Institute of Quantum Matter, Johns Hopkins University, J. DEISENHOFER, University of Augsburg, LIDONG PAN, C.M. MORRIS, Institute of Quantum Matter, Johns Hopkins University, M. SCHMIDT, University of Augsburg, M. JOHNSSON, Stockholm University, V. TSURKAN, University of Augsburg, Academy of Sciences of Moldova, A. LOIDL, University of Augsburg, N.P. ARMITAGE, Institute of Quantum Matter, Johns Hopkins University — Theoretical models of the spin-orbital liquid (SOL) FeSc$_2$S$_4$ have predicted it to be in close proximity to a quantum critical point separating a spin-orbital liquid phase from a long-range ordered magnetic phase. Here, we examine the magnetic excitations of FeSc$_2$S$_4$ through time-domain terahertz spectroscopy under an applied magnetic field. At low temperatures an excitation emerges that we attribute to a single-triplet excitation from the SOL ground state. A three-fold splitting of this excitation is observed as a function of applied magnetic field. Using experimentally obtained parameters, we compare to existing theoretical models to determine FeSc$_2$S$_4$’s proximity to the quantum critical point and establish FeSc$_2$S$_4$ as a SOL with long-range entanglement.

\(^1\)Work at Johns Hopkins was supported by the Gordon and Betty Moore Foundation through Grant GBMF2628, the DOE-BES through DE-FG02-08ER46544, and the ARCS Foundation.

9:00AM L28.00006 Probing hidden orders in frustrated magnets, LUCILE SAVARY, T. SENTHIL, Massachusetts Institute of Technology — We propose a new direct way to experimentally probe some hidden orders, in particular, spin nematic order in magnets. Both the general formulation and particular applications to possible materials with specific hidden orders will be discussed.

9:12AM L28.00007 A continuous Mott transition between a metal and a quantum spin liquid, RYAN V. MISHMASH, Caltech and UCSB, IVAN GONZALEZ, CESGA, ROGER G. MELKO, Waterloo and Perimeter Institute, OLEXEI I. MOTRÜNICH, Caltech, MATTHEW P. A. FISHER, UCSB — More than half a century after first being proposed by Sir Nevill Mott, the deceptively simple question of whether the interaction-driven electronic metal-insulator transition may be continuous remains enigmatic. Recent experiments on two-dimensional materials suggest that when the insulator is a quantum spin liquid, lack of magnetic long-range order on the insulating side may cause the transition to be continuous, or only very weakly first order. Motivated by this, we study a half-filled extended Hubbard model on a triangular lattice strip geometry. We argue, through use of large-scale numerical simulations and analytical bosonization, that this model harbors a continuous (Kosterlitz-Thouless-like) quantum phase transition between a metal and a gapless spin liquid characterized by a spinon Fermi sea, i.e., a “spin Bose metal”. These results may provide a rare insight into the development of Mott criticality in strongly interacting two-dimensional materials and elucidate a mechanism by which spin-liquid phases are stabilized in the vicinity of such transitions.

9:24AM L28.00008 The phase diagram of the XXZ model and the extended Hubbard model on the triangular lattice\(^1\), SEBASTIAN EGGERT, XUE-FENG ZHANG, DANIEL SELLMANN, Univ. of Kaiserslautern, Germany, CLAUDIUS GROS, LUCA TOCCHIO, Univ. of Frankfurt, Germany — The Heisenberg model on the triangular lattice was proposed as the first example of a spin-liquid by Anderson in the early 70’s. Even though the isotropic Heisenberg model is by now well understood and known not to be a spin-liquid in the modern sense, so far the full phase diagram of the xxz model on the triangular lattice has received little attention. We now present DMRG calculations on order parameters and entanglement measures in order to establish the quantitative phase diagram as a function of both field and Ising anisotropy. We then also discuss the effect of introducing spin and charge degrees of freedom by considering the extended Hubbard model on the triangular lattice as a function of filling. In this case there is a very rich phase diagram with several different phases, where a stable charge order coexists with conducting behavior.

\(^1\)Supported by OPTIMAS and the Deutsche Forschungsgemeinschaft via the SFB/TR49

9:36AM L28.00009 Possible spin liquid phase of the $S = 1/2$ J1-J2 triangular Heisenberg model\(^1\), ZHENYUE ZHU, UC Irvine, DAVID HUSE, princeton University, STEVEN WHITE, UC Irvine — We study the $S = 1/2$ Heisenberg model on the triangular lattice with nearest neighbor interaction $J_1$ and next nearest neighbor interaction $J_2$ with the density matrix renormalization group. We are able to study long open cylinders with width up to 9 lattice spacings. At $J_2/J_1 = 0.1$, we find a possible spin liquid (SL) state with short range spin-spin, bond-bond and chiral correlation lengths, bordered by a classical $120^\circ$ Need order pattern at small $J_2$ and a two sub-lattice collinear magnetic ordered state at $J_2 > 0.17$. We identify two quasi-degenerate ground states in the SL phase on long even cylinders, with an energy gap that decreases exponentially with the cylinder width. We also observe a dimerization effect on odd cylinders. We further find a large spin triplet gap. Our evidence supports a fully gapped SL state for the intermediate phase.

\(^1\)Supported by NSF Grant No. DMR-1161348 and Simon foundation on the Many Electron Problem

9:48AM L28.00010 Quantum spin liquid in a $\pi$ flux triangular lattice Hubbard model, STEPHAN RACHEL, Technical University Dresden, MANUEL LAUBACH, University of Wuerzburg, JOHANNES REUther, Dahlem Center for Complex Quantum Systems and Freie Universitaet Berlin, RONNY THOMALE, University of Wuerzburg — We propose the $\pi$ flux triangular lattice Hubbard model ($\pi$-THM) as a prototypical setup to stabilize magnetically disordered quantum states of matter in the presence of charge fluctuations. The quantum paramagnetic domain of the $\pi$-THM which we identify for intermediate Hubbard $U$ is framed by a Dirac semi-metal for weak coupling and by $120^\circ$ Néel order for strong coupling. Generalizing the Klein duality from spin Hamiltonians to tight-binding models, the $\pi$-THM maps to a Hubbard model which corresponds to the $(J_1, J_3) = (-1, 2)$ Heisenberg-Kitaev model in its strong coupling limit. The $\pi$-THM provides a promising microscopic testing ground for exotic finite-$U$ spin liquid ground states amenable to numerical investigation.

10:00AM L28.00011 Quantum Antiferromagnets and Emergent Orders on Spatial Anisotropic Triangular Lattices, JIAN-JIAN MIAO, DONG-HUI XU, YI ZHOU, FU-Chun ZHANG, Zhejiang Univ — Schweniger boson representation and large $N$ expansion technique is applied to the quantum antiferromagnetic Heisenberg model on triangular lattices with spatial anisotropic nearest-neighbor and next-nearest-neighbor coupling. In the large $N$ limit, we found several degenerate ground states with different magnetic ordering on sub-lattices, where the non-zero bonds form honeycomb lattice or dice lattice. Large $\kappa = (N^{-1})$ expansion is used to lift the degeneracy and to obtain the phase diagram. Possible applications to recent discovered compound LiZnMo$_3$O$_8$ are discussed.
10:12AM L28.00012 Magnetism in $S = 1/2$ Double Perovskites with Strong Spin-Orbit Interactions, HIROAKI ISHIZUKA, LEON BALENTS, University of California, Santa Barbara — Motivated by recent studies on heavy-element double-perovskite (DP) compounds, we theoretically studied spin models on a FCC lattice with anisotropic interactions. In these systems, competition/cooperation of spin, orbital, and the lattice degrees of freedoms in the presence of the strong-spin orbit coupling is of particular interest. In a previous theoretical study, the magnetic phase diagrams of DP compounds with $S_1$ electron configuration was studied using a model with four-fold degenerated single-ion state. On the other hand, a recent experiment on a DP material, Ba$_2$Na$_2$OsO$_6$, reported that the compound is likely to be an effective $S = 1/2$ magnet. Inspired by the experimental observation, we considered spin models with symmetry-allowed anisotropic nearest-neighbor interactions. By a combination of various analytical and numerical techniques, we present the magnetic phase diagram of the model and the effect of thermal and quantum fluctuations. In particular, we show that fluctuations induce $(110)$ anisotropy of magnetic moments. We also discuss a possible “nematic” phase driven by spin-phonon couplings.

[1] H. Ishizuka and L. Balents, accepted for publication in PRB.

10:24AM L28.00013 A liquid-gas transition in a 3D Kitaev model, JOJI NASU, Tokyo Institute of Technology — Quantum spin liquid (QSL) is an exotic quantum state of matter in insulating magnets, where long-range ordering is suppressed down to the lowest temperature. Several experimental candidates of QSL have been recently nominated thus far. In their characterization, the absence of thermodynamic anomalies, namely, adiabatic connection from the high-temperature paramagnet (spin gas), is regarded as a hallmark of QSL. Although adiabatic connection between liquid and gas is allowed by bypassing the critical end point in conventional fluids, it is highly nontrivial whether a thermodynamic transition between QSL and paramagnet exists or not in quantum spin systems. The issue is crucial not only for theoretical understanding of QSLs but also for the interpretation of existing and forthcoming experiments. To clarify this problem, we investigate a three-dimensional extension of the Kitaev model [1,2,3]. This model is relevant to the recently found Ir oxides Li$_2$IrO$_3$. The Kitaev model is one of the soluble quantum spin models, where the ground state is given by gapped and gapless QSLs, depending on the anisotropy of the interactions. This model can be rewritten as a free Majorana fermion system coupled with $Z_2$ variables. Using this representation, we perform the Monte Carlo simulation and analyze the thermodynamic properties. We find that the model exhibits a finite-temperature phase transition between the QSLs and paramagnet in the whole parameter range. This result indicates that both gapless and gapped QSL phases at low temperatures are always distinguished from the high-temperature paramagnet by a phase transition. We also find that the difference between QSL and paramagnet comes from the topological nature of the excitations. This work has been done in collaboration with Y. Motome and M. Udagawa in Univ. of Tokyo. [1] J. Nasu, M. Udagawa, and Y. Motome, Phys. Rev. Lett. 113 197205 (2014). [2] J. Nasu et al., Phys. Rev. B 89 115125 (2014). [3] J. Nasu, M. Udagawa, and Y. Motome, preprint (arXiv:1409.4865).

Wednesday, March 4, 2015 8:00AM - 11:00AM — Session L29 GMAG DMP FIAP: Focus Session: Spin Transport and Voltage Control 206A — Ronny Knut, National Institute of Standards and Technology

8:00AM L29.00001 Voltage controlled magnetism in 3d transitional metals, WEIGANG WANG, Univ of Arizona — Despite having attracted much attention in multiferroic materials and diluted magnetic semiconductors, the impact of an electric field on the magnetic properties remains largely unknown in 3d transitional ferromagnets (FMs) until recent years. A great deal of effort has been focused on the voltage-controlled magnetic anisotropy (VCMA) effect where the modulation of anisotropy field is understood by the change of electron density among different d orbitals of FMs in the presence of an electric field. Here we demonstrate another approach to alter the magnetism by electrically controlling the oxidation state of the 3d FM at the FM/oxide interface. The thin FM film sandwiched between a heavy metal layer and a gate oxide can be reversibly changed from an optimally-oxidized state with a strong perpendicular magnetic anisotropy to a metallic state with an in-plane magnetic anisotropy, or to a fully-oxidized state with nearly zero magnetization, depending on the polarity and time duration of the applied electric fields. This is a voltage controlled magnetism (VCM) effect, where both the saturation magnetization and anisotropy field of the 3d FM can be reversibly controlled by voltage in a non-volatile fashion. We will also discuss the impact of this VCM effect on magnetic tunnel junctions and spin Hall switching experiments. This work, in collaboration with C. Bi, Y.H. Liu, T. Newhouse-Illige, M. Xu, M. Rosales, J.W. Freeland, O. Mryasov, S. Zhang, and S.G.E. te Velthuis, was supported in part by NSF (ECCS-1310338) and by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA.

8:36AM L29.00002 Field-dependent perpendicular magnetic anisotropy and interfacial metal-insulator transition in CoFeB/MgO systems, IGOR BARSUKOV, University of California, Irvine, YU FU, INAC/CEA, Grenoble, France, C. SAFRANSKI, YU-JIN CHEN, B. YOUNGBLOOD, University of California, Irvine, A. GONCALVES, L. SAMPAYO, CBPF, Rio de Janeiro, Brazil, R. ARIAS, Universidad de Chile, Santiago, Chile, M. SPASOVA, M. FARLE, CeNIDE, University Duisburg-Essen, Duisburg, Germany, I. KRIVOROTOV, University of California, Irvine — The CoFeB/MgO interface is a central role in magnetic tunnel junction devices due to the high tunneling magnetoresistance ratio. A strong perpendicular anisotropy (PMA) and voltage-controlled anisotropy are beneficial for spintronics application. We study PMA in thin films of Ta$_2$/Co$_{20}$Fe$_{60}$B$_{20}$/MgO in the thickness range of 0.9-2.5 nm and find that it can be best described by the first two order terms. Surprisingly, we find PMA to be strongly field-dependent [1]. Our results show that the field dependence has significant implications for determining and customizing magnetic anisotropy in spintronic applications. Our data suggest that it can be caused by an inhomogeneous interfacial spin pinning with a possibly ferrimagnetic phase at the CoFeB/MgO interface. We perform magnetometry and transport measurements and find a magnetization peak and resistance transitions at 160K, which are consistent with the presence of an interfacial oxide phase undergoing a Morin-like [2] transition. [1] I. Barsukov et al., 105, 152403 (2014) [2] F. J. Morin, Phys. Rev. Lett. 3, 34 (1959)

8:48AM L29.00003 Electric Polarization Controllable Magnetoresistance of Magnetic Ferroelectric Tunnel Junctions, MEI FANG, YANMEI WANG, Fudan University, DAL SUN, University of Utah, XIAOSHAN XU, University of Nebraska at Lincoln, WENTING YANG, LIFENG YING, Fudan University, JIANG LU, HO NYUNG LEE, Oak Ridge National Laboratory, JIAN SHEN, Fudan University, FUDAN UNIVERSITY TEAM, UNIVERSITY OF UTAH COLLABORATION, UNIVERSITY OF NEBRASKA AT LINCOLN COLLABORATION — The tunneling of electrons through ferroelectric material sandwiched by ferromagnetic electrodes, dubbed magnetic ferroelectric tunnel junctions (MFTJs), can be affected by not only the magnetic alignments between the two ferromagnetic electrodes, but also the electric polarization of the ferroelectric layer, which is right for multi-functional device applications. In this work, we investigate the TMR response during the switching process of electric polarization of the ferroelectric layer. Using a parallel connection mode for polarized up and polarized down domains of the PZT layer, the percentage of switched domain and its corresponding TMR are determined. The calculation results agree well with the experiments data.

The work was supported by National Basic Research Program of China (973 Program), National Natural Science Foundation of China and China Postdoctoral Science Foundation.
Voltage controlled magnetocrystalline anisotropy at the Fe/MgO (001) interface. Pavel Lukashev, University of Northern Iowa, Evgeny Tsymbal, University of Nebraska - Lincoln — The effect of electric fields on magnetocrystalline anisotropy energy (MAE) is a promising way to control the magnetization orientation purely by voltage (rather than by current required for a spin transfer torque), which can potentially alleviate the energy dissipation bottleneck of the existing magnetic memory technology. Here we perform density-functional calculations to explore the voltage controlled magnetic anisotropy (VCMA) of a thin film Fe stacked along the [001] direction when an external electric field is applied across an adjacent epitaxial MgO layer. The results are analyzed by evaluating layer and orbital resolved contributions to MAE. We find that MAE is confined to a depth of few atomic layers near the interface, as determined by the metal screening length, indicating that the VCMA is an interface effect. The applied electric field leads to a nearly linear change in the interface MAE due to a change in the 3d-orbital occupancy of the interfacial Fe atoms and is enhanced, as compared to the clean Fe (001) surface, due to a relatively large dielectric constant of MgO. In addition to the electric field screening, there is a notable effect of atomic displacements driven by an applied electric field, when atomic relaxations are taken into account.

First-principles study of electric field and structural strain impact on perpendicular magnetic anisotropy of Fe/MgO interfaces. Fatima Ibrahim, Hongxin Yang, Bernhard Dieny, Mairbek Chshiev, Spintec, CEA/BRGM/Institut Néel, INAC, 38054 Grenoble, France — Electric-field (EF) control of magnetic anisotropy is promising in the context of establishing low-energy consumption memory devices [1] since it allows EF-assisted switching of magnetization in magnetic tunnel junctions with perpendicular magnetic anisotropy (PMA) [2]. Using first-principles calculations, we demonstrate that both the EF and structural strain induce changes of the PMA in Fe/MgO interfaces which originally exhibit strong PMA [3]. Namely, we find that the PMA change in response to strain is much larger than that induced by applied EF. This suggests that the EF control of PMA is caused not only by charge accumulation and depletion mechanism but rather mediated by structural modifications occurring at the interface in agreement with recent experimental reports [4,5]. In addition, using atomic and orbital-resolved analysis of PMA, we elucidate the effect of both the EF and structural strain on PMA showing in particular that it extends beyond the interfacial layer.

Voltage-controlled magnetic tunnel junctions with Gd$_2$O$_3$ barriers. Ty Newhouse-Illige, Charles Stanford, Matthew Gamble, Chong Bi, Hamid Almasi, Weigang Wang, University of Arizona — It is of great importance to investigate magnetic tunnel junction (MTJ) with high-k barriers, with the premise that a large voltage-controlled magnetic anisotropy (VCMA) can be achieved due to the increased charge transfer effect. Gd$_2$O$_3$ has a dielectric constant of 22, which is substantially larger than that of MgO (∼ 9). It is critical to achieve crystalline barrier with cubic phase in order to obtain symmetry-conserved tunneling as in MgO-based MTJs. We have demonstrated that cubic Gd$_2$O$_3$ can be grown on amorphous CoFeB by reactive sputtering under proper conditions. In exchanged-biased MTJs with in-plane anisotropy, magnetotunneling anisotropy (MTA) up to 20 K has been obtained. The sharp switching at near zero field and exchange-bias field higher than 800 Oe indicate the magnetic properties of the CoFeB in these junctions are nearly as good as in MgO-based MTJs. MTJs with interfacial perpendicular magnetic anisotropy (PMA) has been created with TMR ∼ 10%. A very interesting VCMA effect in these Gd$_2$O$_3$-based MTJs has been observed and will be discussed. This work was supported in part by NSF (CCF-1310338) and by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA.

A transition in the magneto-transport in the L1$_0$ MnAl thin films. Linqiang Luo, Jiwei Lu, Nian Diao, Yishen Cui, Stuart A. Wolf, University of Virginia — In this talk we will report on L1$_0$ MnAl thin films with perpendicular magnetic anisotropy prepared on single crystal MgO substrates by co-sputtering Mn and Al targets. A Cr seed layer enabled the epitaxial growth of the MnAl films. The magneto-resistance (MR) of these films was measured using a Hall bar structure. When the external electric field was applied perpendicular to the thin film surface, a change in the magnetic state of the MR was observed as will be discussed below. Above 175K, a negative magneto-oresistance was observed with two maxima occurring at the coercivity fields of the MnAl thin films. Below 175K, the MR became positive, and the MR ratio increased with decreasing temperature. The possible mechanisms for the transition in the MR will be discussed in detail in this talk. They include the effects of inhomogeneity, chemical ordering and the underlying domain structure.

Voltage-controlled magnetocrystalline anisotropy at the Fe/MgO (001) interface. Pavel Lukashev, University of Northern Iowa, Evgeny Tsymbal, University of Nebraska - Lincoln — The effect of electric fields on magnetocrystalline anisotropy energy (MAE) is a promising way to control the magnetization orientation purely by voltage (rather than by current required for a spin transfer torque), which can potentially alleviate the energy dissipation bottleneck of the existing magnetic memory technology. Here we perform density-functional calculations to explore the voltage controlled magnetic anisotropy (VCMA) of a thin film Fe stacked along the [001] direction when an external electric field is applied across an adjacent epitaxial MgO layer. The results are analyzed by evaluating layer and orbital resolved contributions to MAE. We find that MAE is confined to a depth of few atomic layers near the interface, as determined by the metal screening length, indicating that the VCMA is an interface effect. The applied electric field leads to a nearly linear change in the interface MAE due to a change in the 3d-orbital occupancy of the interfacial Fe atoms and is enhanced, as compared to the clean Fe (001) surface, due to a relatively large dielectric constant of MgO. In addition to the electric field screening, there is a notable effect of atomic displacements driven by an applied electric field, when atomic relaxations are taken into account.

First-principles study of electric field and structural strain impact on perpendicular magnetic anisotropy of Fe/MgO interfaces. Fatima Ibrahim, Hongxin Yang, Bernhard Dieny, Mairbek Chshiev, Spintec, CEA/BRGM/Institut Néel, INAC, 38054 Grenoble, France — Electric-field (EF) control of magnetic anisotropy is promising in the context of establishing low-energy consumption memory devices [1] since it allows EF-assisted switching of magnetization in magnetic tunnel junctions with perpendicular magnetic anisotropy (PMA) [2]. Using first-principles calculations, we demonstrate that both the EF and structural strain induce changes of the PMA in Fe/MgO interfaces which originally exhibit strong PMA [3]. Namely, we find that the PMA change in response to strain is much larger than that induced by applied EF. This suggests that the EF control of PMA is caused not only by charge accumulation and depletion mechanism but rather mediated by structural modifications occurring at the interface in agreement with recent experimental reports [4,5]. In addition, using atomic and orbital-resolved analysis of PMA, we elucidate the effect of both the EF and structural strain on PMA showing in particular that it extends beyond the interfacial layer.

Voltage-controlled magnetic tunnel junctions with Gd$_2$O$_3$ barriers. Ty Newhouse-Illige, Charles Stanford, Matthew Gamble, Chong Bi, Hamid Almasi, Weigang Wang, University of Arizona — It is of great importance to investigate magnetic tunnel junction (MTJ) with high-k barriers, with the premise that a large voltage-controlled magnetic anisotropy (VCMA) can be achieved due to the increased charge transfer effect. Gd$_2$O$_3$ has a dielectric constant of 22, which is substantially larger than that of MgO (∼ 9). It is critical to achieve crystalline barrier with cubic phase in order to obtain symmetry-conserved tunneling as in MgO-based MTJs. We have demonstrated that cubic Gd$_2$O$_3$ can be grown on amorphous CoFeB by reactive sputtering under proper conditions. In exchanged-biased MTJs with in-plane anisotropy, magnetotunneling anisotropy (MTA) up to 125 K has been obtained. The sharp switching at near zero field and exchange-bias field higher than 800 Oe indicate the magnetic properties of the CoFeB in these junctions are nearly as good as in MgO-based MTJs. MTJs with interfacial perpendicular magnetic anisotropy (PMA) has been created with TMR ∼ 10%. A very interesting VCMA effect in these Gd$_2$O$_3$-based MTJs has been observed and will be discussed. This work was supported in part by NSF (CCF-1310338) and by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA.

A transition in the magneto-transport in the L1$_0$ MnAl thin films. Linqiang Luo, Jiwei Lu, Nian Diao, Yishen Cui, Stuart A. Wolf, University of Virginia — In this talk we will report on L1$_0$ MnAl thin films with perpendicular magnetic anisotropy prepared on single crystal MgO substrates by co-sputtering Mn and Al targets. A Cr seed layer enabled the epitaxial growth of the MnAl films. The magneto-resistance (MR) of these films was measured using a Hall bar structure. When the external electric field was applied perpendicular to the thin film surface, a change in the magnetic state of the MR was observed as will be discussed below. Above 175K, a negative magneto-oresistance was observed with two maxima occurring at the coercivity fields of the MnAl thin films. Below 175K, the MR became positive, and the MR ratio increased with decreasing temperature. The possible mechanisms for the transition in the MR will be discussed in detail in this talk. They include the effects of inhomogeneity, chemical ordering and the underlying domain structure.

The authors gratefully acknowledge financial support provided by INSPIRE program.

Near Room Temperature Kondo-Suppression of Spin Accumulation in Cu-Based Non-Local Spin Valves. Justin Watts, University of Minnesota, Liam O’Brien, University of Minnesota, University of Cambridge, Paul Crowell, Chris Leighton, University of Minnesota — Recent studies on metallic non-local spin valves have focused on the anomalous temperature dependence of the spin accumulation signal, $\Delta R_{NL}$, which unexpectedly decreases at low temperatures. O’Brien et al. (Nat. Commun. 5, 3927, 2014) advanced an explanation, based on interdiffusion-induced local moments suppressing injected spin polarization via a manifestation of the Kondo effect. Here we extend this work to devices based on Co/Cu, a combination for which the Kondo temperature can exceed 300 K. Non-magnetic channel thicknesses, $L_y$, from 50 to 200 nm have been explored, along with annealing temperatures up to 100 °C. The decrease in spin diffusion length in Cu from 300 nm for $L_y = 50$ nm to 20 nm for $L_y = 200$ nm, and its change upon annealing, will be discussed in detail. Most importantly we find that, despite the limited miscibility of Co in Cu, a significant decrease in $\Delta R_{NL}$ occurs with decreasing temperature as the Cu channel thickness is reduced. In the thinnest channels we find the maximum in $\Delta R_{NL}$ occurs near room temperature. This result implies that local moment formation and the associated Kondo physics can impact the performance of spin transport devices at ambient temperature in a very common and technologically important materials system.

This work was supported by Seagate Technology, the NSF MRSEC and NEB 2020 programs, and the 7th European Community Framework Programme.
10:12AM L29.000010 Asymmetric spin absorption into a nonlocal spin detector. SHUHAN CHEN, CHUAN QIN, YI JJ, University of Delaware — Nonlocal spin detection measures a spin-dependent chemical potential difference associated with a spin accumulation in a nonmagnetic channel. Typically a ferromagnetic spin detector is in contact with the nonmagnetic channel. A spin-dependent voltage is developed between the detector and the channel when a fraction of the spin current in the channel is absorbed into the detector. We explore an unconventional approach for nonlocal spin detection by probing the voltage between the two ends of the ferromagnetic spin detector. The nonlocal spin valves with 150 nm wide Cu channels are fabricated by e-beam lithography. The ferromagnetic Py spin injectors are 250 nm wide and Py spin detectors are 120 nm wide. Low-resistance AlOx barriers are placed between the Py and the Cu. Since the spin absorption across the Cu/AlOx/Py detector interface is not spatially uniform, a net emf is formed near the junction and a net voltage develops between the two ends of the spin detector. This spin-dependent voltage is clearly detectable at room temperature and suggests an unconventional method of detecting nonlocal spin accumulation.

10:24AM L29.00011 Transport properties of $\text{RPtBi (R = Gd, Dy, Tm, and Lu)}$ under applied magnetic fields. EUNDEOK MUN, Simon Fraser University, SERGEY BUD’KO, PAUL CANFIELD, Iowa State University, Ames Laboratory — It has been suggested that the combination of strong spin-orbit coupling and noncentrosymmetric crystal structure make ternary Heusler compounds a strong candidate for 3D topological materials. The crystal structure of rare-earth platinum bismuth ($\text{RPTBi}$) half-Heusler compounds lacks an inversion symmetry, hence the material is a noncentrosymmetric. The earlier electrical resistivity data of $\text{RPTBi}$ revealed a systematic change from a small gap semiconductor for lighter rare-earth to metallic for heavier rare-earth compounds. The angle resolved photoemission spectroscopy showed a clear spin-orbit splitting of the surface bands that cross the Fermi surface. Here we present very large magnetic field dependencies of transport properties in single crystals of $\text{RPTBi}$ ($R =$ Gd, Dy, Tm, and Lu). Successfully grown the high quality $\text{RPTBi}$ single crystals reveal that a large non-saturating magnetoresistance (MR) of as high as 800 % at 2 K and over 300 % at 300 K under a moderate magnetic field of 14 T. In addition to the large MR, the samples exhibit pronounced temperature and magnetic field dependences of Hall coefficient and thermoelectric power. Obtained transport data suggest that the high hole and electron mobility dominate the magnetotransport.

10:36AM L29.00012 Effect of thickness and strain on the metamagnetic transition temperature of ultra-thin epitaxial FeRh films$^1$. ALEJANDRO CEBALLOS, CATHERINE BORDEL, Univ of California - Berkeley, OLIVER SCHNEIDER, Julius-Maximilians-Universitat Wurzburg, FRANCES HELLMAN, Univ of California - Berkeley — The antiferromagnetic to ferromagnetic transition in ultra-thin epitaxial FeRh films was studied as a function of film thickness and substrate-induced strain. The lattice mismatch from MgO, STO and KTO was used to provide different strain states on FeRh films with thicknesses spanning 5 to 22 nm. The interplay of these parameters was studied using magnetometry, diffractometry, atomic force microscopy and energy dispersive spectroscopy. Our results provide insight into the growth mechanisms of FeRh and how the onset of the magnetic transition can be controlled via strain engineering.

$^1$This material is based upon work supported by the National Science Foundation Graduate Research Fellowship and the Department of Energy.

10:48AM L29.00013 Temperature-dependent spin scattering in Pt and at its interfaces. RYAN FREEMAN, ANDREI ZHOLUD, SERGEI URAZHIDIN, Emory Univ — Pt is an important material for spintronic devices, as it exhibits a significant spin Hall effect, enabling its applications as an efficient source of spin currents. Among key parameters describing spin-transport properties are the spin diffusion length (SDL) and the interfacial spin-scattering $\delta$. The reported values of SDL in Pt range from 0.5 to 15nm, likely due to the differences in the measurement approaches and material purity. Little is presently known about $\delta$. We utilized current-perpendicular-to-plane giant magnetoresistance (CPP-GMR) and magnetic nanopillar structures to determine the dependence of $\delta$ and SDL in Pt on temperature T. Both $\delta$ and SDL increase by almost a factor of two between 300K and 7K, implying that the bulk spin scattering decreases while the interfacial spin scattering increases with decreasing T. These opposite trends result in a nonmonotonic dependence of GMRT on T for thin Pt layers. We discuss the possible mechanisms for the unexpected dependence of $\delta$ on T. We also show that the SDL is within a factor of 2 of the mean free path, implying that almost every scattering event is spin flipping. This result provides a simple approach to estimate SDL in Pt and other materials with strong spin-orbit interaction.

Wednesday, March 4, 2015 8:00AM - 11:00AM – Session L31 GMAG DMP FIAP: Focus Session: Spin Dependent Phenomena in Semiconductors: Spin Orbit and Spin Relaxation 207A - Hanan Dery, University of Rochester

8:00AM L31.00001 Spin-orbit coupling in bulk and low dimensional III-V zinc-blende and wurtzite semiconductors from first principles$^1$. MARTIN GMITRA, JAROSLAV FABIAN, University of Regensburg, Germany — We have performed systematic investigations, using first-principles methods, of spin-orbit coupling effects in bulk III-V zinc-blende and wurtzite GaAs, GaSb, InAs, and InSb semiconductors. We have investigated the spin-orbit effects of the surface states of these semiconductors in different technologically important growth directions. Based on symmetry-derived Hamiltonians we have extracted realistic spin-orbit parameters important for spin relaxation, spin transport, optical orientation, and semiconductor-based Majorana states studies.

$^1$This work is supported by DFG SFB 689.

8:12AM L31.00002 ABSTRACT WITHDRAWN —

8:24AM L31.00003 Spin Relaxation in III-V Semiconductors in various systems: Contribution of Electron-Electron Interaction. FATIH DOGAN, HASAN KESSERWAN, AURELIEN MANCHON, King Abdullah University of Science and Technology (KAUST) — In spintronics, most of the phenomena that we are interested happen at very fast time scales and are rich in structure in time domain. Our contribution, on the other hand, is mostly based on energy domain calculations. Many of the theoretical tools use approximations and simplifications that can be perceived as oversimplifications. We compare the structure, material, carrier density and temperature dependence of spin relaxation time in n-doped III-V semiconductors using Elliot-Yafet (EY) and D’yakonov-Perel’ (DP) with real time analysis using kinetic spin Bloch equations (KSBE). The EY and DP theories fail to capture details as the system investigated is varied. KSBE, on the other hand, incorporates all relaxation sources as well as electron-electron interaction which modifies the spin relaxation time in a non-linear way. Since el-el interaction is very fast ($\sim$ fs) and spin-conserving, it is usually ignored in the analysis of spin relaxation. Our results indicate that electron-electron interaction cannot be neglected and its interplay with the other (spin and momentum) relaxation mechanisms (electron-impurity and electron-phonon scattering) dramatically alters the resulting spin dynamics. We use each interaction explicitly to investigate how, in the presence of others, each relaxation source behaves. We use GaAs and GaN for zinc-blend structure, and GaN and AIN for the wurtzite structure,
8:36AM L31.00004 Spin Relaxation in Materials Lacking Coherent Charge Transport$^1$. NICHOLAS HARMON, University of Iowa — As semiconductor spintronics research extends to materials beyond intrinsic or lightly doped semiconductors (e. g. organic materials, amorphous semiconductors, and impurity bands), the need is readily apparent for new theories of spin relaxation that encompass highly disordered materials, where charge transport is incoherent. We describe a broadly applicable theory of spin relaxation in materials with incoherent charge transport. The theory is based on continuous-time-random-walk theory and can incorporate many different relaxation mechanisms. We focus primarily on spin relaxation caused by spin-orbit and hyperfine effects in conjunction with carrier hopping. Analytic and numerical results from the theory are compared in various regimes with Monte Carlo simulations. Three different systems were examined: a polymer (MEH-PPV) $^1$, amorphous silicon $^2$, and heavily doped n-GaAs. In the organic and amorphous systems, we predict spin relaxation and spin diffusion dependences on temperature and disorder for three different mechanisms (hyperfine, hopping-induced spin-orbit, and intra-site spin relaxation). The resulting unique experimental signatures predicted by the theory for each mechanism in these disordered systems provide a prescription for determining the dominant spin relaxation mechanism. We find our theory to be in agreement with available measurements in these materials. We also predict that large disorder modifies certain mechanisms to be algebraic instead of exponential in time. Our results should assist in evaluating the suitability of various disordered materials for spintronic devices. All work done in collaboration with Michael E. Flatté. Timothy Peterson and Paul Crowell collaborated as well on the n-GaAs study.

$^1$This work was supported by an ARO MURI and by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA.

9:12AM L31.00005 Electron spin flips due to scattering off substitutional donors in multivalley semiconductors$^1$. YANG SONG, Department of Electrical and Computer Engineering, University of Rochester, Rochester, New York, 14627, OLEG CHALAEV, Department of Electrical and Computer Engineering, University of Rochester, HANAN DERY, Department of Electrical and Computer Engineering, Department of Physics and Astronomy, University of Rochester — We elucidate the physical origin of donor-driven spin relaxation in multivalley semiconductors with an emphasis on silicon. This spin flip is dominated by intervalley scattering between non time-reversal related valleys and by spin-orbit interaction from the core region of the donors. By a concise and intuitive explanation, we will present how the crystal symmetries and the multivalley nature of the conduction band set the selection rules for spin flips, and how to decisively associate the microscopic contributions with the empirically found strong dependence of the spin relaxation on the donor identity. These analyses and results are quite general for various other materials with multivalley conduction bands, and they are crucial for optimizing spintronics devices especially in the highly doped region near semiconductor-ferromagnet interfaces.

$^1$This work is supported by NSF and DTRA Contracts No. ECCS-1231570 and No. HDTRA1-13-1-0013, respectively.

9:24AM L31.00006 Spin relaxation in strained n-type silicon$^1$. OLEG CHALAEV, YANG SONG, HANAN DERY, University of Rochester — The impurity-induced spin-relaxation mechanism in heavily doped n-type silicon has been recently reported in Phys. Rev. Lett. 113, 167201. The leading contribution to the spin-relaxation rate occurs due to electron transitions between momentum-space valleys that reside on different crystallographic axes (the so-called f-process). This spin relaxation mechanism can be suppressed by applying uniaxial compressive strain that lifts the valley degeneracy. By calculating the next-order contribution to the spin-relaxation rate due to intravalley scattering and intervalley scattering between opposite valleys (the so-called g-process), we find a significant enhancement of the spin lifetime.

$^1$Supported by NSF and DTRA Contracts No. ECCS-1231570 and HDTRA1-13-1-0013

9:36AM L31.00007 Theory of copper induced spin-orbit coupling in graphene: substrate, clusters, and adatoms$^1$. TOBIAS FRANK, Univ Regensburg, SUSANNE IRMER, DENIS KOCHAN, MARTIN GMITRA, JAROSLAV FABIAN, University of Regensburg — We present a DFT study of graphene functionalized by copper adatoms and clusters, as well as of graphene on the (111) Cu surface, focussing on spin-orbit coupling effects. In the single copper adatom limit we study two energetically favored adsorption positions: the top and bridge positions and their corresponding diffusion barrier. Based on symmetry arguments we propose an effective tight-binding model Hamiltonian to describe low energy electronic states and determine realistic orbital and spin-orbit coupling parameters. We consider also copper clusters adsorbed on graphene and graphene on the Cu (111) surface, for which we as well fit to a model Hamiltonian to extract Rashba and intrinsic spin-orbit coupling strengths.

$^1$This work is supported by the DFG GRK 1570, SFB 689, and European Union Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

9:48AM L31.00008 Intervalley mixing and skew scattering in graphene systems$^1$. MAHMOUD M. ASMAR, SERGIO E. ULLOA, Ohio University — The scattering of electrons in graphene from impurities that preserve the point symmetries of the lattice is known to be anisotropic, with a transport to elastic time ratio $\xi \approx 2$ at low energies [1]. In systems in which the spin orbit interactions (SOI) are locally enhanced and do not lead to K-K' intervalley mixing, we have shown that the scattering becomes isotropic, and can be experimentally detected through the drop in $\xi \approx 1$ at low carrier concentrations [2]. These systems have been also shown to exhibit skew scattering and associated spin Hall Effect (SHE) [3]. In this study we extend our analysis to defects described by time reversal invariant interactions (TRIs) that reduce the lattice symmetries of graphene and may cause intervalley scattering. We show that the presence of such defects also leads to the suppression of $\xi$, with carrier concentration dependence similar to those produced by the intrinsic SOI, but qualitatively different from the effects of Rashba SOI, allowing their simultaneous determination. Finally, we show the effects of such defects on skew scattering, and the dependence of the SH angle on the relative strength of such disorder.


$^1$Supported by NSF DMR MWN/CIAM.
10:00AM L31.00009 Extrinsic Spin Hall Effect Induced by Resonant Skew Scattering in Graphene

1. AÑES FERREIRA², Graphene Research Centre and Department of Physics, National University of Singapore, 2 Science Drive 3, Singapore 117546, Singapore. TATIANA G. RAPPOPORT, Instituto de Física, Universidade Federal do Rio de Janeiro, CP 68.528, 21941-972 Rio de Janeiro, RJ, Brazil, MIGUEL A. CAZALILLA, Department of Physics, National Tsing Hua University, and National Center for Theoretical Sciences (NCTS), Hsinchu City, Taiwan. A.H. CASTRO NETO, Graphene Research Centre and Department of Physics, National University of Singapore, 2 Science Drive 3, Singapore 117546, Singapore. — We show that the extrinsic spin Hall effect can be engineered in monolayer graphene by decoration with small doses of adatoms, molecules, or nanoparticles originating local spin-orbit perturbations. The analysis of the single impurity scattering problem shows that intrinsic and Rashba spin-orbit local couplings enhance the spin Hall effect via skew scattering of charge carriers in the resonant regime. The solution of the transport equations for a random ensemble of spin-orbit impurities reveals that giant spin Hall currents are within the reach of the current state of the art in device fabrication. The spin Hall effect is robust with respect to thermal fluctuations and disorder averaging.

²The author acknowledges support from the National Research Foundation-Competitive Research Programme through Grant No. R-144-000-295-281

10:12AM L31.00010 Weyl Nodes in Trigonal Tellurium and Selenium

MOTOAKI HIRAYAMA, Nanosystem Research Institute, AIST, RYO OKUGAWA, Department of Physics, Tokyo Institute of Technology, SHOJI ISHIBASHI, Nanosystem Research Institute, AIST, SHUICHI MURAKAMI, Department of Physics, Tokyo Institute of Technology, TIES, Tokyo Institute of Technology, TAKASHI MIYAKE, Nanosystem Research Institute, AIST. — Singular points in the momentum space (Dirac nodes) have been under intensive investigation recently. Among various Dirac systems, materials having three-dimensional Dirac nodes without spin degeneracy (Weyl nodes) are of particular interest because of their topological nature. We study trigonal Te and Se as systems having both strong spin-orbit interaction (SOI) and broken inversion symmetry, which is necessary for the Weyl node. We calculate the electronic structure by using QMAS [1] based on relativistic density functional theory, and add the self-energy correction in the GW approximation. Te and Se are insulating at ambient pressure. The conduction bands have a spin splitting similar to the Rashba splitting around the H points, but unlike the Rashba splitting the spin directions are radial, forming a hedgehog spin texture. The energy gap decreases with increasing pressure. In the metallic phase, the spin rotates twice around H on the k₉ = ±π/c plane, which can be explained by the motion of the Weyl nodes under pressure [2]. We also find that trigonal Te shows the Weyl semimetal phase with time-reversal symmetry under pressure [2].


10:24AM L31.00011 Spin relaxation and transport mechanisms in ZnO thin films

MEGAN PRESTGARD, GENE SIEGEL, University of Utah. Department of Materials Science and Engineering, ROBERT ROUNDY, MIKHAIL RAIKH, University of Utah, Department of Physics, ASHUTOSH TIWARI, University of Utah, Department of Materials Science and Engineering — Zinc oxide has been widely used in optoelectronic and lasing application due to its wide-bandgap and large exciton binding energy. In recent studies, it has also been studied for spintronic device applications due to its relatively large spin-orbit coupling and potential as a dilute magnetic semiconductor. However, a fundamental understanding of spin transport and relaxation mechanisms has not yet been reached. Knowledge of these mechanisms is required in order to accurately explain and enhance spin-based effects in ZnO. To study spin transport and relaxation in ZnO, four-probe non-local Hanle measurements were performed on thin film samples. These samples were grown using a pulsed laser deposition technique under low ambient oxygen pressure. Under these conditions, the films grown are degenerately doped, with a carrier concentration on the order of 10¹⁹ cm⁻³. Taking this into account, the spin lifetime results can be explained by Dyakonov-Perel (DP) relaxation mechanisms using Fermi-Dirac statistics.

10:36AM L31.00012 Hyperfine-induced spin relaxation of a hopping carrier: implications for spin transport in 1-D vs 3-D organic semiconductors

1. VAGHARSH MKHITARYAN, VIATCHESLAV DOBOVITSKI, Ames Laboratory, Iowa State University, Ames, Iowa 50011. 0 TEAM — The hyperfine coupling of a carrier spin to a nuclear spin bath is a predominant channel for the carrier spin relaxation in organic semiconductors. We investigate the hyperfine-induced spin relaxation of a carrier performing a random walk on a d-dimensional regular lattice theoretically, in a transport regime typical for organic semiconductors. We show that in d=1 and d=2 the time dependence of spin polarization, P(t), is dominated by a superexponential decay, crossing over to an exponential tail at long times. The faster decay is attributed to multiple self-intersections (returns) of the random walk trajectories, which occur more often in lower dimensions. We also show, analytically and numerically, that the returns lead to sensitivity of P(t) to external electric and magnetic fields, and this sensitivity strongly depends on dimensionality of the system (d = 1 vs. d = 3). Furthermore, we consider the coordinate dependence of spin polarization, σ(r), in a hypothetic lateral or vertical organic spin-valve device. We demonstrate that, while σ(r) is essentially exponential, the effect of multiple self-intersections can be identified in transport measurements from the specific field-dependence of spin relaxation length.

²This work was supported by the Department of Energy-Basic Energy Sciences under Contract No. DE-AC02-07CH11358

10:48AM L31.00013 Dissecting the mechanisms of magnetocrystalline anisotropy in alloys: Electronic structure analysis tools and applications to (Feₓ₋₀₂ Coₓ)₀₂₋₀₂, Liₓ₋₀₂, Feₓ, N alloys

KIRILL BELASHCHENKO, University of Nebraska - Lincoln, VLADIMIR ANTRPOPOV, Ames Laboratory — We describe a first-principles code and a set of tools providing detailed information about the mechanisms of the magnetocrystalline anisotropy (MCA) in alloys. The spin-orbit coupling (SOC) is included in the Green’s function-based linear muffin-tin orbital (LMTO) method combined with the coherent potential approximation. Third-order correspondence with the LMTO Hamiltonian is formally demonstrated. The analysis tools include the identification of contributions from different spin channels, single-ion and two-ion terms and alloy components by computing the SOC energy with scaled SOC parameters, as well as a full reciprocal-space resolution of MCA in the Brillouin zone. Application of these tools is illustrated for the (Feₓ₋₀₂ Coₓ)₀₂₋₀₂ system, where the complicated non-monotonic concentration dependence of MCA is attributed to the combination of band filling and SOC selection rules. For Liₓ₋₀₂, Feₓ, N we demonstrate the interplay between chemical disorder, orbital polarization, and correlation effects in a doubly degenerate impurity band.

³Work at UNL supported by NSF Grant DMR-1308751.
8:00AM L32.00001 Huge spin-driven polarizations at room temperature in bulk BiFeO₃. JUN HEE LEE, RANDY FISHMAN, Oak Ridge National Laboratory — Although BiFeO₃ is one of the most investigated multiferroics, its magnetoelectricity and spin-driven polarizations are barely understood on an atomistic level. By combining a first-principles approach with a spin-cyclod model, we report hidden but huge spin-driven polarizations at room temperature in bulk BiFeO₃. One of the polarizations reaches \( \sim 0.03 \text{ C/m}^2 \), which is larger than any other spin-driven polarization in a bulk material by one order of magnitude. By comparing our results with intrinsic measurements such as neutron scattering, Raman spectroscopy, IR directional dichroism, and high magnetic-field measurements, we disentangle all the hidden spin-driven polarizations due to exchange-striction, spin-current, and single-ion-anisotropy. We find that the broken inversion symmetry of the J3c structure of BiFeO₃ induce the strong response of the magnetic couplings to an electric field and are responsible for the associated huge spin-driven polarizations.

1This research is sponsored by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division and by the Scientific User Facilities Division, Office of Basic Energy Sciences, US Department of Energy.

8:12AM L32.00002 Theory for the Spectroscopic Mode Frequencies and THz Absorption of Multiferroic BiFeO₃. RANDY FISHMAN, JUN HEE LEE, Oak Ridge National Laboratory — A microscopic model for BiFeO₃ that includes two Dzyaloshinskii-Moriya interactions and easy-axis anisotropy along the ferroelectric polarization predicts both the zero-field spectroscopic modes as well as their splitting and evolution in a magnetic field [1]. Due to simultaneously broken time-reversal and spatial-inversion symmetries, the absorption of light changes slightly as the magnetic field or the direction of light propagation is reversed. We discuss three sets of physical mechanisms that contribute to the THz absorption and directional dichroism (DD) of BiFeO₃: spin current, magnetostriction, and anisotropy. First-principles calculations are used to obtain relationships among some of the polarization matrix elements induced by broken inversion symmetries in J3c structure. While our model nicely describes the DD along the magnetic field direction [1-1,0], it fails to predict the weak DD observed for field along [1,1,0].


8:24AM L32.00003 Atomic-Scale Tunneling Spectra across BiFeO₃/La₄/3Sr₇/3MnO₃ Heterointerfaces. YA-PING CHIU, Department of Physics, National Taiwan Normal University, Taipei, 116, Taiwan, BO-CHAO HUANG, Institute of Physics, Academia Sinica, Taipei 105, Taiwan, PU YU, State Key Laboratory of Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University, CHIA-SENG CHANG, YING-HAO CHU, Institute of Physics, Academia Sinica, Taipei 105, Taiwan. — Atomic-level evolution of electronic structures across BiFeO₃/La₄/3Sr₇/3MnO₃ complex oxide heterointerfaces has been demonstrated by cross-sectional scanning tunneling microscopy and spectroscopy in this work. Analysis of scanning tunneling spectroscopy results exploits how the change in the terminated interface brings the influence to the electrostatic configurations across the BiFeO₃/La₄/3Sr₇/3MnO₃ heterointerfaces. Spatially unit-cell-by-unit-cell resolved electronic states at the atomic level reveal that the control of material interfaces at the atomic level determines the ferroelectric polarization in BiFeO₃. The precise electronic information therefore provides a clear realization about the electronic state at these complex-oxide heterointerfaces, which is crucial to understand and design a host of novel functionalities at complex oxide heterointerfaces.

1Affiliation 2: Department of Materials Science and Engineering, National Chiao Tung University, Hsinchu 300, Taiwan

8:36AM L32.00004 Structural evolution from Bi₄/3K₀.8Fe₂O₉₋δ nanobelts to BiFeO₃ nanochains and their multiferroic properties. SINING DONG, Univ of Notre Dame, XIAOGUANG LI, Univ of Sci and Tech of China, XINYU LIU, MALGORZATA DOBROWOLSKA, JACEK FURDYNA, Univ of Notre Dame — In this study, we reported the structural evolution of Bi₄/3K₀.8Fe₂O₉₋δ nanobelts to BiFeO₃ nanochains and the related variations of multiferroic properties. By using in-situ transmission electron microscopy with comprehensive characterization, it was found that the layered perovskite multiferroic Bi₁₄/3K₀.8Fe₂O₉₋δ nanobelts were very unstable in a vacuum environment with Bi being easily removed. Based on this finding, a simple vacuum annealing method was designed which successfully transformed the Bi₁₄/3K₀.8Fe₂O₉₋δ nanobelts into one-dimensional BiFeO₃ nanochains. Both the Bi₁₄/3K₀.8Fe₂O₉₋δ nanobelts and the BiFeO₃ nanochains showed multiferroic behaviors, with their ferroelectric and ferromagnetic properties clearly established by piezoresponse and magnetic measurements, respectively. Interestingly, the BiFeO₃ nanochains exhibited a surprisingly large exchange bias with small training effects. This one-dimensional BiFeO₃ multiferroic nanostructure characterized by a relatively stable exchange bias offers important functionalities that may be attractive for device applications.

8:48AM L32.00005 Correlated Switching Dynamics in the Nanoscale Proximity of 90° Ferroelectric Domain Walls. SHIMING LEI, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA, United States., XUEYUN WANG, S.W. CHEONG, Department of Physics and Astronomy and Rutgers Center for Emergent Materials, Rutgers University, Piscataway, NJ, United States., L.Q. CHEN, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA, United States., SERGEE KALININ, The Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee, VENKATRAMAN GOPALAN, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA, United States. — Ferroelectrics are materials which have a built in polarization in their crystal structure even in the absence of an electric field. Domain walls themselves can possess dramatically different properties than the bulk ferroelectrics themselves. Previously we discovered that the universally present 180° walls have an order of magnitude lower domain switching threshold field than the bulk. This effect extends up to many microns around a wall, though the wall itself is unit cell thick. Here we present new results on 90° walls in PbTiO₃ single crystals that show similar proximity effect and correlated switching. Our SSSPFM imaging across the a/c/a domain walls suggests a strong correlated switching behavior in the proximity of the inclined 90° domain walls, even at a small AC driving voltage of 1V without DC bias on the tip. Consistent with phase-field modeling results, the inclined extended domain walls is found to act as nucleation sites in ferroelectric materials, and give rise to the domain wall asymmetrical broadening across the domain wall.

9:00AM L32.00006 Magnetic-induced polarization in charge-ordered CaMnO₁₂₋δ system. DIOMEDES SALDANA-GRECO, JIN SOO LIM, ANDREW M. RAPPE, University of Pennsylvania — The electronic properties of CaMnO₁₂₋δ yield interesting physical phenomena including charge-ordering, non-collinear magnetism, and improper ferroelectricity. The charge-ordered CaMnO₁₂₋δ is a complex quadruple perovskite whose chemical formula is (CaM₃₋δ)₃(Mn⁺³₋δMn⁺⁹/₁₂)O₁₂ where three Mn⁺³ are on the A-site (Mn₁), three Mn⁺³ on the B-site (Mn₂), and one Mn⁺³ on the B-site (Mn₃). Three parallel c-chains with alternating Mn₁ and Mn₂ form a Kagome lattice with either Mn₃ or Ca at the center of the hexagonal rings. The non-collinear magnetic structure consists of spin moments lying on the ab-plane, forming a helical pattern along the c-axis. Our DFT+U+J study shows that the Mn₃ spins adopt a (90°-30°) spin configuration with respect to the surrounding (Mn₁,Mn₂) spins, breaking the inversion symmetry and generating a Berry-phase computed ferroelectric polarization of 2975 μC/m² along the c-axis. We demonstrated that when the magnetic helicity of the system is reversed, the ferroelectric polarization flips. This study aims to explore how the electronic and magnetic properties are intertwined to give rise to a multiferroic, charge-ordered state.
9:12AM L32.00007 Giant spin-driven ferroelectric polarization and magnetoelectric effect in perovskite rare-earth maganifies under high pressure. TSUYOSHI KIMURA, Osaka University — The discovery of ferroelectricity in TbMnO$_3$ triggered extensive studies on a type of multiferroics, “spin-driven ferroelectrics.” Unlike conventional ferroelectrics such as BaTiO$_3$, spin-driven ferroelectrics exhibit remarkable magnetoelectric (ME) effects. However, the ferroelectric polarization $P$ in spin-driven ferroelectrics ever reported ($< 10^{-3}$µC/cm$^2$) is much smaller than that in conventional ferroelectrics (typically $10^0 - 10^3$µC/cm$^2$). Thus, the quest for robust magnetically-controllable $P$ comparable to that in conventional ferroelectrics is still a major challenge in the research on multiferroics. In this study, we utilized the “high-pressure” to attain a magnetically-controllably spin-driven $P$ with its magnitude being comparable to that in conventional ferroelectrics [T. Aoyama et al., Nature Commun. 5, 4927 (2014)]. With a home-made high-pressure measurement system with a diamond anvil cell, we investigated high-pressure effects on ME properties of perovskite TbMnO$_3$ ($R =$ Gd, Tb, and Dy). Our study revealed that these magnanites exhibit a pressure-induced ME phase transition and that the high-pressure phase shows the largest $P$ (e.g., 1 µC/cm$^2$ in TbMnO$_3$) among spin-driven ferroelectrics ever reported. Moreover, $P$ is further enhanced by applying a magnetic field. Our study demonstrates that it is possible to attain giant spin-driven ferroelectric polarization which comes close to that in conventional ferroelectrics, and to control it magnetically.

This work has been done in collaboration with T. Aoyama, K. Yamauchi, A. Iyama, S. Picozzi, A. Miyake, and K. Shimizu.

9:48AM L32.00008 Terahertz electromagnons in spin-diluted cupric oxide: dynamics of twisted spin states. JAMES LLOYD-HUGHES, University of Warwick, SAMUEL JONES, University of Oxford, NICOLA WURZ, MICHELE FAILLA, CHRIS MCCONVILLE, University of Warwick, DHARMALINGHAM PRABHAKARAN, University of Oxford — Understanding the physics of magnetoelectric materials may lead to their application in actuators, sensors and solid state memories. Improper multiferroics also have novel quasiparticle excitations: electromagnons form when spin-waves become electric-dipole active. We investigated magnons, electromagnons and spin-lattice coupling in Cu$_{1-x}$Zn$_x$O (0<x<0.05), an improper ferromagnet. Terahertz time-domain spectroscopy demonstrated electromagnons only in the multiferroic phase, and established the selection rule and that the oscillator strength tracks the static polarisation [1]. The impact of non-magnetic Zn-substitution on lattice dynamics was elucidated by Raman and Fourier-transform spectroscopy, showing strong spin-lattice coupling in Cu$_{1-x}$Zn$_x$O. While the phonon and magnon modes broaden and shift as a result of alloy-induced disorder, the electromagnon was found to be insensitive to Zn substitution and the induced disorder in the local spin structure. The results demonstrate that electromagnon excitations and dynamic magnetoelectric coupling can be maintained even in disordered spin systems, and at elevated temperatures [2]. [1] Nature Communications 5, 3787 (2014). [2] Physical Review B 90, 064405 (2014).

10:00AM L32.00009 Terahertz study of potential multiferroic materials Sr$_2$FeSi$_2$O$_7$ and BaFe$_2$O$_4$[1], THUC T. MAI, M.T. WARREN, J. BRANGHAM, Center for Emergent Materials, Department of Physics. The Ohio State University. Columbus, OH 43210, T-H. HWAN, POSTECH, South Korea, S-W. CHEONG, Department of Physics, Rutgers University. J. YAN, Oak Ridge National Laboratory and University of Tennessee Knoxville. R. VALDES AGUILAR, Center for Emergent Materials, Department of Physics. The Ohio State University. Columbus, OH 43210 — We present data on the complex dielectric function of two iron-based quantum magnets in the terahertz frequency range. We study the phase transitions in Sr$_2$FeSi$_2$O$_7$ at low temperature when it becomes a collinear antiferromagnet, in contrast with the canted antiferromagnetic state of iso-structural multiferroic Ba$_2$CoGe$_2$O$_7$. We compare the terahertz response of these two materials in light of the recent observation of electromagnon excitations in Ba$_2$CoGe$_2$O$_7$. We have also studied BaFe$_2$O$_4$, a hexagonal ferromagnet that is predicted to have an antiferroelectric state. We will report experiments at terahertz frequencies probing this predicted state.

1 Work partially supported by the NSF MRSEC Center for Emergent Materials under grant DMR-1420451.

10:12AM L32.00010 Enhancement of Magnetoelectric Coupling in CoGa$_2$Fe$_{2-x}$O$_4$/BaTiO$_3$ Composite[1], YAN NI, ZHEN ZHANG, DAVID JILES, Department of Electrical and Computer Engineering, Iowa State University, CAJETAN NLEBE-DIM, Ames Laboratory, U.S. Department of Energy — Multiferroic materials exhibit magnetoelectric coupling and promise new device applications including magnetic sensors, generators and filters. An effective method for developing magnetoelectric (ME) materials with enhanced ME effect is achieved by the coupling through the interfacial strain between piezoelectric and magnetostrictive materials. In this study, enhancement of magnetoelectric coupling was found by systematically studying the electrical and magnetic properties of CoGa$_2$Fe$_{2-x}$O$_4$/BaTiO$_3$ composite. It is found that Ga doping not only stabilizes the magnetic phase of composites but also increases the sensitivity of magnetoelastic response by 30%. Moreover, Ga doping reduces the electrical conductivity and the dielectric loss of composite. An enhancement of magnetoelectric coupling was found to be significant in the composite as compared to the constituent materials. The results indicate that the interfacial strain can significantly enhance the magnetoelectric coupling.

1 This work was supported by the USDoE, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. The research was performed at Ames Laboratory, operated for the USDoE by Iowa State University (contract # DE-AC02-07CH11358).

10:24AM L32.00011 Ultrafast Optical Spectroscopy of BiFeO$_3$-BaTiO$_3$ Based Structures[1], B.A. MAGILL, M.A. MEEKER, G.A. KHODAPARAST, S. PRIYA, Y. ZHOU, HYUN-CHEOL SONG, Virginia Tech. M. BISHOP, S. MCGILL, National High Magnetic Field Laboratory, Florida — Ultrafast optical spectroscopy can provide insight into fundamental microscopic interactions, dynamics and the coupling of several degrees of freedom. Pump/ probe studies can reveal the answer to questions like “What are the achievable switching speeds in multiferroics?” In this talk, we report on two color (400/800nm) pump-probe differential reflectance spectroscopy of BiFeO$_3$-BaTiO$_3$ based structures to probe the coupling between optical and acoustic phonons to spin waves, in these material systems. We present the results of several different time resolved transient reflectivity measurements to probe both the carrier and spin dynamics.

1 This work was supported by the AFOSR through grant FA9500-14-1-0376. Also supported by the Institute of Critical Technology and Applied Sciences (ICTAS) at Virginia Tech.

10:36AM L32.00012 Linear to quadratic magnetoelectric effect in Fe langasite, SERGEY ARTYUKHIN, DAVID VANDERBILT, SANG-WOOK CHEONG, Rutgers University — Materials with coexisting and interacting switchable ferroic orders – multiferroics – are the subject of intense investigations due to their existing and potential applications in spintronics and information storage technology. Here we investigate the much debated magnetically induced polarization and magneto-electric effect in the hexagonal Fe-langasite Ba$_3$NbFe$_3$Si$_2$O$_{11}$ with distorted triangular layers of magnetic Fe ions. We propose a simple model for these phenomena, and discuss how application of the magnetic field induces a toroidal moment, responsible for the peculiar magnetoelectric effect in this material.
Euglena’s diverse perspectives led. I will demonstrate how this process led to improved curricular design, refined assessment objectives, and new design heuristics.

at multiple-time scales. In this presentation I will detail our process of collecting systematic data, listening to and valuing students’ reasoning, and bridging in instructor to teaching in a large lecture hall with multiple instructors. We have used a design-based research approach to support critical reflection of the course learning environment that bridges the disciplinary domains of biology and physics. Across the three years we have gone from teaching in a small class with one — but they often see these courses as disconnected. Over the past three years the NEXUS/Physics course has been working to develop an interdisciplinary — and charge screening in fluids. We also introduce the students to research-grade equipment and modern physics analysis tools in contexts relevant to biology, — via construction and via play – and it provides an engaging theme for a formal biophysics devices class as well as to be presented in informal outreach activities; its low cost requirements make it especially suitable for use in resource-limited settings.

This work is supported by NSF-TUES DUE 11-22818, the HHMI NEXUS grant, and a NSF Graduate Research Fellowship (DGE 0750616).

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Wednesday, March 4, 2015 8:00AM - 10:48AM

Session L33 DBIO FED: Focus Session: Undergraduate Teaching at the Intersection of Physics and Biology

8:00AM L33.00001 Rethinking Physics for Biologists: A design-based research approach

8:18AM L33.00002 Introductory Physics Laboratories for Life Scientists – Hands on Physics of Complex Systems

8:48AM L33.00003 A biotic video game smart phone kit for formal and informal biophysics education

9:00AM L33.00004 Hands-on-Entrophy, Energy Balance with Biological Relevance

9:36AM L33.00005 A Low-Cost, Hands-on Module to Characterize Antimicrobial Compounds Using an Interdisciplinary, Biophysical Approach
9:48AM L33.00006 An undergraduate course, and new textbook, on “Physical Models of Living Systems”
PHILIP NELSON, Univ Pennsylvania — I’ll describe an intermediate-level course on “Physical Models of Living Systems.” The only prerequisite is first-year university physics and calculus. The course is a response to rapidly growing interest among undergraduates in several science and engineering departments. Students acquire several research skills that are often not addressed in traditional courses, including: basic modeling skills, probabilistic modeling skills, data analysis methods, computer programming using a general-purpose platform like MATLAB or Python, dynamical systems, particularly feedback control. These basic skills, which are relevant to nearly any field of science or engineering, are presented in the context of case studies from living systems, including: virus dynamics; bacterial genetics and evolution of drug resistance; statistical inference; superresolution microscopy; synthetic biology; naturally evolved cellular circuits. Publication of a new textbook by WH Freeman and Co. is scheduled for December 2014.

1Supported in part by EF-0928048 and DMR-0832802.

10:00AM L33.00007 Teaching Optics to Biology Students Through Constructing a Light Microscope
JENNIFER ROSS, Univ of Mass - Amherst — The microscope is familiar to many disciplines, including physics, materials science, chemistry, and the life sciences. It demonstrates fundamental aspects of ray and wave optics, making it an ideal system to help students in the basic concepts of optics and in measurement principles and techniques. We present an experimental system developed to teach students the basics of ray and wave optics. The students design, build, and test a light microscope made from optics components. We describe the equipment and the basic measurements that students can perform to develop experimental techniques to understand optics principles. Students measure the magnification and test the resolution of the microscope. The system is open and versatile to allow advanced projects such as epi-fluorescence, total internal reflection fluorescence, and optical trapping. We have used this equipment in an optics course, an advanced laboratory course, and graduate-level training modules.

10:12AM L33.00008 What Physics do Biophysicists Need to Know? JONATHON HOWARD, Yale University — No abstract available.

Wednesday, March 4, 2015 8:00AM - 11:00AM — Session L34 GERA: Thin Film Photovoltaics (Perovskites, etc) 210A -

8:00AM L34.00001 Hybrid Perovskite Solar Cells with Copper Iodide as Hole Transportlayer
ROSS HAROLDSON, ZANE OLDS, ALEXANDER B COOK, ANVAR ZAKHIDOV, Univ of Texas - Dallas — Hybrid organo-metallic solar cells based on perovskite-structured nanocrystals have had steadily improving power conversion efficiencies over the past several years, and within this short period of time are capable of achieving efficiencies over 19%. In our work we show that dopants thin layer of Copper iodide (Cul) on top of a hole transport layer such as PEDOT:PSS increases the open circuit voltage, of the devices. Cul is a p-type hole conducting material with a large band gap that has been used before for hole transport layers by itself. We demonstrate that Cul as the working hole transport layer increases the Voc about 10% increase.

8:12AM L34.00002 Morphological Optimization of Perovskite Thin Films via Dynamic Zone Annealing
YAN SUN, KAI WANG, XIONG GONG, ALAMGIR KARIM, University of Akron — Organolead Halide Perovskites have been proved to be excellent candidates for application in low-cost high-efficient solar cells owing to their superior desired optical and electrical properties, as well as compatibility with low-temperature solution-processed manufacturing. However, most perovskites applications in photovoltaics require high quality perovskite films. Although tremendous works on tuning perovskite film morphology have been reported previously, it is still a challenge to realize high quality perovskite film with controllable film uniformity and surface coverage, neither the mechanisms in the formation of perovskite. To address the issues above, here we demonstrate the effect of Dynamic Zone Annealing (DZA) on perovskite morphologies, which is proved as an efficient method to control the structure and morphology in crystalline polymer and block copolymers. Via applying the DZA method, the mechanism in perovskite film formation is studied. Furthermore, by optimizing DZA parameter such as maximum temperature, temperature gradient and zone velocity to control dendritic morphology and the grain growth, enhanced device performance was realized eventually.

equal contribution

8:24AM L34.00003 Photovoltaic properties of low band gap ferroelectric perovskite oxides
XIN HUANG, Southeast University, TULA PAUDEL, University of Nebraska-Lincoln, SHUAI DONG, Southeast University, EVGENY TSYMBAL, University of Nebraska-Lincoln — Low band gap ferroelectric perovskite oxides are promising for photovoltaic applications due to their high absorption in the visible optical spectrum and a possibility of having large open circuit voltage. Additionally, an intrinsic electric field present in these materials provides a bias for electron-hole separation without requiring p-n junctions as in conventional solar cells. High quality thin films of these compounds can be grown with atomic layer precision allowing control over surface and defect properties. Initial screening based on the electronic band gap and the energy dependent absorption coefficient calculated within density functional theory shows that hexagonal rare-earth manganites and ferrites are promising as photovoltaic absorbers. As a model, we consider hexagonal TbMnO_3. This compound has almost ideal band gap of about 1.4 eV, very high ferroelectric Curie temperature, and can be grown epitaxially. Additionally hexagonal TbMnO_3 offers possibility of coherent structure with transparent conductor ZnO. We find that the absorption is sufficiently high and dominated by interband transitions between the Mn d-bands. We will present the theoretically calculated photovoltaic efficiency of hexagonal TbMnO_3 and explore other ferroelectric perovskite oxides.

8:36AM L34.00004 Infrared spectrum and normal-mode assignment in methyl-ammonium lead halide perovskite CH_3NH_3PbI_3
MIGUEL ANGEL PEREZ OSORIO, MARINA FILIP, Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, UK — CALLUM DOCHERTY, LAURA HERZ, MICHAEL JOHNSTON, Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford, OX1 3PU, UK — FELICIANO GIUSTINO, Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, UK — Solar cells based on MAPbI_3 (MA=CH_3NH_3) have attracted enormous attention during the past two years owing to their high energy-conversion efficiency, reaching up to 19.3% in record devices. A detailed understanding of the structure/property relations of this compound may help us explain its extraordinary performance. Here, we investigate the vibrational modes and infrared (IR) absorption spectrum of MAPbI_3 by combining first-principles calculations and experiment. Our calculations indicate that the normal modes at high frequency, 400-3100 cm^{-1}, correspond to internal vibrations of the MA cations, whereas those at low frequency, up to 180 cm^{-1}, can be assigned either to vibrations of the PbI network or to the libration and spinning of the cations. Using a factor group analysis we establish the symmetry of the normal modes and predict which mode will be IR or Raman active. In order to confirm these assignments we explicitly calculate the IR spectrum of the MAPbI_3. The calculated spectrum is in good agreement with experiment, therefore we now have a complete characterization of the vibrational properties of MAPbI_3. This work will serve as a solid reference for future structural and characterization studies of hybrid organic-inorganic perovskites.
8:48AM L34.00005 Nanoscale charge localization induced by random orientations of organic molecules in hybrid perovskite CH₃NH₃PbI₃. JIE MA, LIN-WANG WANG, Lawrence Berkeley National Lab — Perovskite-based solar cells have achieved high solar-energy conversion efficiencies and attracted wide attentions nowadays. Despite the rapid progress in solar-cell devices, many fundamental issues of the hybrid perovskites have not been fully understood. Experimentally, it is well known that in CH₃NH₃PbI₃, the organic molecules CH₃NH₃ are randomly oriented at the room temperature, but the impact of the random molecular orientation has not been investigated. Using linear-scaling ab-initio methods, we have calculated the electronic structures of the tetragonal phase of CH₃NH₃PbI₃ with randomly oriented organic molecules in large supercells up to ~ 20,000 atoms. Due to the dipole moment of the organic molecule, the random orientation creates a novel system with long-range potential fluctuations unlike alloys or other conventional disordered systems. We find that the charge densities of the conduction-band minimum and the valence-band maximum are localized separately in nanoscales due to the potential fluctuations. The charge localization causes electron-hole separation and reduces carrier recombination rates, which may contribute to the long carrier lifetime observed in experiments. We have also proposed a model to explain the charge localization.

9:00AM L34.00006 Dynamics of CH₃NH₃PbI₃ from first principles simulations1, ALI KACHMAR, MARCELO CARIGNANO, Qatar Environment and Energy Research Institute, Qatar Foundation, PO Box 5825, Doha, Qatar — We study the dynamical and optical properties of CH₃NH₃PbI₃ using density functional calculations based on forces calculated with density functional theory. We have studied the three stable phases of CH₃NH₃PbI₃ but most of the effort was dedicated to the intermediate tetragonal phase, which is stable at standard ambient conditions. In this case, two different system sizes have been considered, one with 8 unit cells (384 atoms) and a larger one with 27 unit cells (1296 atoms). The total simulated time reached 40 ps. Our findings reveal the interplay between the thermal energy of the system and the electronic degrees of freedom. For example, the organic molecule undergoes relatively fast rotations and the energy band gap, approximated by the LUMO-HOMO energy difference, fluctuates around the equilibrium value of ~1.5 eV with a width of 0.2 eV. The rotation of the CH₃NH₃ molecule is not isotropic, and more importantly, it is quite sensitive to the size of the simulation box. Our study also provides a quantitative measure for the finite size effects affecting the calculated properties and provides a contextual scenario in which to analyze the more typical density functional theory studies based on static calculations on optimal structures.

1The authors acknowledge the HPC resources of Texas A&M University at Qatar.

9:12AM L34.00007 Bandstructure, optical spectra, and mean free paths in the room-temperature structure of CH₃NH₃PbI₃ from many-body perturbation theory1, DEREK VIGIL-FOWLER, MARCO BERNARDI, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — The organometallic halide perovskites have generated enormous interest due to the rapidly increasing efficiency of solar cells fabricated from these materials. Most research on the organometallic halide perovskites has been experimental due to the challenges posed by these materials to theoretical study, including the size of the unit cell, the presence of many defects, the orientational disorder in of the methyammonium (MA) cation, and the heavy atoms involved with the corresponding large spin-orbit coupling (SOC). We study the room-temperature tetragonal structure of CH₃NH₃PbI₃ using density functional theory (DFT) and a many-body Green’s functions approach. We use DFT to study the effect of the dependence of the bandstructure on the orientation of the MA cation, while we perform GW and GW plus Bethe-Salpeter equation (GW-BSE) calculations to study the quasiparticle bandstructure and optical spectra, respectively, paying close attention to convergence and the effect of SOC. We particularly investigate the existence of a proposed charge-transfer state in this material. We also briefly discuss the mean free paths due to electron-photon and electron-electron scattering in the ideal structure.

1This work was supported by NSF Grant No. DMR10-1006184, and U.S. DOE Contract No. DE-AC02-05CH11231 and the DOE SciDAC program. Computational resources were provided by NERSC. D.V.-F. acknowledges funding from the NSF’s Blue Waters Fellowship.

9:24AM L34.00008 Exciton Binding energies and effective masses in Organo-lead Tri-Halide Perovskites, OLIVER PORTUGALL, ATSUKIKO MIYATA, ANATOL MITIOGLU, PAULINA PLOCHOCKA, LNCMI TOULOUSE, JACOB TSE-WEI WANG, SAMUEL STRANKS, HENRY SNAITH, ROBIN NICHOLAS, Oxford University, LNCMI TOULOUSE TEAM, OXFORD UNIVERSITY TEAM — Solid-state perovskite-based solar cells have made a dramatic impact on emerging PV research with efficiencies of over 17% already achieved. However, to date the basic electronic properties of the perovskites such as the electron and hole effective masses and the exciton binding energy are not well known. We have measured both for methyl ammonium lead tri-iodide using magneto absorption in very high magnetic fields up to 150T showing that the exciton binding energy at low temperatures is only 16 meV, a value three times smaller than previously thought and sufficiently small to completely transform the way in which the devices must operate. Landau level spectroscopy shows that the reduced effective mass of 0.104 me is also smaller than previously thought. In addition by using a fast pulse 150T magnet we measure the band structure change due to the structural phase transition that occurs in this system at around 160K. We also observe Landau levels in the high temperature phase as used for device production, which has a very similar effective mass and the analysis suggests an exciton binding energy which is even smaller than in the low temperature phase.

9:36AM L34.00009 Ferritin-based nanocrystals for solar energy harvesting1, JOHN COLTON, STEPHEN ERICKSON, CAMERON OLSEN, JACOB EMBLEY, TREVOR SMITH, RICHARD WATT, Brigham Young University — Ferritin is a 12 nm diameter hollow protein with an 8 nm cavity that can be filled with a variety of nanocrystals (ferrihydrite being native). We report on several experiments with ferritin-based nanocrystals designed to utilize ferritin for solar energy harvesting. First, we have shown that the native band gap can be altered by controlling nanocrystal size, by replacing the native iron oxide core with other metal oxides, and by depositing halides and oxo-anions with the iron oxide core. This gives available band gaps of 1.6 to 2.3 eV. Theoretical efficiency calculations based on these band gaps show that the efficiency of a multi-junction solar cell based on layered structures using a fast pulse 150T magnet we measure the band structure change due to the structural phase transition that occurs in this system at around 160K. We also observe Landau levels in the high temperature phase as used for device production, which has a very similar effective mass and the analysis suggests an exciton binding energy which is even smaller than in the low temperature phase.

1This research was partially supported by the Utah Office of Energy Development, Governor’s Energy Leadership Scholars Program.

9:48AM L34.00010 Tuning Fermi Level Beyond the Intrinsic Equilibrium Doping Limit through Quenching: the Case in CdTe1, JI-HUI YANG, JI-SANG PARK, JOONGOO KANG, WYATT METZGER, TERESA BARNES, SU-HUAI WEI, National Renewable Energy Lab — The ability to tune the Fermi levels is of great importance for many electronic device applications. However, the Fermi level is often limited to a certain range in the band gap due to the existence of certain intrinsic compensating defects. Here, we demonstrate that quenching can be used as an effective way to overcome this limit and tune the Fermi levels in a much wider range. Taking a photovoltaic material, CdTe, as a prototype example, we analyzed the physical origin behind the Fermi level pinning and explain why growing the sample at high temperature and then rapidly quenching it to room temperature can overcome the self-compensation limit. We show that for CdTe, quenching can enlarge the Fermi level range from only 0.6 eV to 1.1 eV, which has a great potential in improving CdTe solar cell performance. Our proposed strategy of tuning Fermi level positions beyond intrinsic equilibrium doping limit is general and can be applied to other semiconductor systems.

1The Work at NREL is supported by the U.S. Department of Energy, EEERE/SunShot program, under Contract No. DE-AC36-08GO28308.
10:00AM L34.00011 Photovoltaic efficiency of an indirect bandgap material, MICHELLE TOMASIK, NÍALL MANGAN, JEFFREY GROSSMAN, MIT — Photovoltaic materials with direct band gap transitions absorb light more readily than those with indirect gaps, allowing for thinner devices. However, direct bands also suffer faster rates of radiative recombination than indirect bandgap materials. Some novel photovoltaic absorber materials, such as tin sulfide, have both direct and indirect gaps. Such materials raise the question of whether the multiple energy states benefit or harm device efficiency. We develop a model for current in a device with direct and indirect band gaps using detailed balance, similar to the Shockley-Queisser model for direct band photovoltaics. We explore the effects of the following on device performance: transition probability of carriers between the direct and indirect state, and relative transport rate in each band.

10:12AM L34.00012 Ab initio modeling of the optical properties in organometallic halide perovskites for photovoltaic applications1, AMANDA NEUKIRCH, WAN YI NEI, Los Alamos National Laboratory, LAURENT PEDESSEAU, JACKY EVEN, Université Européenne de Bretagne, CLAUDINE KATAN, CNRS, Institut des Sciences Chimiques de Rennes, ADITYA MOHITE, SEGREGI TRETIAK, Los Alamos National Laboratory — The need for an inexpensive, clean, and plentiful source of energy has generated large amounts of research in an assortment of solution processed organic and hybrid organic-inorganic solar cells. A relative newcomer to the field of solution processed photovoltaics is the lead halide perovskite solar cell. In the past 5 years, the efficiencies of devices made from this material have increased from 3.5% to nearly 20%. Despite the rapid development of organic-inorganic perovskite solar cells, a thorough understanding of the fundamental photophysical processes driving the high performance of these devices is not well understood. I am using state-of-the-art ab initio computational techniques in order to characterize the properties at the interface of perovskite devices in order to aid in materials design and device engineering. I will present an in-depth analysis of the electronic and optical properties of bulk and surface states of pure and mixed halide systems. The high-level static quantum mechanical calculations, including spin-orbit-coupling and the many body GW approach, identify the key electronic states involved in photinduced dynamics. This knowledge provides important information on how the optical properties change with variations to the system.

1Supported by the DOE, the LANL LDRD program XW11, and CNLS.

10:24AM L34.00013 Band-Gap Tuning in Perovskite-type Ferroelectric ZnSnO₃ by Doping and Core-Shell Approach for Solar Cell Applications, CORISA KONS, ANUJA DATTA, Florida Cluster for Advanced Smart Sensor Technologies and Department of Physics, University of South Florida, PRITISH MUKHERJEE, Center for Integrated Functional Materials and Department of Physics, University of South Florida — Ferroelectric (FE) perovskite materials are an emerging class of potential absorbers in next generation solar cells due to their spontaneous polarization which facilitates electron-hole separation and drive charge carriers at opposite ends. With a large remnant polarization of \( \approx 59 \ \mu \text{C/cm}^2 \), perovskite-type LiNbO₃ (LN)-ZnSnO₃, containing earth abundant elements is of much interest as a high performance solar absorber. However, the wide band-gap in ZnSnO₃ (\( \sim 3.7 \) eV) is unsuitable to absorb the broad solar range, which can be overcome by band-gap engineering. Here, we discuss band-gap tuning through substitutional doping (Sb, Cu, Ca, Ba) in LN-type ZnSnO₃ nanorods, synthesized by a facile solvothermal process. A band-gap as low as 2.5 eV was obtained in 5 at.% Ca doped ZnSnO₃ nanorods showing superior FE properties. The current-voltage (\( I-V \)) measurements under light revealed multiple orders of enhancement as compared to the dark. The band-gap in ZnSnO₃ is also found to be a strong function of the lattice constant which is tuned by introducing a slight strain through lattice mismatching using a core shell approach. A detailed structural, optical, and FE analyses are predicted to predict the future of this technologically important material in next generation FE photovoltaics.

10:36AM L34.00014 Nanoscale optimization of quantum dot solar cells, YANSHU LI, ANDREI SERGEEV, NIZAMI VAGIDOV, VLADIMIR MITIN, State Univ of NY - Buffalo, KIMBERLY SABLON, Army Research Laboratory, STATE UNIV OF NY - BUFFALO TEAM, ARMY RESEARCH LABORATORY TEAM — Quantum dots (QDs) offer possibilities for nanoscale control of photoelectron processes via engineering the band structure and potential profile. Nanoscale potential profile (potential barriers) and nanoscale band engineering (AlGaAs atomically thin barriers) effectively suppress the photoelectron capture to QDs. QDs also increase conversion efficiency of the above-bandgap photons due to extraction of electrons from QDs via Coulomb interaction with hot electrons that excited by high-energy photons. To study the effects of the band structure engineering and nanoscale potential barriers on the photovoltaic performance we fabricated 3-\( \mu \text{m} \) base GaAs devices with various InAs quantum dot media and selective doping. All quantum dot devices show improvement in conversion efficiency compared with the reference cell. Quantum efficiency measurements allow us to associate the spectral characteristics of photoresponse enhancement with nanoscale structure of QD media. The dark current analysis provides valuable information about recombination in QD solar cells. The two-diode model well fit the scope of data and recovers the measured open circuit voltage.

10:48AM L34.00015 Theoretical study on single-phase stability and intrinsic defects in different Cu₂ZnSn(Se₁₋ₓSₓ)₄ (x = 0.25, 0.5, 1) alloys, PRANAB SARKER, MUHAMMAD N. HUDA, Department of Physics University of Texas at Arlington, Texas 76019 — Cu₂ZnSn(Se₁₋ₓSₓ)₄ (CZTSSe) alloy has been emerged as a potential next generation commercialized photovoltaic cell because of its higher solar-to-current efficiency (12.6 %) over parent compounds Cu₂ZnSnS₄ (CZTS) and Cu₂ZnSnSe₄ (CZTSe). However, the values of composition \( x \) in higher efficient CZTSSe (>1%) are not known yet. It has been inferred from the recent theoretical and experimental evidences that 0.375 \( \leq x \leq 0.625 \) (\( x = \text{alloy ratio per unit cell} \)) could be the range that poses to ensure higher PV efficiency in CZTSSe. The crystal structure of CZTSSe at those \( x \) values were determined using density functional theory. In addition, the probability of forming different intrinsic defects in those different CZTSSe alloys were evaluated at various growth conditions determined from chemical potential landscape analysis for the first time. Chemical potential landscape analysis further reveals that CZTSSe alloys have higher single phase stability than that of their parent structures.

1This work is partially supported by NREL.

Wednesday, March 4, 2015 8:00AM - 10:36AM
Session L35 DFD: Turbulence and Instabilities

8:00AM L35.00001 Information theory used to study the turbulent cascade, RORY CERBUS, Okinawa Institute of Science and Technology, Fluid Mechanics Unit, WALTER GOLDBURG, University of Pittsburgh, Department of Physics and Astronomy — The simplest picture of turbulence is the one imagined by Richardson and Kolmogorov. In their theory there is a cascade of energy from large scales to small scales. Here we present a new tool to study this picture using simple ideas borrowed from information theory. We use the conditional entropy (conditioned uncertainty) of velocity fluctuations on one scale conditioned on another larger or smaller scale. By varying the scale of the velocity fluctuations used in the conditioning, we can test both direction and locality. The ideas are tested on both experimental and numerical simulation data. This tool can be applied to 3D turbulence or 2D turbulence and because it has nothing to do with the Navier-Stoke’s equation, it can be used for any other system where there is a similar cascade-like phenomenon.

1This work is supported by NSF Grant No. 1044105 and by the Okinawa Institute of Science and Technology (OIST).
8:12AM L35.00002 Mutually independent cascades in anisotropic soap-film turbulence, CHIEN-CHIA LIU, GUSTAVO GIOIA, PINAKI CHAKRABORTY, Okinawa Institute of Science and Technology — Computational, experimental and field data amassed to date indicate that in 2D turbulence the spectrum of longitudinal velocity fluctuations, \( E_1(k_1) \), and the spectrum of transverse velocity fluctuations, \( E_2(k_1) \), correspond always to the same cascade, consistent with isotropy, so that \( E_1(k_1) \propto k^{-5/3} \) and \( E_2(k_1) \propto k^{-5/3} \). The "spectral exponent" \( \alpha \) is either 5/3 (for the inverse-energy cascade) or 3 (for the enstrophy cascade). Here, we carry out experiments on turbulent 2D soap-film flows in which \( E_1(k_1) \propto k^{-5/3} \) and \( E_2(k_1) \propto k^{-5/3} \), as if two mutually independent cascades were concurrently active within the same flow. To our knowledge, this species of spectrum has never been observed or predicted theoretically. Our finding might open up new vistas in the understanding of turbulence.

8:24AM L35.00003 The spectral link in mean-velocity profile of turbulent plane-Couette flows, DONGRONG ZHANG, GUSTAVO GIOIA, PINAKI CHAKRABORTY, Okinawa Institute of Science and Technology — In turbulent pipe and plane-Couette flows, the mean-velocity profile (MVP) represents the distribution of local mean (i.e., time-averaged) velocity on the cross section of a flow. The spectral theory of MVP in pipe flows (Gioia et al., PRL, 2010) furnishes a long-surmised link between the MVP and turbulent energy spectrum. This missing spectral link enables new physical insights into an imperfectly understood phenomenon (the MVP) by building on the well-known structure of the energy spectrum. Here we extend this theory to plane-Couette flows. Similar to pipe flows, our analysis allows us to express the MVP as a functional of the spectrum, and to relate each feature of the MVP relates to a specific spectral range: the buffer layer to the dissipative range, the log layer to the inertial range, and the wake (or the lack thereof) to the energetic range. We contrast pipe and plane-Couette flows in light of the theory.

8:36AM L35.00004 Reinforcement of steady streaks for consecutive transition delay\(^1\), SOHRAB S. SATTARZADEH, JENS H. M. FRANSSON, Linnaeus Flow Centre, KTH Mechanics — Miniature vortex generators (MVGs) are recently proven efficient as passive control devices to delay the transition to turbulence on a flat plate boundary layer by modulating the base flow in the spanwise direction, through generating steady streamwise elongated streaks, and hence reducing the skin-friction drag. As the MVGs are localized in the streamwise direction, a shortcoming of the passive laminar control is the recovery of the two-dimensional boundary layer which force the control effects to fade away. In the present study we show that by placing a second array of MVGs downstream of the first one the streamwise extent of the control can be prolonged by reinforcing the steady streaks in the streamwise direction. The reinforced passive control strategy results in consecutive turbulence transition delay with obtaining a net skin-friction drag reduction of 65\%, for the present measurement conditions, compared to the smooth plate boundary layer.

\(^1\)Support from the European Research Council (ERC) is acknowledged.


8:48AM L35.00005 Numerical study of turbulent transport at high Reynolds number in Richtmyer-Meshkov instability in an ICF like geometry, POOJA RAO, JEREMY MELVIN, RYAN KAUFMAN, HYUNKYUNG LIM, YAN YU, JAMES GLIMM, Stony Brook University, DAVID SHARP, Los Alamos National Lab — We study mixing in high Reynolds (Re) number flows in numerical simulations of a Richtmyer-Meshkov instability in an idealized ICF geometry. We propose that LES simulations of these turbulent flows have an underlying dependence on the numerical algorithm and this possible non-uniqueness emphasize the need for parameter free models to allow extrapolation from validation of Re in the experimental range. Using the front-tracking code FronTier (validated for Rayleigh-Taylor data at Re=35k) in combination with the dynamic subgrid-scale models proposed by Germano, we achieve a parameter free model to allow for this extrapolation step. Under this simulation framework, we discuss the properties of the mixing and document the sensitivity of the subgrid terms to the numerical algorithm.

9:00AM L35.00006 Measuring the orientation and rotation rate of 3D printed particles in turbulent flow, GREG VOTH, Wesleyan Univ, STEFAN KRAMEL, BRENDAN COLE, Wesleyan University — The orientation distribution and rotations of anisotropic particles plays a key role in many applications ranging from icy clouds to papermaking and drag reduction in pipe flow. Experimental access to time resolved orientations of anisotropic particles has not been easy to achieve. We have found that 3D printing technology can be used to fabricate a wide range of particle shapes with smallest dimension down to 300 \( \mu \)m. So far we have studied rods, crosses, jacks, tetrads, and helical shapes. We extract the particle orientations from stereoscopic video images using a method of least squares optimization in Euler angle space. We find that in turbulence the orientation and rotation rate of many particles can be understood using a simple picture of alignment of both the vorticity and a long axis of the particle with the Lagrangian stretching direction of the flow.

9:12AM L35.00007 Lattice-Boltzmann Simulation of Tablet Dissolution in Complex Hydrodynamic Environment, JIAOLOONG JIANG, NING SUN, Materials Science and Engineering Department, Stony Brook University, Stony Brook, NY, 11794, USA, TAESHN PARK, GLEN H. KO, RES Group Inc., 1 Broadway, Cambridge, MA, 02142, USA, DILIP GERSAPPE, Materials Science and Engineering Department, Stony Brook University, Stony Brook, NY, 11794, USA — Using the Lattice-Boltzmann method, we developed a 3D model to study the tablet dissolution process in a complex hydrodynamic environment involving spatially varying velocity and shear forces. The results show that a turbulent flow is formed in the region above the tablet, which has been obtained by visualization experiments. The dissolution profiles were obtained by incorporating detailed kinetics, showing good agreement with case studies from literature. After studying the influence of the paddle speed and the size of the system, we simulated the dissolution process for multicomponent tablets. Our results indicate how the hydrodynamic environment would affect the dissolution process by changing the local concentration of components near the tablet as well as by the particle erosion under high fluid velocity. Since the code was successfully parallelized, the simulation for comparatively large systems is possible now.

9:24AM L35.00008 Three Dimensional Characterization of Quantum Vortex Dynamics in Superfluid Helium, DAVID MEICHLE, DANIEL LATHROP, University of Maryland — Vorticity is constrained to line-like topological defects in quantum superfluids, such as liquid Helium below the Lambda transition. We have invented a novel method to disperse fluorescent nanoparticles directly into the super-fluid which become trapped on the vortex cores, providing optical tracers. Using a newly constructed multi-camera stereographic microscope, we present data dynamically characterizing vortex reconnections and the subsequent emission of Kelvin waves fully in three dimensions. Statistics of thermally driven counterflow will be compared in 3D to previous measurements in projection.

9:36AM L35.00009 The Importance of Nonlocal Terms in Superfluid Turbulence, RENA ZIEVE, OWEN DIX, University of California, Davis — Simulations of vortex motion in superfluid helium based on the Biot-Savart law plus vortex reconnections can model homogeneous superfluid turbulence. However, the quantitative properties of the turbulent tangle are disturbingly sensitive to details of how the computations are carried out, and in some cases the tangle degenerates unphysically into an arrangement of parallel straight vortices. These problems have been attributed to the reconnection procedure, to the periodic boundary conditions used for most calculations, and to the localized induction approximation (LIA) which often replaces the (non-local) Biot-Savart integral. Previous work using numerical calculation of the complete Biot-Savart integral does not show the same issues as the LIA calculations, but these are time-consuming calculations. We show here that numerical integration over a relatively small region can suffice, as long as the size of the region exceeds the typical intervortex spacing. This result explains why the non-local contribution has a strong effect. It contributes an attraction between nearby vortices that ultimately leads to reconnections, which prevent the vortices from settling into an array of parallel lines.
9:48AM L35.00010 Study of Grid Turbulence in Superfluid He\textsuperscript{4} in a Large Square Channel\textsuperscript{1}.

JHIEE YANG, GARY C. IHAS, University of Florida, WILLIAM F. VINE, University of Birmingham — Studying quantum turbulence in superfluid helium can lead us to a deeper understanding in classical turbulence. We study grid-generated turbulence in liquid helium in the temperature range 1.4 K-2.1 K for homogeneous and isotropic turbulence (HIT). Using a conventional second sound attenuation method, the decay of vorticity ($\omega$) is observed in a long, square cross-section channel. Theories assume that energy is injected on the scale of the grid mesh size, and predict that when the energy containing eddies are growing, the vorticity decays as $\omega \sim t^{-11/6}$ for $\omega \sim t^{-17/14}$. When they saturate at the channel size, the vorticity begins decaying as $\omega \sim t^{-11/2}$. Previous experiments have been performed in 1 cm$^2$ square channels, with a limited range of mesh sizes. We have used a larger channel and various mesh sizes to investigate grid mesh size effects and decay before saturation. A novel phase and amplitude locked feedback system ensures fast, stable attenuation data without disturbances from temperature fluctuations.

\textsuperscript{1}US NSF DMR #1007937 and EPSRC EP /H04762X/1.

10:00AM L35.00011 Observation of the Stratorotational Instability in Flow between Rotating Concentric Cylinders\textsuperscript{1}.

RYU IBANEZ, HARRY L. SWINNEY, University of Texas at Austin, BRUCE RODENBORN, Centre College — We study the stratorotational instability in a Taylor-Couette system with a radius ratio $\eta = r_o/r_i = 0.877$. The system is vertically stratified with a constant buoyancy frequency, $N = \sqrt{-g/(\rho_o/\rho_i)(\partial \rho/\partial z)}$. We determine when the flow becomes unstable as the ratio of the outer to inner cylinder rotation rates, $\mu = \Omega_o/\Omega_i$, is decreased from unity (solid body rotation), for Reynolds numbers $Re = \Omega_i r_i (r_o - r_i)/\nu$ ranging from 450 to 4000 and $N/2r = 0.3$ to 1.0 Hz. The axial and azimuthal frequencies, obtained from spatiotemporal spectral analysis of digital movies, yield the observed modes at different Re and $\mu$ for fixed $N$. We find for sufficiently large buoyancy frequency, $N/2r > 0.5$ Hz, the stratorotational instability occurs even above the $\mu = \eta$ stability limit obtained from theory developed in the Boussinesq (small $N$) approximation [cf. the review by D A Shalybkov, \textit{Physics Uspekhi} 52, 915 (2009)]. The frequencies we obtain for the azimuthal modes are close to multiples of the average frequency of rotation of the cylinders, while the axial wavelengths are found to vary linearly with Froude number, $Fr = \Omega_i/N$.

\textsuperscript{1}Supported by The Sid W. Richardson Foundation

10:12AM L35.00012 Stability analysis of an electrified liquid jet in the presence of an externally coflowing liquid. VENKAT GUNDABALA, VIKRANT MODI, Indian Institute of Technology Bombay, GUNDABALA MICROFLUIDICS GROUP TEAM — Traditionally, electrospraying and electrospaying are carried out with either air or vacuum as external medium. Recently, it has been shown that electrospRAY can be successfully implemented in the presence of an external flowing liquid. We envisage that implementation of electrospraying process in the presence of an external liquid coflowing with the electrospraying solution will allow greater control on the fiber deposition and morphology. In the present work, to gain fundamental understanding on the behaviour of an electrified liquid jet in the presence of an externally coflowing liquid, we perform stability analysis on the system. The classical Rayleigh-Plateau instability and an electrically induced axisymmetric instability were identified. The effect of the viscosity, velocity, and permittivity of the ambient liquid on the stability of the two instabilities was studied. It was found that both the growth rate and the critical wavenumbers were strongly influenced by the above parameters. An operating diagram predicting the transition from drop generation mode to fiber generation mode as a function of external liquid properties is generated.

10:24AM L35.00013 An adaptive selective frequency damping method\textsuperscript{1}. BASTIEN JORDI, COLIN COTTER, SPENCER SHERWIN, Imperial College London — The selective frequency damping (SFD) method is used to obtain unstable steady-state solutions of dynamical systems. The stability of this method is governed by two parameters that are the control coefficient and the filter width. Convergence is not guaranteed for arbitrary choices of these parameters. Even when the method does converge, the time necessary to reach a steady-state solution may be very long. We present an adaptive SFD and show that by modifying the control coefficient and the filter width along the solver execution, we can reach an optimum convergence rate. This method is based on successive approximations of the dominant eigenvalue of the flow studied. We design a one-dimensional model to select SFD parameters that enable us to control the evolution of the least stable eigenvalue of the system. These parameters are then used for the application of the SFD method to the multi-dimensional flow problem. We apply this adaptive method to a set of classical test cases of computational fluid dynamics and show that the steady-state solutions obtained are similar to what can be found in the literature. Then we apply it to a specific vortex dominated flow (of interest for the automotive industry) whose stability had never been studied before.

\textsuperscript{1}Seventh Framework Programme of the European Commission - ANADE project under grant contract PITN-GA-289428

Wednesday, March 4, 2015 8:00AM - 11:00AM – Session L36 GSOFT: Focus Session: Reconfiguring and Actuating Soft Matter I: Metamaterials

8:00AM L36.00001 Buckling in a topological metamaterial. ANINE MEEUSSEN, JASYN PAULOSE, VINCENZO VITTELLI, Univ of Leiden — Controlling the nonlinear response of mechanical metamaterials paves the way toward designing materials with adaptive and tunable mechanical properties. Buckling, a change in load-bearing state from axial compression to off-axis deformation, is a ubiquitous nonlinear instability that is often exploited to change the local or global mechanical response in metamaterials composed of slender elements. We create localized buckling regions in cellular metamaterials by engineering states of self-stress, regions where the response is dominated by stretching or compression of the constituent beams rather than bending at the stiff hinges connecting them. Unique to our approach is the use of topological states of self-stress, which originate in a topological invariant that characterizes the vibrational spectrum of the repeating unit cell. Unlike typical states of self-stress which result from additional geometric constraints induced by excess beams in a region, these topological states do not change the number of beams at each hinge. We demonstrate the phenomenon through numerical calculations of the linear response of the proposed metamaterial, and through experiments probing the nonlinear regime including localized buckling at specific regions.

8:12AM L36.00002 Holey Sheet! A Programmable Mechanical Metamaterial. BASTIAAN FLORIJN, CORENTIN COULAI, MARTIN VAN HECKE, Leiden University — We probe the mechanics of BiHolar metamaterials, 2D elastic media with a square lattice of circular holes of two different sizes. Biaxial loading of these BiHolar structures leads to a wealth of mechanical responses, including mechanically switchable hysteresis and memory effects. We show that we can program the mechanical response with the loading force and the hole size ratio\textsuperscript{[1]}

\textsuperscript{[1]}Bastiaan Florijn, Corentin Coulais, and Martin van Hecke, Phy. Rev. Lett. 113, 175503 (2014)
Tunable acoustic metamaterials

D. ZEB ROCKLIN, University of Michigan, Department of Physics, BRYAN CHEN, Instituut-Lorentz, Leiden University, MARTIN FALK, Massachusetts Institute of Technology, TOM LUBENSKY, University of Pennsylvania, Physics and Astronomy, VINCENZO VITELLI, Instituut-Lorentz, Leiden University — Mechanical lattices under periodic boundary conditions with coordination $z = 2d$, where $d$ is the spatial dimensionality, and with a gapped phonon spectrum at all wavenumbers not equal to zero are isostatic. When cut, these lattices with $N$ sites in two dimensions necessarily have of order $N^{1/2}$ zero modes on their boundaries. Recently, Kane and Lubensky showed that these systems can be described by a super-symmetric Hamiltonian analogous to that of the Su-Schrieffer model for polyacetylene and they identified a topological invariant, the topological polarization, that determines on which edges zero modes lie in finite systems. We show that a family of two-dimensional four-site-per-unit-cell isostatic lattices possess topologically protected bulk zero modes. These “Weyl modes” are novel, tunable low-energy mechanisms of the mechanical lattice. They are the analogs of the zero-energy electronic modes of topological semimetals. We discuss how adjusting the lattice parameters induces Weyl modes and alters their wavevectors (generally incommensurate with the lattice) and how they can transport zero modes from one edge to an opposite one as surface wavenumber varies. An accompanying talk discusses the novel dynamical properties of the system.

Reversible Shape Memory Optical Gratings

QIAOXI LI, CARY TIPPETS, YULAN FU, Univ of NC - Chapel Hill, EUGENE DONEV, Seawee: The University of the South, SARA TURNER, VALERIE ASHBY, RENE LOPEZ, SERGEI SHEIKO, Univ of NC - Chapel Hill — Recent advancements in the understanding of the mechanisms that control shape memory in semi-crystalline polymers, has led to the development of protocols that allow for reversibility in complex shape transformations. The shift between two programmable shapes is reversible without applying any external force. This is made possible by thermodynamically driven relaxation of extended polymer chains on heating is then inverted by kinetically preferred pathways of polymer crystallization on cooling. Reversible shape-shifting was applied to modulation of photonic gratings to create hands-free reversibly tunable optical elements. We have fabricated a sub-micron ratio optical square grating that presents reversible magnitude changes of its diffraction intensity (up to about 38% modulation) when subject to changes in temperature. This result is attributed to programmable changes in the grating height due to reversible shape memory and is repeatable over multiple cycles. Besides, roughness-induced variations in scattering signal observed upon heating-cooling cycles may offer another way to monitor kinetics of polymer melting and crystallization. Grants: NSF DMR-1407645, A. CHEN, R. SOORYAKUMAR, Ohio State Univ - Columbus — Photonic crystals and diffraction gratings are key components in color displays, bio/chemical sensors and security coded documentation, among others. Most magnetically responsive photonic crystals rely on electrostatic repulsion and magnetic attraction between constituent particles to tune the inter-particle spacing and thus, their resulting optical signatures. We present a 2D tunable diffraction device based on an all magnetic confinement and manipulation scheme previously developed for fluid borne magnetic dipoles (Scientific Reports 3, 3124 (2013)). The confinement platform consists of thin-film permanent magnets patterned on a silicon surface and a precessing magnetic field. By adjusting the orientation of the field, inter-particle dipolar and trap confinement forces are tuned, thereby enabling the confined magnetic beads to repel or attract one another. A bench top epi-illumination microscope delivers a narrow incident light cone that is diffracted and subsequently imaged. We investigate the white light diffraction from beads in various overall confining potentials, as a function of the orientation of the magnetic field. The presence of the confining potential and field-tunable inter-particle spacing gives rise to a wide range of tunable diffraction patterns.

Effects of graphene on electro-optic switching and spontaneous polarization of a ferroelectric liquid crystal

RAJ TARANT BASU, US Naval Academy — A small quantity of graphene flakes was doped in a ferroelectric liquid crystal (FLC), and the field-induced ferroelectric electro-optic switching was found to be significantly faster in the FLC+graphene hybrid than that of the pure FLC. Further studies revealed that the suspended graphene flakes enhanced the FLC’s spontaneous polarization by improving smectic-C ordering resulting from the pi-electron stacking, and reduced rotation viscosity by trapping some of the free ions of the FLC media. These effects coherently impacted the FLC-switching phenomenon, enabling the FLC molecules to switch faster on reversing an external electric field.

Effects of graphene on electro-optic response and ion-transport in a nematic liquid crystal

DANIEL KINNAMON, ALFRED GARVEY, RAJ TARANT BASU, US Naval Academy — A small quantity of graphene flakes was doped in a nematic liquid crystal (LC), and the nematic electro-optic switching was found to be significantly faster in the LC+graphene hybrid than that of the pure LC. Additional studies revealed that the presence of graphene reduced the free ion concentration in the nematic media by ion-trapping process. The reduction of mobile ions in the LC was found to have subsequent impacts on the LC’s conductivity and rotational viscosity, allowing the nematic director to respond faster on switching the electric field on and off.
10:00AM L36.00011 Sound and Noisy Light: Optical Control of Phonons in Photo-switchable Structures. SOPHIA SKLAN, JEFFREY GROSSMAN, Massachusetts Inst of Tech-MIT. We present a novel means of controlling phonons via optical tuning. Taking as a model an array of photoresponsive materials (photowitches) embedded in a matrix, we numerically analyze the vibrational response of an array of bistable harmonic oscillators with stochastic spring constants. Changing the intensity of light incident on the lattice directly controls the composition of the lattice and therefore the speed of sound. Furthermore, modulation of the phonon bandstructure at high frequencies results in a strong confinement of phonons. The applications of this regime for phonon wave-guides, vibrational energy storage, and phononic transistors is examined.

1Support provided by NSF GRF Grant No. 112374

10:12AM L36.00012 Meta-Atom Interactions and Coherent Response in rf SQUID Metamaterials. MELISSA TREPANIER, DAIMENG ZHANG, University of Maryland, OLEG MUKHANOVA, Hynes, PHILIPP JUNGSUSANNE BUTZ, Karlsruhe Institute of Technology, V.P. KOSELETS, IEEE, ALEXEY USTINOVA, Karlsruhe Institute of Technology, STEVEN ANLAGEA, University of Maryland. An rf SQUID (radio frequency superconducting quantum interference device) metamaterial can be modeled as an array of coupled nonlinear oscillators with resonant frequencies that are extremely tunable with temperature, dc magnetic field, and rf current. The metamaterial is driven by an external rf field and its response to that field defines its metamaterial characteristics. In the presence of disorder (nonuniform applied dc magnetic flux for instance) the SQUIDs may or may not oscillate coherently in response to the external rf field. Since we are interested in metamaterial applications, a strong coherent response is desirable. The coherence is affected by a variety of factors including flux uniformity, array size, degree of coupling, strength of the driving field, and uniformity in SQUID parameters. In this talk we will present experimental and simulation results exploring the effect of these parameters on coherence.

1This work is supported by the NSF-GOALI and OISE programs through grant # ECCS-1158644, and CNAM.

10:24AM L36.00013 ABSTRACT WITHDRAWN —

10:36AM L36.00014 Combinatorial 3D Mechanical Metamaterials. CORENTIN COULAIS, Univ of Leiden, EIAL TEOMY, Tel-Aviv University, KOEN DE REUS, Univ of Leiden, YAIR SHOKEF, Tel-Aviv University, MARTIN VAN HECKE, Univ of Leiden / AMOLF. We present a class of elastic structures which exhibit 3D-folding motion. Our structures consist of cubic lattices of anisotropic unit cells that can be tiled in a complex combinatorial fashion. We design and 3d-print this complex ordered mechanism, in which we combine elastic hinges and defects to tailor the mechanics of the material. Finally, we use this large design space to encode smart functionalities such as surface patterning and multistability.

10:48AM L36.00015 Mechanical topological matter. LISA NASH, DUSTIN KLECKNER, University of Chicago, VINCENTO VITHELLI, Instituut-Lorentz, Leiden University, ARI M. TURNER, Johns Hopkins University, WILLIAM T.M. IRVINE, University of Chicago. Topologically protected states can arise in electronic systems with broken time-reversal symmetry. We present a classical mechanical model for a solid in which broken time-reversal symmetry gives rise to topologically protected edge-modes, analogous to the edge modes in the quantum Hall effect. We will discuss numerical and experimental observations of these chiral edge-modes, their topological characterization, robustness and broader phenomenology.

Wednesday, March 4, 2015 8:00AM - 11:00AM –
Session L37 GQI: Focus Session: Semiconductor Qubits - Electrically Controlled Quantum Dots 212A - Charles Marcus, University of Copenhagen

8:00AM L37.00001 Addressable single-spin control in multiple quantum dots coupled in series. TAKASHI NAKAJIMA, RIKEN Center for Emergent Matter Science – Electron spin in semiconductor quantum dots (QDs) is promising building block of quantum computers for its controllability and potential scalability [1]. Recent experiments on GaAs QDs have demonstrated necessary ingredients of universal quantum gate operations: single-spin rotations by electron spin resonance (ESR) which is virtually free from the effect of nuclear spin fluctuation [2], and pulsed control of two-spin entanglement [3]. The scalability of this architecture, however, has remained to be demonstrated in the real world. In this talk, we will present our recent results on implementation of single-spin-based qubits in triple, quadruple, and quintuple QDs based on a series coupled architecture defined by gate electrodes. Deterministic initialization of individual spin states and spin-state readout were performed by the pulse operation of detuning between two neighboring QDs. The spin state was coherently manipulated by ESR, where each spin in different QDs is addressed by the shift of the resonance frequency due to the inhomogeneous magnetic field induced by the micro magnet deposited on top of the QDs. Control of two-spin entanglement was also demonstrated. We will discuss key issues for implementing quantum algorithms based on three or more qubits, including the effect of a nuclear spin bath, single-shot readout fidelity, and tuning of multiple qubit devices. Our approaches to these issues will be also presented. This research is supported by Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST) from JSPS, IARPA project “Multi-Qubit Coherent Operations” through Copenhagen University, and Grant-in-Aid for Scientific Research from JSPS.


8:36AM L37.00002 Multi-qubit read-out of spin qubits in GaAs in a CCD like manner: the Spin qubit CCD. TIM BAART, MOHAMMAD SHAFIEI, JULES VAN OVEN, Kavli Institute of Nanoscience, Delft University of Technology, CHRISTIAN REICHL, WERNER WEGSCHEIDER, Solid State Physics Laboratory, ETH Zurich, LIENEN VANDERSYPEN, Kavli Institute of Nanoscience, Delft University of Technology. Efficient implementation and characterization of quantum information protocols requires the ability to measure multiple qubits individually and in a single-shot manner. We reported a succesful demonstration of two-qubit read-out in [1]. We now demonstrate the next step by reading out three individual spin qubits formed by a linear array of three quantum dots where each electron forms a single spin qubit. We introduce several strategies for multi-qubit measurements in dot arrays and demonstrate and implement the following protocol experimentally. We first read-out the right qubit using standard spin-to-charge conversion [2]. Next we shuttle the centre electron to the right dot and read out its spin state. Afterwards we shuttle the left qubit through the centre dot to the right, and complete the three-qubit read-out. Due to its resemblance with reading out a CCD, we coin this the Spin qubit CCD. This is the first demonstration of reading out multiple qubits through the same reservoir and allows scaling to larger arrays of qubits.


Biasing modes, the Hamiltonian has an especially simple form, which can directly generate a wide range of different entangling gates including the iSWAP gate. In which the system can be biased, and use the representation of its nonlocal properties in terms of local invariants. We find that, in one of the possible trajectories. Furthermore, we prepare different states using these gates and determine their fidelities. In our experiment this calibration routine succeeds in removing systematic gate errors to a high degree while increasing the pulses’ decoherence. We extract the Bloch sphere trajectories of the resulting gate sequences using self-consistent state tomography and find good agreement with the theoretically predicted trajectories. 


Fernando Calderon-Vargas, Jason Kestner, University of Maryland Baltimore County — In view of recent experimental demonstration of entanglement in capacitively coupled singlet-triplet qubits, we address the open question of what type of entangling gates the system’s Hamiltonian can produce directly via a single square pulse. In the analysis we consider the system’s Hamiltonian from first principles, incorporating the three different ways in which the system can be biased, and use the representation of its nonlocal properties in terms of local invariants. We find that, in one of the possible biasing modes, the Hamiltonian has an especially simple form, which can directly generate a wide range of different entangling gates including the iSWAP gate. 

Moreover, using the complete form of the Hamiltonian we find that, for any biasing mode, a CNOT gate can be generated directly.


Xin Wang, Condensed Matter Theory Center, University of Maryland, College Park, Edwin Barnes, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland, College Park — Precise execution of quantum gates acting on two or multiple qubits is essential to quantum computation. For semiconductor spin qubits coupled via capacitive interaction, the best fidelity for a two-qubit gate demonstrated so far is around 70%, insufficient for fault-tolerant quantum computation. In this talk we present control protocols that may substantially improve the robustness of two-qubit gates against both nuclear noise and charge noise. Our pulse sequences incorporate simultaneous dynamical decoupling protocols and are simple enough for immediate experimental realization. Together with existing control protocols for single-qubit gates, our results constitute an important step toward scalable quantum computation using spin qubits.

This work is done in collaboration with Sankar Das Sarma and supported by LPS-NSA-CMTCT and IARPA-MQCO.

Jeroen Danon, Mark Rudner, Niels Bohr Inst. — We study multi-photon resonances in a strongly-driven three-level quantum system, where one level is periodically swept through a pair of levels with constant energy separation $E$. Near the multi-photon resonance condition $n \omega_0 = E$, where $n$ is an integer, we find qualitatively different behavior for $n \geq 2$. We explain this phenomenon in terms of families of interfering trajectories of the multi-level system. Remarkably, the behavior is insensitive to fluctuations of the energy of the driven level, and survives deep into the strong dephasing regime. The setup can be relevant for a variety of solid state and atomic or molecular systems. In particular, it provides a clear mechanism to explain recent puzzling experimental observations in strongly-driven double quantum dots.

Peter Stano, Riken Center for Emergent Matter Science, Wako, Saitama, Japan, Jelena Klinovaja, Floris Braakman, Department of Physics, Kinglerbergstrasse 82, University of Basel, Switzerland, Lieven Vandersypen, Kavli Institute of Nanoscience, TU Delft, 2600 GA Delft, The Netherlands, Daniel Loss, Department of Physics, Kinglerbergstrasse 82, University of Basel, Switzerland — We investigate theoretically the long-distance coupling and spin exchange in an array of quantum dot spin qubits in the presence of microwaves. We find that photon assisted tunnelling is boosted at resonances between photon and energy of virtually occupied excited states and show how to make it spin selective. We identify configurations that enable fast switching and spin echo sequences for efficient and non-local manipulation of spin qubits. We devise configurations in which the near-resonantly boosted tunnelling provides non-local coupling which, up to certain limit, does not diminish with distance between the manipulated dots before it decays weakly with inverse distance.

9:48AM L37.00008 Efficient suppression of Overhauser field fluctuations with DNP. Robert McNeil, Tim Botzem, Stefanie Tenberg, JARA Institute for Quantum Information, RWTH-Aachen University, Sebastian Rubbert, Kavli Institute of Nanoscience Delft, Delft University of Technology, Hendrik Bluhm, JARA Institute for Quantum Information, RWTH-Aachen University — In certain spin-qubit schemes the Overhauser field is a tuned control parameter and in many spin qubits this fluctuating nuclear field is a significant factor limiting coherence. Nuclear spins can be driven via dynamic nuclear polarisation (DNP) to a chosen field and selective feedback applied narrowing the distribution of nuclear Overhauser field fluctuations[1]. The achievable narrowing of the Overhauser field is related to the maximum pump rate and previous experiments on gated GaAs quantum dots were limited by the pump rate of the pumping mechanism used. We present a method to reduce nuclear fluctuations by increasing the maximum achievable pump rate. Sequentially applying two ac electric fields with frequencies slightly detuned from the desired Larmor frequency results in a pump curve with a stable fixed point. In the absence of spin-orbit interaction, driving electron spin flips via electric dipole spin resonance (EDSR)[2] will also drive nuclear spin flips and this scheme is expected to result in stronger pumping and efficient suppression of the Overhauser field fluctuations. We will present experimental evidence of this driven nuclear polarization including tracking of EDSR resonances. 1. Bluhm, et al. PRL 105, 216803 ('10) 2. Laird, et al. PRL 99, 246601 ('07)

10:00AM L37.00009 Anisotropy and quadrupolar effects on dephasing in two-electron spin qubits in GaAs. Tim Botzem, Robert McNeil, Hendrik Bluhm, JARA-Institute for Quantum Information, RWTH Aachen University. D-52074 Aachen, Germany — Understanding the dynamics of nuclear spins causing decoherence of gate-defined two-electron spin qubits in GaAs is a crucial prerequisite for a potential use in quantum computation. We present B-field dependent Hahn echo measurements giving new insight on the mechanism causing dephasing due to the nuclear spin bath of the host material GaAs. By rotating the magnetic field inplane we discover two effects ultimately limiting coherence times. We find that the anisotropy of the nuclear spins and electrical fields contributes to broadening of the nuclear Lamor frequencies, which in turn degrades electron coherence. By rotation the magnetic field towards the [100] direction, we can minimize this effect, but an additional envelope modulation that can be attributed to a electron g-factor anisotropy occurs.
Pumping of Dynamic Nuclear Polarization in GaAs Double Quantum Dots

Supported by NSF grant DMR-1207298

Wednesday, March 4, 2015 8:00AM - 11:00AM
Session L38 GQI: Focus Session: Quantum Algorithms 212B - Nathan Wiebe, Microsoft Research
8:48AM L38.00005 Quantum learning robust to noise1, JOHN SMOLIN, ANDREW CROSS, GRAEME SMITH, IBM T J Watson Res Ctr — Noise is often regarded as anathema to quantum computation, but in some settings it can be an unlikely ally. We consider the problem of learning the class of n-bit parity functions by making queries to a quantum example oracle. In the absence of noise, quantum and classical parity learning are easy and almost equally powerful, both information-theoretically and computationally. We show that in the presence of noise this story changes dramatically. Indeed, the classical learning problem is believed to be intractable, while the quantum version remains efficient. Depolarizing the qubits at the oracle’s output at any constant nonzero rate does not increase the computational (or query) complexity of quantum learning more than logarithmically. However, the problem of learning from corresponding classical examples is the Learning Parity with Noise (LPN) problem, for which the best known algorithms have superpolynomial complexity. This creates the possibility of observing a quantum advantage with a few hundred noisy qubits. The presence of noise is essential for creating this quantum-classical separation.

1AWC and JAS acknowledge support from ARPA under contract W911NF-10-1-0324

9:00AM L38.00006 Quantum algorithm for topological and geometric analysis of data, SETH LLOYD, MIT, PAOLO ZANARDI, University of Southern California, SILVANO GARNERONE, IQC University of Waterloo — Topological methods for analyzing data sets provide a powerful technique for extracting useful information from data. Data that represents geometric features of the world typically gives a distorted picture of those features, if only because the devices and systems that sense the world and that generate the data by their very nature induce distortions. By definition, topological features are those that persist under continuous distortions of the data. Topological methods can therefore identify features of the real system from which the data was collected, but that have been distorted by the data collection process. Persistent homology is a sophisticated tool for identifying such topological features—connected components, holes, or voids—and for determining how such features persist as the data is viewed at different scales. This talk presents quantum machine learning algorithms for calculating Betti numbers in persistent homology, and for finding eigenvectors and eigenvalues of the combinatorial Laplacian (the quantities that famously allow one to “hear the shape of a drum”). The algorithms provide an exponential speedup over classical algorithms for topological and geometrical data analysis.

9:12AM L38.00007 On the Chemical Basis of Trotter-Suzuki Errors in Quantum Chemistry Simulation, RYAN BABBUSH, JARROD MCCLEAN, Harvard University, DAVE WECCKER, Microsoft Research, ALÁN ASPURU-GUZIK, Harvard University, NATHAN WIEBE, Microsoft Research — Although the simulation of quantum chemistry is one of the most anticipated applications of quantum computing, the scaling of known upper bounds on the complexity of these algorithms is daunting. Prior work has bounded errors due to Trotterization in terms of the norm of the error operator and analyzed scaling with respect to the number of spin-orbitals. However, we find that these error bounds can be loose by up to sixteen orders of magnitude for some molecules. Furthermore, numerical results for small systems fail to reveal any clear correlation between ground state error and number of spin-orbitals. We instead argue that chemical properties, such as the maximum nuclear charge in a molecule and the filling fraction of orbitals, can be decisive for determining the cost of a quantum simulation. Our analysis motivates several strategies to use classical processing to further reduce the required Trotter step size and to estimate the necessary number of steps, without requiring additional quantum resources. Finally, we demonstrate improved methods for state preparation techniques which are asymptotically superior to proposals in the simulation literature.

9:24AM L38.00008 Simulating Hamiltonian Dynamics with a Truncated Taylor Series, ROLANDO SOMMA, Los Alamos National Laboratory — One of the main motivations for quantum computers is their ability to efficiently simulate the dynamics of quantum systems. Since the mid-1990s, many algorithms have been developed to simulate Hamiltonian dynamics on a quantum computer, with applications to problems such as simulating spin models and quantum chemistry. While it is now well known that quantum computers can efficiently simulate Hamiltonian dynamics, ongoing work has improved the performance and expanded the scope of such simulations. In this talk, I will describe a very simple and efficient algorithm for simulating Hamiltonian dynamics on a quantum computer by approximating the truncated Taylor series of the evolution operator. This algorithm can simulate the time evolution of a wide variety of physical systems. The cost of this algorithm depends only logarithmically on the inverse of the desired precision, and can be shown to be optimal. Such a cost also represents an exponential improvement over known methods for Hamiltonian simulation based on, e.g., Trotter-Suzuki approximations. Roughly speaking, doubling the number of digits of accuracy of the simulation only doubles the complexity. The new algorithm and its analysis are highly simplified due to a technique for implementing linear combinations of unitary operations to directly apply the truncated Taylor series. This is joint work with Dominic Berry, Andrew Childs, Richard Cleve, and Robin Kothari.

10:00AM L38.00009 Scaling of Quantum Walks on Complex Networks1, STEFAN BOETTCHER, STEFAN FALKNER, Physics Dept., Emory University, RENATO PORTUGAL, Laboratório Nacional de Computação Científica — I will describe the renormalization group method (RG) as applied to master equations with a unitary propagator. It allows to determine many asymptotic properties of quantum walks, although I will focus here on the walk dimension d_w, which describes the similarity solution, p(x,t) ∼ f(|x|/d_w)^t, for the probability density function p. We can calculate d_w to arbitrary accuracy for a number of networks, such as the dual Sierpinski gasket, small-world Hanoi networks, or Migdal-Kadanoff lattices, which we have verified with direct simulations. However, due to unitarity, the asymptotic solution of the RG equations as well as procedures to implement RG approximately for arbitrary walks remain elusive. Yet, based on the exact RG for the nearest neighbor walk, we can conjecture a few general conclusions, for instance, that d_w for a discrete-time quantum walk is always half of that for the random walk on the same r-regular network, when driven with the Grover coin. (This talk summarizes our work in http://dx.doi.org/10.1103/PhysRevA.90.032324 and http://arxiv.org/abs/1410.7034.)

1We acknowledge financial support from the U. S. National Science Foundation through grant DMR-1207431.

10:12AM L38.00010 An Easy Method for Finding the Scattering Coefficients of Quantum Graphs and Some Applications, SETH COTTRELL, New York Univ NYU — Quantum walks are roughly analogous to classical random walks, and like classical walks they have been used to find new (quantum) algorithms. When studying the behavior of large graphs or combinations of graphs it is often useful to find the response of a subgraph to signals of different frequencies. In this talk I’ll be presenting a simple technique for quickly finding the scattering coefficients of any quantum graph. This is done by imitating the scattering states using normalizable states on a modified version of the graph. These scattering coefficients can be expressed entirely in terms of the characteristic polynomial of the graph’s time-step operator. With these coefficients in hand we can replace an entire subgraph with a single vertex whose behavior is frequency dependent. This gives us a powerful set of tools for rapidly understanding the behavior of more complex structures. Time permitting, I will apply these tools to several types of graphs (star, complete, tree) demonstrating how we can gain information about the structure of these graphs by bouncing signals off of them, describing the limitations on what information cannot be accessed, and even show how to construct some computations using quantum walks that can be run in faster than classical time.

10:24AM L38.00011 Variational Quantum Eigensolver: How to Use Any Quantum Device in Your Lab to Perform Quantum Simulation, JARROD MCCLEAN, Harvard University — Quantum devices offer a way to simulate and study states that currently cannot be efficiently stored or manipulated on classical computers. Unfortunately, many quantum algorithms designed to simulate such states are prohibitively expensive in terms of quantum resources such as coherence time. In this talk I will review a recently introduced technique, the Variational Quantum Eigensolver, that has minimal coherence and can utilize any quantum device capable of basic state preparation and measurement for a quantum advantage in the simulation of physical quantum states. I will also introduce the problem of simulation of molecular systems in quantum chemistry and discuss recent advances in understanding and reducing the costs associated with this problem in our and related algorithms.
HENDRIK MEIER, RICHARD T. BRIERLEY, ANGELA KOU, STEVEN M. GIRVIN, LEONID I. GLAZMAN, Yale University — We investigate a long chain of inductively coupled Josephson junctions penetrated by an external magnetic field. In the limit of infinite junction capacitances, we determine the classical ground state and find that the competition between Josephson and inductive forces leads to a rich phase diagram as a function of magnetic flux per plaquette $\phi_0$ and the ratio $F = E_J/E_L$ of Josephson ($E_J$) and inductive ($E_L$) energies. At large $\ell$, kinks in the superconducting phase set in as a function of $\phi_0$, similarly to vortices in type-II superconductors. Upon further increasing $\phi_0$, the interplay between kink-kink interaction and pinning on the lattice leads to a Frenkel-Kontorova-type (devil’s) staircase of phases distinguished by different rational kink densities. At $\phi_0$, equal to half a flux quantum, the system bears similarity to a classical Ising antiferromagnet, possibly with a long-ranged exchange. Inclusion of a finite junction capacitances is similar to placing the Ising chain in a transverse magnetic field (the quantum Ising model). Using this similarity, we investigate the quantum dynamics of a chain of fluxonium qubits.

8:12AM L39.00002 Ground states and excitations of inductively coupled fluxonium qubits, R.T. BRIERLEY, H. MEIER, A. KOU, I.I. GLAZMAN, S.M. GIRVIN, Yale University — We consider fluxonium qubits arranged in a one dimensional array, where the inductors are shared between neighboring qubits. For an infinite system with small charging energies, there are a series of different phases that depend on the applied magnetic flux and the ratio of the inductive and Josephson energies. For small flux and large Josephson energy, the behavior of the classical ground state is similar to the Frenkel-Kontorova model, while when the flux is half a flux quantum it is similar to an Ising antiferromagnet. A realistic finite system will not exhibit a phase transition but some features of the infinite-size limit should persist. We investigate theoretically the ground and low-lying excited states for experimentally relevant parameters. We discuss how the nature of the ground state changes, and what experimental signatures would be expected.

8:24AM L39.00003 Reentrant Behavior in A Multi-connected Superconducting Jaynes-Cummings Lattice, LIN TIAN, KANGJUN SEO, School of Natural Sciences, University of California, Merced, CA 95343, USA — Superconducting quantum devices have excellent connectivity, tunable coupling and long decoherence time as demonstrated by recent experiments. These devices provide a powerful platform for constructing analog quantum simulators to study novel many-body effects. Here we present a multi-connected Jaynes-Cummings lattice model, where the qubits and the resonators are connected alternately. In a one-dimensional configuration, this model bears an intrinsic symmetry between the left and the right qubit-resonator couplings under a mirror reflection. Different from the coupled cavity array (CCA) model, the qubit-resonator couplings in this model induce both onsite Hubbard nonlinearity and hopping of the excitations along the lattice. By analyzing this model in the limiting cases of very different couplings, we show that this model demonstrates a Mott insulator–superfluid–Mott insulator transition at commensurate fillings with symmetric critical points. The reentry to the Mott insulator phase originates from the symmetry between the couplings.

8:36AM L39.00004 Phase Diagram of A Multi-connected Superconducting Jaynes-Cummings Lattice at Commensurate and Incommensurate Fillings, KANGJUN SEO, LIN TIAN, School of Natural Sciences, University of California, Merced, CA 95343, USA — A multi-connected superconducting Jaynes-Cummings lattice can be constructed with alternatively-connected superconducting qubits and resonators. In a one-dimensional configuration, this model bears an intrinsic symmetry between the left and the right qubit-resonator couplings. Here we study the quantum phase transition of this model using the exact diagonalization method. At commensurate fillings, the off-diagonal long range order of the single-particle density matrix and the energy gap are calculated. We obtain the phase diagram of this model, which demonstrates a symmetry between the couplings and a reentry to the Mott insulator phase. For a system with given chemical potential, the density of the excitations contains integer-valued plateaus between critical chemical potentials that define the boundaries of different many-body phases and indicate the phase transition. We also discuss the implementation of this model with superconducting devices, including the state preparation and detection schemes.

8:48AM L39.00005 Simulating an Interacting Quantum Gas with Superconducting Circuits, CHRISTOPHER EICHLER, JONAS MLYNEK, JONAS BUTSCHER, PHILIPP KURPIERS, ETH Zurich, TOBIAS OSBORNE, Gottfried Wilhelm Leibniz Universität Hannover, ANDREAS WALLRAFF, ETH Zurich — The high level of control achievable over quantized degrees of freedom have turned superconducting circuits into one of the prime physical architectures for quantum computing and simulation. While conventional approaches towards quantum information processing mostly rely on unitary time evolution, more recently open-system dynamics are considered for quantum simulations. In this talk, I will present experiments in which we use an open cavity QED system with tunable interactions to simulate the ground state of an interacting Bose gas confined in one dimension [1,2]. These experiments rely on the ability to efficiently measure higher order photon correlations of the cavity output field. For this purpose we have developed a quantum limited amplifier achieving phase-preserving amplification at large bandwidth and high dynamic range [3]. Our results explore a different path towards the simulation of complex quantum many-body physics based on the controlled generation and detection of nonclassical radiation in an open quantum system.

9:00AM L39.00006 Many-body localization in a quantum system subject to a local periodic drive, CANRAN XU, MAXIM VAVILOV, Univ of Wisconsin, Madison — We consider a one dimensional spin chain system with quenched disorder and in the presence of a local harmonic drive. We study the time evolution of the system in the Floquet basis and evaluate the Bures displacement of the system in the Hilbert space caused by the drive per one period. This displacement can be used to identify two phases of the system: (1) the many-body localized phase, in which the distribution of the distance exhibits long tails while its average value decreases rapidly as disorder increases; and (2) the ergodic phase, in which the displacement distribution is narrow and its average value weakly depends on disorder. This distinction in the average value of the displacement between the two phases develops readily for system with ten or more spins. Therefore, recently built networks of superconducting qubits subject to a local microwave drive can simulate dynamics of a system in the many-body localization regime.

1Supported by NSF Grants No. DMR-1105178 and DMR-0955500.
9:12AM L39.00007 Localization vs. delocalization of waves in circuit QED. BRUNO G. TAKETANI, FRANK K. WILHELM, Saarland University — Wave localization in disordered media is an important phenomenon arising from the destructive interference of waves from the many scatterers in the medium. However, interaction between localized modes may counteract this effect and lead to a localization-delocalization transition. Understanding this interplay between disorder and interaction is of great importance. We investigate this interplay using quasiperiodic JJA.

9:24AM L39.00008 Site-wise manipulations induced phase transitions of interacting photons using superconducting circuit simulators1, XIUHAO DENG, School of Natural Sciences, University of California Merced, CHUNJING JIA, Department of Applied Physics, Stanford University, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator, CHIH-CHUN CHIEN, School of Natural Sciences, University of California Merced — The Bose Hubbard model (BHM) of interacting bosons in a lattice has been a paradigm in many body physics. Here a quantum simulator of the BHM using a superconducting circuit is proposed. Specifically, a superconducting transmission line resonator supporting microwave photons is coupled to a charge qubit to form one site of the BHM, and adjacent sites are connected by a tunable coupler. To obtain a mapping from the superconducting circuit to the BHM, we focus on the dispersive regime where the excitations remain photon-like. Standard perturbation theory is implemented to locate the parameter range where the BHM can be simulated. This simulator allows single-site manipulations and we illustrate this feature by considering two scenarios where a single-site manipulation can drive a Mott insulator-superfluid transition. The critical point of the transition can be located by mean-field analyses and the exact diagonalization method was implemented to provide accurate results. The variance of the density and the fidelity metric clearly show signatures of this transition. Experimental realizations and other possible applications of this simulator are also discussed.

9:36AM L39.00009 Classical chaos and its correspondence in superconducting qubits. C. NEILL, B. CAMPBELL, Z. CHEN, B. CHIARO, A. DUNSWORTH, M. FANG, I. HOI, J. KELLY, A. MEGRANT, P. O’MALLEY, C. QUINTANA, A. VAINSENCHER, J. WENNER, T. WHITE, UC Santa Barbara, R. BARENDRES, YU CHEN, A. FOWLER, E. JEFFREY, J. MUTUS, P. ROUSHAN, D. SANK, J.M. MARTINIS, Google, Santa Barbara — Advances in superconducting qubits have made it possible to experimentally investigate quantum-classical correspondence by constructing quantum systems with chaotic classical limits. We study the quantum equivalent of a classical spinning top using three fully coupled qubits that behave as a single spin-3/2 and subject the spin to a sequence of non-linear rotations. The resulting entanglement bears a striking resemblance to the classical phase space, including bifurcation, and suggests that classical chaos manifests itself as quantum entanglement. Studying the orientation of the spin-3/2 reveals that the rotations which generate chaos and entanglement are at the same time the source of disagreement between the quantum and classical trajectories. Our experiment highlights the correspondence between classical non-linear dynamics and interacting quantum systems.

9:48AM L39.00010 Quantum simulation with arrays of transmon qubits: Ising dynamics1. VINAY RAMASESH, SHAY HACOHEN-GOURGY, QNL, University of California, Berkeley, THOMAS KIENDL, FLORIAN MARQUARDT, Institut for Theoretical Physics, Universität Erlangen-Nürnberg, Staudtstraße 7, D-91058 Erlangen, Germany, NATHAN SIWAK, CHRISTOPHER RICHARDSON, Laboratory for the Physical Sciences - University of Maryland, College Park, IRFAN SIDDIQI, QNL, University of California, Berkeley — Chains of coupled qubits are known to realize the transverse-field Ising Hamiltonian in the two-level approximation. In this model, the qubit transition frequencies map onto the external magnetic field, so the ground and excited states play the role of spin-up and spin-down atoms. We implement this structure in a planar, on-chip architecture, with a one dimensional linear array of capacitively-coupled transmon qubits, where the two terminal qubits are dispersively coupled to microwave independent resonators for state readout. We present spectroscopic data and describe coherent manipulations in the array.

1This work is supported by the AFOSR.

10:00AM L39.00011 Quantum simulation with an array of transmon qubits: Bose-Hubbard model1. SHAY HACOHEN-GOURGY, VINAY RAMASESH, QNL, University of California, Berkeley, CLAUDIA DE GRANDI, STEVEN GIRVIN, Departments of Physics and Applied Physics, Yale University, IRFAN SIDDIQI, QNL, University of California, Berkeley — Chains of capacitively-coupled transmons can emulate the Bose-Hubbard Hamiltonian when one considers the full level-structure of the circuit. Here, each individual transmon plays the role of a lattice site, with the excitation level of each transmon corresponding to the number of bosons occupying that particular site. The transmon’s anharmonicity gives rise to the attractive contact-interaction term, while the capacitive coupling realizes the hopping amplitude. We implement such a chain of 3 capacitively-coupled transmons in a single 3D microwave cavity. In our parameter regime, the ground state of the 3-excitation subspace is one in which all excitations lie on a single qubit. Using cavity-assisted bath engineering, it should be possible to cool from an initial state in this subspace to the ground state. We present the current status of this goal.

1This work is supported by AFOSR, Army Research Office W911NF1410011 and NSF DMR-1301798

10:12AM L39.00012 Perturbative scanning probe microscopy on a Kagome lattice of superconducting microwave resonators, DEVIN UNDERWOOD, Princeton University, WILL SHANKS, IBM, ANDY C.Y. LI, JENS KOCH, Northwestern University, ANDREW HOUCK, Princeton University — Microwave photons confined to a lattice of coupled resonators, each coupled to its own superconducting qubit have been predicted to exhibit matter like quantum phases. Realizing such a lattice-based quantum simulator presents a daunting experimental challenge; as such, new tools and measurement techniques are a necessary precursor. Here, we present measurements of the internal mode structure of microwave photons on a 49-site Kagome lattice of capacitively-coupled coplanar waveguide resonators without qubits. By scanning a probe with a sapphire tip over the surface of a single lattice site, the resonant frequency was detuned, thus forming a local defect in the lattice. This perturbation resulted in measurable shifts in the lattice spectrum, which were used to extract the mode weights at the perturbed site. By perturbing each lattice site it was possible to reconstruct a complete map of different normal mode weights within the entire lattice. Additionally we present experimental evidence of a frustrated flat band that arises from the Kagome lattice geometry.

10:24AM L39.00013 Perturbative study of interacting photons in open lattices, ANDY C.Y. LI, Northwestern University, FRANCESCO PETRUCCIONE, University of KwaZulu-Natal and National Institute for Theoretical Physics, JENS KOCH, Northwestern University — Quantum simulation realized in the circuit QED architecture is an emerging direction to study many-body physics in open lattice systems. Among several models of interacting photons, the driven-dissipative Jaynes-Cummings (JC) lattice is commonly employed to investigate the steady-state and dynamical behavior. While there is a wealth of analytical and numerical tools applicable to closed lattice systems in thermal equilibrium, the number of methods to treat open lattice systems is rather limited. Hence, many properties of open lattices remain an open question. Here, we formulate a general perturbation theory and an infinite-order resummation scheme applicable to open lattices. We then apply this theory to the driven-dissipative JC lattices to predict steady-state expectation values. This allows us to explore the rich features due to photon-qubit interaction and compare results obtained for finite chains and infinite lattices.
10:36 AM L39.00014 Experimental Study of a Disordered Jaynes-Cummings Lattice , MATTIAS FITZPATRICK, DEVIN UNDERWOOD, DARIUS SADRI, Princeton University, JENS KOCH, Northwestern University, ANDREW HOUCK, Princeton University — Circuit quantum electrodynamics (cQED) is an exciting testbed for simulation of open quantum systems. Effective photon-photon interactions can be mediated by a superconducting qubit strongly coupled to a microwave transmission line cavity. Many-body quantum simulators can be realized using Jaynes-Cummings systems, where a competition is induced between onsite interactions and hopping between sites. In this experiment, we present measurements of a Kagome lattice consisting of 49 microwave cavity resonators and 49 transmon qubits. We fabricate each qubit with random area superconducting quantum interference devices (SQUIDs) to create qubits with different sensitivity to magnetic field. This allows us to simultaneously tune all of the qubits randomly with the application of a single external magnetic field, enabling a systematic study of the effects of disorder. We will present preliminary experimental results from this Kagome lattice as well as future directions of quantum simulation using Jaynes-Cummings lattices.


Wednesday, March 4, 2015 8:00AM - 11:00AM – Session L41 DPOLY DMP: Focus Session: Organic Electronics and Photonics - Transport in Polymer Thin Films 214A - Barry Rand, Princeton University

8:00 AM L41.00001 Changes in the Solution Behavior of Conjugated Polymers with Light Absorption , MARK DADMUN, BRIAN MORGAN, University of Tennessee — Conjugated polymers are well established as functional materials in a broad range of applications including organic photovoltaics, chemical sensors, and organic light emitting diodes. This functionality is mainly derived from their ability to create electron-hole pair excitons through photoexcitation. The presence of these entities on the polymer chains may alter the chain conformation, solution behavior, and ultimately macroscopic morphology, of the conjugated polymer. Previous studies have shown significant changes in properties such as viscosity and photooluminescence upon exposure of select conjugated polymer films to white light. In order to expand upon these preliminary findings, we have performed small angle neutron scattering experiments on solutions of several semiconducting, conjugated polymers in both the presence and absence of incident light. Substantial differences are observed between the light vs dark samples, the magnitude of which are dependent on polymer dispersion, solvent choice, and solution concentration. Analysis of the neutron curves shows real difference in Kuhn lengths and radius of gyration of the polymer, suggesting possible rearrangement of polymer chain conformation or alteration of polymer chain-solvent interactions.

8:12 AM L41.00002 Correlating Transport with Nanostructure and Chemical Identity in Radical Polymer Conducting Glasses , BRYAN BOUDOURIS, LIZBETH ROSTRO, ADITYA BARADWAJ, MARTHA HAY, Purdue University — Radical polymers are an emerging class of macromolecules that are composed of non-conjugated backbones which bear stable radical groups at the pendant positions. Because of these stable radical sites, these glassy materials are able to conduct charge in the solid state through a series of oxidation-reduction (redox) reactions. Importantly, the redox-active behavior is controlled by both the local chemical environment of the radical polymer groups and by the nanoscale structure of the materials. Here, we demonstrate that proper control of the pendant group chemical functionality allows for the fabrication of transparent and conducting amorphous thin films which have solid-state hole mobility and electrical conductivity values on the same order as those seen in common conjugated, semicrystalline polymer systems [e.g., poly(3-hexylthiophene) (P3HT)]. Furthermore, we show that control of the nanostructure of the materials aids in facilitating transport in these radical polymer thin films. In turn, we implement simultaneous spectroscopic and electrical characterization measurements in order to elucidate the exact mechanism of charge transport in radical polymers. Finally, we demonstrate that, because there is ready control over the molecular properties of these materials, developing bendable and stretchable transparent conducting thin films is relatively straightforward with this unique class of organic electronic materials.

8:24 AM L41.00003 Using NEXAFS spectroscopy to probe the Biaxial Orientation of a Pyridal[2,1,3]thiadiazole-containing Donor-Acceptor Polymer , SHRAYESH PATEL, GREG SU, CHAN LUO, MING WANG, ALAN HEEGER, GUILLERMO BAZAN, MICHAEL CHABINYC, EDWARD KRAMER, UC Santa Barbara; Mitsubishi Chemical - Center for Advanced Materials — Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy is a powerful tool to probe the molecular orientation of conjugated polymer thin films. Here, we report on the biaxial orientation of a high mobility donor-acceptor copolymer coated on uniaxial nanogrooved substrates. The polymer system under investigation is regioregular PCDTPT based on cyclopenta[2,1-b:3,4-b]dithiophene (CDT) and pyridal[2,1,3]thiadazole (PT) structural units. In partial electron yield mode, NEXAFS spectroscopy is a surface sensitive technique (~2-3 nm). This is particularly useful as we are interested in probing the orientation near the interface between the polymer and the substrate. While the carbon K-edge is commonly used for NEXAFS experiments, we can take advantage of the PT unit and use the nitrogen K-edge to probe the biaxial orientation of our films. We will present the biaxial orientation of films coated on substrates with and without uniaxial nanogrooves. The results indicate that the presence of uniaxial nanogrooves are important in obtaining films with high level of orientation. Lastly, anisotropic field-effect transistor mobility values will be presented for various coating conditions.

8:36 AM L41.00004 Percolation, tie-lines, and the microstructural determinants of charge transport in semicrystalline conjugated polymers , ANDREW SPAKOWITZ, Stanford University — Semiconducting polymers play an important role in a wide range of optical and electronic material applications. It is widely accepted that the polymer ordering impacts charge transport in such devices. However, the connection between molecular ordering and device performance is difficult to predict due to the current need for a mathematical theory of the physics that dictates charge transport in semiconducting polymers. Here, we present a new analytical and computational description in which the morphology of individual polymer chains is dictated by well-known statistical models and the electronic coupling between units is determined using Marcus theory. This effort combines our research group’s modeling efforts in polymer conformational properties and reaction-diffusion phenomena to address the multiscale dynamics of charge transport in a heterogeneous material. The resulting model is capable of bridging molecular-level charge transport mechanisms to large scale transport behavior, thus facilitating direct comparison with experiments. The multiscale transport of charges in these materials (high mobility at short length scales, low mobility at long length scales) is naturally described with our framework. Additionally, the dependence of mobility with electric field and temperature is explained in terms of conformational variability and spatial correlation. Our model offers a predictive approach to connecting processing conditions with transport behavior.
9:12AM L41.00005 Charge motion in Poly(3-hexylthiophene-2,5-diyl) studied with Scanning Probe Microscopy1, JASON MOSCATELLO, CHLOE CASTANEDA, KATHERINE AIDALA, Mount Holyoke College — Organic semiconductors like poly(3-hexylthiophene-2,5-diyl) offer the promise of solution-processable, flexible electronics, but the charge motion in these disordered films is not fully understood. We use Kelvin Probe Force Microscopy (KPFM) to study trapped charges in the channel of inverted field effect transistors and have developed a technique to measure real time screening. The tip of the AFM is placed at a specific location above the sample with grounded source and drain electrodes, and the potential of the surface is recorded using KPFM. When a voltage is applied to the back gate, charges will move to screen this potential. For materials with relatively low charge density and mobility, it will take some time of amount to fully screen. The tip will initially measure the potential of the voltage applied to the back-gate, which will decrease as charges enter the film. The shape and timescales of this decrease reveal information about injection barriers and traps in the material. Our data suggest that we are observing holes entering and exiting trap states as the gate voltage is turned on and off. Other factors, such as aging, increase the timescales of the screening.

1Supported by NSF DMR-1207924

9:24AM L41.00006 Probing charge delocalization in a semi-crystalline supramolecular polymer, KEEHOON KANG, SHUN WATANABE, KATRINA BROCH, Cavendish Laboratory, University of Cambridge, Cambridge, U.K., DAIUSKE MATSUMOTO, KAZUHIRO MARUMOTO, Division of Materials Science, University of Tsukuba, Japan, HISAAKI TANAKA, SHIN-ICHI KURODA, Department of Applied Physics, Nagoya University, Japan, MARTIN HEENEY, Department of Chemistry, Imperial College, London, U.K., HENNING SIRRINGHAUS, Cavendish Laboratory, University of Cambridge, Cambridge, U.K. — Various doping methods have achieved metallic conductivity in π-conjugated polymer but most of them suffer from dopant-induced disorder. We developed a simple and effective method of doping a high mobility semi-crystalline polymer, poly(2,5-bis(3-hexadecylthiophen-2-yl)-thieno[3,2-b]thiophene) (pBTBT) by forming a bi-layer with a small-molecule acceptor, 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4-TCNQ). The doping realizes an efficient charge transfer between pBTBT and F4-TCNQ (conductivity over 150 S/cm), while preserving the structural order of a pristine pBTBT. The charges are discovered to be sufficiently delocalized to give rise to a nearly-ideal Hall effect, and therefore, a coherent transport in a wide temperature range. Graphene was used as the back contact material, and the charge density was measured to be approximately 8 cm-2 per room temperature. The combination of a Pauli magnetic susceptibility and magnetococonductance signatures strengthen the evidence of weak localization in the supramolecular system. Comparison with other amorphous conducting polymers elucidates the role of structural order as an indicator of the degree of charge delocalization.

9:36AM L41.00007 A Blend Approach to P3HT Based Field Effect Transistor Performance Enhancement via Inclusion of 2,5-bis(3-dodecylthiophen-2-yl)thieno[3,2-b]thiophene: PING-HSUN CHU, Georgia Institute of Technology, LEI ZHANG, University of Massachusetts, Amherst, JUNG OK PARK, MOHAN SRINIVASARAO, Georgia Institute of Technology, ALEJANDRO L. BRISEÑO, University of Massachusetts, Amherst, ELSA REICHMANIS, Georgia Institute of Technology — Improved OFET performance through a polymer-small molecule semiconductor blend approach was demonstrated. However, a number of serious issues remain. For example, the threshold voltage (Vth) of the blend OFETs is still at a relatively high value (Vth) > 10V), which is incompatible with most of portable electronics. Moreover, electrode treatment or thermal annealing is required to avoid a sacrifice in the device performance. However, a small molecule, 2,5-bis(3-dodecylthiophen-2-yl)thieno[3,2-b]thiophene (BTTT), is proposed to be incorporated within poly(3-hexylthiophene) (P3HT) polymer thin-films and is demonstrated to lead to over 50% improvement in charge carrier mobility. The resultant blend OFETs exhibit approximately 5-fold increase in charge carrier mobility, 10-fold increase in on-off current ratio and concomitantly, controlled the Vth as low as 1.7 V. It is worth noting that no pre- or post-treatment is required during the blend OFET fabrication process. Further, the thin-film deposition was conducted under ambient conditions using a volatile low boiling point solvent, suggesting a promising method for low-cost, high-throughput, large-area flexible device fabrication under non-stringent conditions.

9:48AM L41.00008 Probing electric fields within organic transistors by nonlinear optics1, PAULO B. MIRANDA, SILVIA G. MOTTI, DOUGLAS J. C. GOMES, Instituto de Fisica de Sao Carlos, Universidade de Sao Paulo, Brazil — Organic field-effect transistors (OFETs) are important building blocks in many organic devices, but further improvements in their performance will require a detailed knowledge of their operation mechanism. Thus mapping the electric fields in OFETs, both in the active organic layer and inside the gate dielectric, will allow a direct comparison with theoretical OFET models and guide advances in device engineering. The nonlinear optical processes of sum-frequency generation (SFG) and second-harmonic generation (SHG) may be used to probe electric fields in OFETs. With a proper choice of pump wavelength, SHG can selectively probe the field component along the OFET channel, inside the organic semiconductor. In contrast, SFG may probe the field within any organic material by selecting a specific molecular vibration and monitoring the field-enhanced SFG signal. Here we investigate OFETs fabricated with a polythiophene derivative (P3HT) on silicon substrates and with the insulating polymer PMMA for the dielectric layer. Both the strength and sign of the electric field in PMMA can be determined, yielding a direct probe of charge accumulation along the OFET channel. An extension of this technique to map the spatial distribution of accumulated charge along the channel will also be discussed.

1Work funded by FAPESP and CNPq (Brazil)

10:00AM L41.00009 Sub-threshold charge transport in polymer transistors, SEOHEE KIM, The University of Texas at Austin, TAE-JUN HA, Kwangwoon University, PRASHANT SONAR, Queensland University of Technology, ANANTH DODABALAPUR, The University of Texas at Austin — Research on polymer transistors has taken center stage due to their promise for use in displays, large-area electronics, and sensors. Most transistors with disordered semiconductor active layers such as amorphous silicon and polymers, have a large density of bulk trap states. Sub-threshold conduction in such transistors is very important. In particular, charge transport in the drift-limited sub-threshold regime is important and has not been adequately investigated. In this work, we will present an analysis of sub-threshold charge transport in polymer transistors with active layers based on the diketopyrrolopyrrole (DPP) core. Such transistors possess room temperature field-effect mobilities of over 2 cm2/Vs. We present an analysis of both above threshold and below threshold charge transport and show how the transport mechanisms change with temperature and charge density. We will also discuss a method to correctly calculate the density of trap states by sub-threshold modeling.

10:12AM L41.00010 High Performance Short-Channel Organic Field-Effect Transistors with Graphene Electrodes1, NARAE KANG, SAIFUL I. KHONDAKER, NanoScience Technology Center and Department of Physics, University of Central Florida — Organic Field-Effect Transistors (OFETs) have received a great deal of attention due to their easy-processing, low-cost, flexibility, and transparency that can lead to future electronic applications such as flexible display, solar cell, and sensors. One of the major challenges in fabricating high-performance OFETs is to reduce a large injection barrier formed at metal/organic interface, which results in poor electrical transport performance. In order to overcome this issue, graphene has been suggested as a promising electrode material for OFETs due to its unique electronic properties as well as strong π-π interaction with organic molecular, which can reduce the injection barrier at the electrode/organic interface. In this study, we fabricated short-channel OFETs using mechanically exfoliated graphene electrodes, and performed temperature dependent transport studies. We will present the detailed temperature dependent data and discuss the charge carrier injection mechanism at graphene/organic interface.

1US NSF Grant No. ECCS 1102228
10:24AM L41.00011 Charge transport in ion-gel gated IDTBT transistors. SHUN WANG, BEI BAO, XIANYI SHAO, LIU TAN, YUESHEN WU, LIBIN WEN, XUXU BAI, XIAOJUN GUO, YING LIU, Shanghai Jiao Tong University — Ionic liquids (ion gels) have been employed as the gate dielectric for polymer transistors due to its ultra-high capacitance. At high charge carrier density provided by ionic liquid gating, polymers like P3HT and PBTTT can exhibit very high mobility. We have fabricated ion-gel gated IDTBT transistors and measured its charge transport properties. We found that the mobility of ion-gel gated IDTBT transistors is greatly suppressed compared to the Cytop gated devices. At carrier density on the order of $10^{14}/$cm$^2$, IDTBT shows mobility of about 0.05 cm$^2$/V/s. Detailed analysis of the temperature dependence of resistivity shows 3D Mott variable range hopping in IDTBT at such carrier density, indicating a different charge transport mechanism from Cytop gated device.

10:36AM L41.00012 Conditions for the Formation of P3HT Organogels During Spin-Coating: Tuning Electrical Properties in Thin Films. CAMERON S. LEE, WEN YEN, Department of Chemistry, University of Texas, Austin — Development of hole-transporting copolymers for use in bulk heterojunctions (BHJs) has significantly improved organic solar cell performance. Despite advances on the materials side, the physics of charge carrier transport remains unsettled. Intrigued by its ability to maintain high fill factors in thick active layers, we studied the copolymer poly[(5-(4,4-diocytyl-4H-silolo)[3,4-b:5,6-b']dithiophen-2yl)-3-tetradecylthiophen-2-yl)] blended with P3HT:BM. Results show mobilities which are carrier-concentration-dependent and characterized by a negative Poole-Frenkel effect. Such behavior is not described by current carrier transport models. Established transport mechanisms like multiple-trap-and-release or variable range hopping yield dependence of mobility on carrier concentration. However, a more basic model like Gaussian distribution model (GDM) is needed to produce the negative Poole-Frenkel effect, though GDM cannot describe carrier-concentration-dependent mobility. We have combined key aspects of existing models to create a unified transport model capable of describing phenomena observed in P3TSiTzTz:PC$_7$BM. This model can be used to address open questions about transport physics of organic BHJ materials.

10:48AM L41.00013 Insights from transport modeling of unusual charge carrier behavior of PDTSiTzTz:PC$_7$BM bulk heterojunction materials. OLEKSIY SLOBODYAN, SARAH MOENCH, KELLY LIANG, ERIC DANIELSON, BRADLEY HOLLIDAY, ANANTH DODABALAPUR, Univ of Texas, Austin — Development of hole-transporting copolymers for use in bulk heterojunctions (BHJs) has significantly improved organic solar cell performance. Despite advances on the materials side, the physics of charge carrier transport remains unsettled. Intrigued by its ability to maintain high fill factors in thick active layers, we studied the copolymer poly[(5-[(4,4-diocytyl-4H-silolo)[3,4-b:5,6-b']dithiophen-2yl)-3-tetradecylthiophen-2-yl)] blended with P3HT:BM. Results show mobilities which are carrier-concentration-dependent and characterized by a negative Poole-Frenkel effect. Such behavior is not described by current carrier transport models. Established transport mechanisms like multiple-trap-and-release or variable range hopping yield dependence of mobility on carrier concentration. However, a more basic model like Gaussian distribution model (GDM) is needed to produce the negative Poole-Frenkel effect, though GDM cannot describe carrier-concentration-dependent mobility. We have combined key aspects of existing models to create a unified transport model capable of describing phenomena observed in P3TSiTzTz:PC$_7$BM. This model can be used to address open questions about transport physics of organic BHJ materials.

Wednesday, March 4, 2015 8:00AM - 11:00AM
Session L42 DPOLY: Focus Session: Renewable and Sustainable Polymers 214B - Megan Robertson, University of Houston

8:00AM L42.00001 Ecobionanocomposites: Hierarchical supramolecular materials incorporating stereocomplexation. JOHN DORGAN, Colorado School of Mines — Polyactides (PLAs) are a leading class of renewable plastics with several favorable sustainability metrics. However, for many applications basic PLA has insufficient properties. The combination of nanoscopic filler particles can be combined with the phenomena of stereocomplexation to create a new class of hierarchically structured materials. Recent progress on the development of these novel ecobionanocomposites is discussed.

8:12AM L42.00002 Insights from transport modeling of unusual charge carrier behavior of PDTSiTzTz:PC$_7$BM bulk heterojunction materials. OLEKSIY SLOBODYAN, SARAH MOENCH, KELLY LIANG, ERIC DANIELSON, BRADLEY HOLLIDAY, ANANTH DODABALAPUR, Univ of Texas, Austin — Development of hole-transporting copolymers for use in bulk heterojunctions (BHJs) has significantly improved organic solar cell performance. Despite advances on the materials side, the physics of charge carrier transport remains unsettled. Intrigued by its ability to maintain high fill factors in thick active layers, we studied the copolymer poly[(5-[(4,4-diocytyl-4H-silolo)[3,4-b:5,6-b']dithiophen-2yl)-3-tetradecylthiophen-2-yl)] blended with P3HT:BM. Results show mobilities which are carrier-concentration-dependent and characterized by a negative Poole-Frenkel effect. Such behavior is not described by current carrier transport models. Established transport mechanisms like multiple-trap-and-release or variable range hopping yield dependence of mobility on carrier concentration. However, a more basic model like Gaussian distribution model (GDM) is needed to produce the negative Poole-Frenkel effect, though GDM cannot describe carrier-concentration-dependent mobility. We have combined key aspects of existing models to create a unified transport model capable of describing phenomena observed in P3TSiTzTz:PC$_7$BM. This model can be used to address open questions about transport physics of organic BHJ materials.

8:36AM L42.00002 Positive effect of biaxial stretching on the mechanical behavior of PLA-Talc nanocomposites. SAADIA OUCHIAR, GREGORY STOCLET, Université de Lille 1 - UMET, CYRILLE CABARET, Ecomeris, VINCENT GLOAGUEN, Université de Limoges - LCSN, JEAN-MARC LEFEBVRE, Université de Lille 1 - UMET, UMET - ENGINEERING POLMER SCIENCE TEAM, UMET / ECMERIS COLLABORATION, UMET / LCSN COLLABORATION — Poly (Lactic acid) (PLA), a biodegradable polyester issued from renewable resources, appears as a good candidate for the replacement of petrochemical-based materials due to its good combination of physical properties. However, major drawbacks of PLA are its brittle behavior and its low thermal stability. One way to outclass these lacks consists in adding nanofillers into PLA. It is also recognized that the mechanical and barrier properties can be improved by biaxial drawing process. Consequently, this study deals with the enhancing effect of biaxial stretching on mechanical properties of Talc based PLA nanocomposites. The Talc content was varied between 0 to 30 wt%. This high level of talc results in a decrease in material cost, in addition to the enhancement of various physical properties. A main result is that neat PLA, which initially exhibit a brittle behavior upon uniaxial stretching at room temperature, become ductile after being biaxially stretched under appropriate conditions. More surprising is that the same behavior is observed for the filled samples. The origin of these enhancing properties will be also discussed.

8:48AM L42.00003 Manipulating Interactions in Cellulose Nanocrystal/Waterborne Epoxy Composites through Physical Mixing. MEISHA L. SHOFNER, School of Materials Science and Engineering, Georgia Institute of Technology, NATALIE M. GIROUARD, J. CARSON MEREDITH, School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, GREGORY T. SCHUENEMAN, Forest Products Laboratory, USDA Forest Service — The objective of this research is to more fully understand the relationships between component interactions and processing pathways in cellulose nanocrystal (CNC)/polymer composite materials. Specifically, wood-derived CNC/waterborne epoxy composites with CNC loadings up to 15 wt.% were produced using two different protocols. Through relatively simple changes in processing, significant differences in CNC dispersion and composite physical properties were seen, and these changes were attributed to an association between the CNCs and the epoxy emulsion, similar in nature to colloidal halogen. Considering literature results available for CNC nanocomposites, as well as other types of polymer nanocomposites, these results support the assertion that the processing-structure-property relationships in such nanocomposites are diverse and can be used to design materials for a range of applications. Additionally, these results put into context the properties that can be expected in composites containing wood-based CNCs produced at a pilot scale facility as compared to CNCs from other cellulose sources produced a few grams at a time, making these results relevant to the production of CNC-based composites at larger volumes.

1Research supported by the USDA Forest Service (11-JV-11111129-117)
9:00AM L42.00004 Epoxy thermost set networks derived from vegetable oils and their blends1  
CHANG RYU, MATTHEW RAVALLI, Rensselaer Polytechnic Institute — Epoxidized vegetable oils (EVOs), such as epoxidized soybean oil and linseed oils were prepared by the partial oxidation of the unsaturated double bonds in vegetable oils and used as monomers for preparing epoxy thermost set materials based on the cationic polymerization. These EVOs have been used to prepare epoxy thermost sets of different network densities by cationic polymerization using onium salt catalyst. The crosslinked epoxy thermost sets provide an ideal platform to study the structure-property-relationships of networked polymers. In particular, rheological studies on the epoxidized vegetable oil thermost sets have been performed to measure the molecular weights between crosslinks (Mx) in the epoxy thermost sets and to ultimately elucidate the role of functionality of epoxy groups in EVO on the mechanical and thermophysical properties of the epoxy thermost set materials.

1 NSF DMR POLYMERS 1308617

9:12AM L42.00005 Structure-Property Relationships in Thiol-Ene Networks Composed of Plant-Derived Chemistry Ac. GUOZHEN YANG, HIRUY TESEFAY, MEGAN ROBERTSON, Univ of Houston — Polymer films prepared through thiol-ene chemistry are attracting increasing attention due to their ease of preparation and superior physical properties. We are investigating the properties of thiol-ene films which contain plant-derived allylated phenolic acids as substitutes to traditional petroleum-derived ene-bearing components. Phenolic acids are readily available through a variety of plant sources and contain rigid aromatic rings which contribute mechanical strength to the resulting polymer films. In this study, the properties of polymer films containing four phenolic acids were explored: salicylic acid, 4-hydroxybenzoic acid, gentisic acid and gallic acid. The allylated phenolic acids vary in the relative number and placement of the allyl groups used in the preparation of the polymer films, which impacts the resulting crosslinking density, glass transition temperature, and mechanical behavior of the polymer films. We have developed relationships between the chemical structures of the phenolic acids and the thermal and mechanical behavior of the polymer films.

9:24AM L42.00006 Polyester Vitrimers from Biosourced Lactones1  
JACOB BRUTMAN, PAULA DELGADO, MARC HILLMYER, University of Minnesota - Twin Cities — Crosslinked polymers with controllable healing characteristics have received significant attention over the last decade. However, there is still much to be developed with these materials in the sustainability arena. Herein, we studied the healing capabilities of crosslinked bioderived poly(lactones) through Lewis acid catalyzed transesterification reactions. Materials that use isodesmic reactions (e.g., transesterification) for healing are termed vitrimers and have been reported using a diverse range of chemistries. Our initial studies focused on the healing properties of amorphous star-shaped poly((±)-lactide) crosslinked with methylenediphenyl disocyanate in the presence of stannous(II) octoate. These materials exhibited remarkably fast stress relaxation rates when compared with previously reported polyester-based vitrimers, and exhibited similar stress relaxation rates at temperatures 140°C lower. Furthermore, the materials were able to recover their original tensile strengths post-healing by heating the system at 140°C for only 30 min. These results will be described in this presentation, as well as our ongoing research efforts on utilizing renewable crosslinkers, a variety of Lewis acid catalysts, and other amorphous polyesters derived from substituted lactates.

1 We acknowledge the Center for Sustainable Polymers at the University of Minnesota, a National Science Foundation supported Center for Chemical Innovation (CHE-1136607).

9:36AM L42.00007 Short-Range Correlation of Successive Helical Jump Motions of Poly(L-Lactic Acid) Chains as Revealed by Solid State NMR1  
WEI CHEN, TOSHIKAZU MIYOSHI, Department of Polymer Science, the University of Akron — Polylactide (i.e. Polyactic acid, PLA) is a renewable and biocompatible thermoplastic material, owning the largest market share among all biodegradable polymeric materials. Thus, understanding of microscopic structure and dynamics are definitively important subjects in further application. The helical jump motion in semi-crystalline polymers was proposed by Hoffmann et al to explain the αc relaxation in the crystalline region. So far, solid-state NMR proved that several semi-crystalline polymers such as polyethylene, isotactic-polypropylene, etc, show large amplitude motions in the crystalline regions. Additionally, successive helical jump motions may lead to long-range chain diffusions. Actually, chain diffusions are determined in terms of combinations of the overall jump rates and coupling degree of the jumps. Thereby, elucidations of correlations of the individual helical jump motions are also scientifically and practically important in further understanding dynamic nature of the crystalline chains and the structural evolutions of polymer crystals. Here, we utilize enter-bands only detection of exchange (CODEX) and 2D exchange NMR to characterize molecular dynamics of the crystalline chains in PLLA α phase. Dynamic geometry, correlation time, and short-range correlation of individual chain dynamics of PLLA in the crystalline region are for the first time reported.

1 This work was financially supported by the National Science Foundation (Grant no. DMR-1105829) and by UA startup funds.

9:48AM L42.00008 Rayleigh-Taylor Instability Analysis at Biobased Composite Interfaces1  
RICHARD WOOL, XINTIAN SU, Univ of Delaware — The Rayleigh-Taylor (RT) instability occurs when a light fluid (such as a gas) of density ρL forms an unstable interface with a heavy fluid of density ρH due to gravitational forces g in the heavy-over-light unstable configuration. The RT instability produces bubbles and spikes which grow with amplitude H ~ [gkM]1/2 in the linear region (Hk<<1) which evolves in a complex manner in the non-linear region (Hk>>1). Here, the wavenumber k = 2π/λ, λ = wavelength between instabilities, t = time, and the Atwood number A = (ρL−ρH)/(ρL+ρH). The RT instability is common in Inertial Confinement in Fusion reactions, Super Novas and for the first time reported here, in the interface of natural fibers with a liquid molding resin (soyoil) where the gas emitted from the natural fibers at T > 100°C explicitly forms and traps the bubbles and spike instabilities in the curing resin. The non-equilibrium spikes that form with A = 0.999 (Hk=1) are self-similar and behave as H = H0 + βtλ, where the initial instability height H0 = 11.6 micron and β = 1.0 (50 µm/s) for soy-based resins (ρL = 1.1 g/cm3). The RT spikes are typical of natural fibers less than 50 µm in diameter. The RT instability is a well-known phenomenon in other fields: the eco-leather is substantially lower viscosity compared to natural leather, polyurethane and PVC (Funded by EPA).

1Supported by EPA and ELC.

10:00AM L42.00009 Thermodynamic Interactions and Shear Alignment of Sustainable Tri-block Copolymers  
SHU WANG, MEGAN ROBERTSON1  
University of Houston, SAMEER VAJJALA KESAVA, ENRIQUE GOMEZ, Pennsylvania State University — Fatty acid-derived acrylates, lauryl acrylate (LAc) and stearyl acrylate (SAc), were utilized in the preparation of polystyrene-b-(LAc-co-SAc)-b-styrene) triblock copolymers. The thermodynamic interactions between polystyrene and the polycrylates were probed through rheology (determination of the order-disorder transition), cloud point measurements, and small angle neutron scattering. The Flory-Huggins interaction parameter was independent of the alkyl side-chain length when the side-chain contained greater than 10 carbon atoms. The thermal and mechanical properties of the triblock copolymers, which behave as thermoplastic elastomers, could be readily tuned by varying the acrylate composition, without changing the order-disorder transition temperature. Structural analysis revealed non-equilibrium spherical morphologies of the triblock copolymers, which transformed to highly-ordered cylindrical microstructures under large amplitude oscillatory shear at a temperature well below the order-disorder transition.

1 Corresponding Author
10:12 AM L42.00010 Structure and phase behavior of aqueous methylcellulose solutions, JOHN MCALLISTER, PETER SCHMIDT, TIMOTHY LODGE, FRANK BATES, University of Minnesota — Cellulose ethers (CE) constitute a multi-billion dollar industry, and have found end uses in a broad array of applications from construction materials, food products, personal care products, and pharmaceuticals for more than 80 years. Methylcellulose (MC, with the trade name METHOCEL TM) is a CE in which there is a partial substitution of –OH groups with –O–CH3 groups. This results in a polymer that is water-soluble at low temperatures, and aqueous solutions of MC display gelation and phase separation at higher temperatures. The nature of MC gelation has been debated for many years, and this project has made significant advances in the understanding of the solution properties of CEs. We have characterized a fibrillar structure of MC gels by cryogenic transmission electron microscopy (cryo-TEM) and small angle neutron scattering (SANS). Using light scattering, turbidity measurements, and dynamic mechanical spectroscopy (DMS) we report that MC microphase separates by nucleation and growth of fibril aggregates, and is a different process from LCST phase separation.

10:24 AM L42.00011 Water in Renewable Polymers: Nonequilibrium Thermodynamics1, YOSSEF ELABD, Texas A&M University — The design of polymers derived from sustainable resources (renewable plastics) as replacements to nonrenewable plastics for various applications will require an accurate assessment and fundamental understanding of the dynamics water sorption in glassy polymers. In this work, water sorption and diffusion in a number of glassy polymers (including the renewable polymer poly(lactide)) were measured using gravimetric and spectroscopic techniques. Non-Fickian diffusion was observed in all polymers studied, which was indicated by rapid, initial water uptake (driven by a concentration gradient), followed by continuous, gradual uptake of water at later experimental times (driven by slow polymer relaxation). Additionally, water sorption in these glassy polymers was predicted using two nonequilibrium thermodynamic models, where excellent agreement between the model prediction and experimental data was achieved for both models. Furthermore, contrasting physical pictures of water clustering were obtained between the Zimm-Lundberg theory and direct measurements.

1 National Science Foundation

Wednesday, March 4, 2015 8:00AM - 11:00AM — Session L43 DPOLY GSOFT GSNP: Focus Session: Stable Glasses, Fluids Under Confinement and at Interfaces 214C - Zahra Fakhraui, University of Pennsylvania

8:00AM L43.00001 Observation of Charge Inversion and Divalent Ion Transport in Nanochannels1, XIN LI, Department of Physics, Yale University, WEIHUA GUAN, Department of Electrical Engineering, Penn State University, BEN WEINER, Department of Physics, Yale University, MARK REED, Department of Electrical Engineering, Department of Applied Physics, Yale University — Ion transport in nanochannels has attracted increasing attention in recent years, with potential applications ranging from ionic control and biosensing to energy storage and conversion. Exciting phenomena occur from the nanoscale confinement of fluids and new models are expected. While most of the previous work in the field has focused on simple monovalent electrolytes, we report a systematic study of divalent ion transport in a well-defined nanochannel fabricated via standard semiconductor methods. Inversion of net surface charge at the fluid/solid interface has been observed by a novel method of open potential work in the field. Moreover, the relation of this charge inversion phenomena with the strong correlated liquid (SCL) theory has been deeply discussed. Intriguing observations from conductance measurement reveal ion-surface interactions and ion-ion correlations.

8:12AM L43.00002 Electrostatic effects of dielectric interfaces on confined electrolyte1, YUFEI JING, Applied Physics Program, Northwestern University, Evanston, IL 60208, VIKRAM JADHAO, Department of Physics & Astronomy, Johns Hopkins University, Baltimore, MD 21218, JOS W. ZWANIKKEN, MONICA OLVERA DE LA CRUZ, Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208 — The behavior of ions in liquids confined between interfaces characterized by different dielectric permittivities is crucial to many nanoscale assembly processes in synthetic and biological materials. The presence of multiple interfaces and associated dielectric heterogeneities often complicates the desired ionic distributions via simulations or theory. Electrostatic correlation effects in a system with electrolyte confined by two planar dielectric interfaces are systematically studied by Car-Parrinello molecular dynamics simulations and liquid state theory. Results for ionic density profiles for various electrolyte concentrations, stoichiometric ratios and dielectric contrasts are presented. We also investigate the interactions between two planar surfaces and effects of the dielectric interfaces on the double layer structure near the interfaces which lies at the heart of soft matter physics.

8:24AM L43.00003 Squeezeout of a model ionic liquid under confinement and charging1, ERIO TOSATTI, SISSA and ICTP, Trieste, Italy, ROSARIO CAPOZZA, SISSA, Trieste, Italy, ANDREA BENASSI, Empa, Duibendorf, Switzerland, ANDREA VANOSSI, CNR-IOM Democritos and SISSA, Trieste, Italy — Electrical charging of parallel plates confining a model ionic liquid down to nanoscale distances yields a variety of charge-induced changes in the structural features of the confined film, including even-odd switching of the structural layering, and important changes of planar ordering within layers. By means of molecular dynamics simulations, we explore this variety of phenomena in the simplest charged Lennard-Jones coarse-grained model including the effect a neutral tail attached to one of the model ions. Using open, grand-canonical-like conditions which allow the flow of ions in and out of the interplate gap, we simulate the liquid squeezeout and obtain the distance dependent forces between the plates during their adiabatic approach under load. Effective free energy curves obtained by integration of these forces versus interplate distance show the local minima that correspond to layering, and predict the switching between one and another under squeezing and charging.

1Partly sponsored under SNSF Sinergia grant CRSII2 136287/1, EU ERC grant No. 320796 MODPHYSFRICT, EU COST Action MP1303.

8:36AM L43.00004 Electrical charging effects on sliding lubrication properties of a model confined ionic liquid, ROSARIO CAPOZZA, International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy, ANDREA BENASSI, Empa, Materials Science and Technology, Überlandstrasse 129, 8600 Dübendorf, Switzerland, ANDREA VANOSSI, CNR-IOM Democritos National Simulation Center. Via Bonomea 265, 34136 Trieste, Italy, ERIO TOSATTI, International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy — Ionic liquids lubricants, used under conditions of nanometric confinement between parallel plates or tip-surface gaps, explore the dependence of friction upon charging, suggestive of some electrical control of friction. Using a simple ionic liquid model, we first study by molecular dynamics the friction between parallel plates under conditions of successive layering reached by squeezeout under an increasing inter-plate force. We then simulate the frictional changes brought about by different charging states of the plates, related to charging-induced switches corresponding to squeezeout (or suck-in) transitions between different layering states as predicted by local minima in the charge-dependent enthalpy curves. Although the actual frictional behavior obtained does depend upon the assumed features and parameters of the model liquid and its interaction with the plates, the broader scenario obtained for charging effects, its relationship to the equilibrium layering and its enthalpy characterization appear of general value.
8:48AM L43.00005 Crossover in the local diffusive dynamics of equilibrium and supercooled confined fluids, JONATHAN BOLLINGER, THOMAS TRUSKETT, University of Texas at Austin — Confined fluids are ubiquitous in natural and technological contexts, and relating emergent structural motifs to dynamics is critical to facilitate the inverse design of nano- and micro-fluidic systems. Crucially, such thin film systems are frequently tuned between equilibrium and glassy states, as during, e.g., processing of polymer thin films. We use molecular dynamics simulations and a Fokker-Planck equation based method to examine the position-dependent diffusive dynamics of binary hard-sphere fluids confined to slit pores that are designed to mimic realizable thin films [Nugent et al. PRL 2007, 99]. At moderate densities, local single-particle mobilities normal to the direction of confinement are higher in regions of high local packing fraction. However, as the average packing fraction is increased into the supercooled regime, this local positive correlation between packing fraction and mobility is reversed. We discuss the outlook for a universal mechanistic framework that can unite these disparate local correlations between packing and mobility and also predict average diffusivities of the inhomogeneous fluids. Auxiliary measurements of the simulated films suggest that this behavioral dichotomy should also emerge in structurally similar experimental colloidal suspensions.

9:00AM L43.00006 Geometrical frustration and correlated capillary instabilities among concentric polymer toroids, ZHENG ZHANG, Univ of Colorado - Boulder, GENE HILTON, National Institute of Standards and Technology, YIFU DING, Univ of Colorado - Boulder — We present the first study on the simultaneous capillary instability among concentric viscous toroids. An array of concentric polystyrene (PS) toroids were lithographically fabricated with a constant radial spacing between neighboring toroids. The toroids were confined in a poly (methyl methacrylate) (PMMA) matrix. PS and PMMA were used because of their immiscibility and well-characterized physical properties. The glass transition temperature ($T_g$) of the pattern are well above room temperature. We found that the radial contraction mode of toroids (Pairam & Fernández-Nieves, PRL 2009) was depended due to substrate confinement. Upon further annealing, the toroids ruptured along the circumferential direction at a finite wavelength. Depending on the relative value of PS, the rupture behavior of each toroid (with different aspect-ratios) can be non-correlated or correlated radially. In the correlated case, geometric frustration due to the toroidal curvature was observed, which led to an intriguing branching behavior in the correlated instability and closely resembles a Cayley tree with fractal coordination number of 3.

9:12AM L43.00007 Ultrastable Glasses and the Random First Order Transition Theory of Glasses, PETER WOLYNES, Rice University — I will discuss the implications of the RFOF theory for the dynamics of ultrastable glasses focusing on the achievable limits to stability and the heterogeneous and homogenous mechanisms of their rejuvenation.

9:48AM L43.00008 Probing the Dynamics of Thin TPD Glass Films via Dewetting$^1$, YUE ZHANG, ETHAN GLOR, TIANYI LIU, CHEN LI, ZAHRA FAKHRAEI, Department of Chemistry, University of Pennsylvania — Enhanced mobility of surface layer has been observed in both polymer glasses and small molecule organic glasses. In polymers, the mobile surface layer is believed to have great effects on the properties of thin films. Similar studies in small molecule glasses are significantly more challenging due to dewetting. Understanding the dynamics of this mobile layer, and its effect on thin film dynamics can be important in understanding heterogeneous dynamics in glassy systems. In this work, we investigate the properties of the mobile layer and its effect on the overall properties of thin glass films of small molecule organic glasses. We show that thin (thickness below 30nm) TPD (N,N’-Bis(3-methylphenyl)-N,N’-diphenylbenzidine) films prepared by physical vapor deposition (PVD), can be unstable and dewet in a hole growth manner due to enhanced mobility at temperatures as low as Tg-35K. By following the kinetics of dewetting, we investigate the mobility changes with temperature and film thickness. These studies can elucidate the relation between the enhanced mobility and the stability of thick films of the same materials prepared at similar deposition temperatures and thus the formation mechanisms and unique properties of physical vapor deposited glasses.

$^1$Department of Chemistry, University of Pennsylvania; National Science Foundation

10:00AM L43.00009 Dewetting of a Liquid-Liquid System, STEFAN BOMMER, NIKOLAS BECKER, Experimental Physics, Saarland University, 66041 Saarbruecken, Germany, SEBASTIAN JACHALSKI, DIRK PESCHKA, Weierstrass Institute for Applied Analysis and Stochastics, 10117 Berlin, Germany, BARBARA WAGNER, Institute for Mathematics, Technical University Berlin, 10623 Berlin, Germany, RALF SEEMANN, Experimental Physics, Saarland University, 66041 Saarbruecken, Germany — In recent years a thorough understanding of thin film dewetting from solid substrates was developed. However, the understanding of a thin liquid film dewetting from another liquid remained scarce. By in situ AFM studies we explore the dewetting dynamics and the morphologies of liquid polystyrene (PS) dewetting from liquid polymethyl-methacrylate (PMMA). Using a selective solvent allows to remove the dewetted PS layer and to image the liquid/liquid interface at selected times. Combining the PS/air and the PS/PMMA interfaces we obtain the full three dimensional shape of the dewetting morphologies. The characteristic shapes of the rim profiles, the equilibrating droplets and their dewetting dynamics depend not only on the ratios of viscosity and surface tension of the two liquids but also on the relative height of the underlying layer. The latter originates from the flow field of the dewetting liquid which penetrates surprisingly deep into the lower liquid it is dewetting from.

10:12AM L43.00010 Coupling the coffee-ring effect to phase separation in drying polymer-nanocrystal deposits. ERIK K. HOBIE, NDSU, JOSEPH B. MILLER, Rice University, AUSTIN C.P. USSELMAN, NDSU, REBECCA J. ANTHONY, UW E. KORTSHAGEN, UMN, ALEXANDER J. WAGNER, ALAN R. DENTON, NDSU — The coupling between the coffee-ring effect and liquid-liquid phase separation is examined for ternary mixtures of solvent, polymer and colloidal nanocrystal. Using real-space imaging and spectroscopic techniques, we resolve the kinetic morphology of the drying front for varied molecular weight of the polymer. Our results demonstrate that the size of the polymer chain has a significant impact on the nature of the coupling between the two instabilities, and we relate these observations to simulations, measured and predicted binodal curves, and the observed shape of the flow field in the confined region at the contact line. The results inform a blade coating process that we exploit to print homogeneous or periodically patterned microscopic wires of nanocomposite material.


$^1$NSF (DMR-1206724, DMREF-1234320)
8:00AM L44.00001 Extremes in systems with linear and nonlinear memory by the return-interval approach\textsuperscript{1} , ARMIN BUNDE, Institute of Theoretical Physics, Giessen University — The occurrence of extreme events above a certain threshold $Q$ in time series can be characterized by their return intervals $r$. Here we review recent work on the distribution $P_Q(r)$ of the return intervals and their correlation properties (i) in systems with linear long-term memory and (ii) in systems with non-linear memory. Examples for (i) are temperature records, examples for (ii) are financial records. The distribution of the return intervals is an important quantity in risk estimation since it enables one to calculate the probability that an extreme event occurs in the next period of time. We discuss the different functional forms of $P_Q(r)$ that range from simple exponential (random systems) to stretched exponentials (systems with long-term memory) and $q$-exponentials (systems with non-linear memory). We show that both linear and non-linear memory lead to return intervals in the return time series, which then results in a clustering of the extreme events. Both the distribution of the return intervals and their correlation properties can be used as a test bed for computer models.

\textsuperscript{1}This work has been supported by the Deutsche Forschungsgemeinschaft

8:36AM L44.00002 Rare Event Extinction on Stochastic Networks\textsuperscript{1} , IRA SCHWARTZ\textsuperscript{2}, Naval Research Lab, LEAH SHAW, College of William and Mary, BRANDON LINDLEY, R. D. Wagner Associates, Inc. — We consider the problem of extinction processes on random networks with a given structure. For sufficiently large well-mixed populations, the process of extinction of one or more state variable components occurs in the tail of the quasi-stationary probability distribution, thereby making it a rare event. Here we show how to extend the theory of large deviations to random networks to predict extinction times. In particular, we use the theory to find the most probable path leading to extinction. We apply the methodology to epidemic models and discover how mean extinction times scale with epidemiological and network parameters in Erdos-Renyi networks. The results are shown to compare quite well with Monte Carlo simulations of the network in predicting both the most probable paths to extinction and mean extinction times.

\textsuperscript{1}BL was a National Research Council post doctoral fellow. IBS was supported by NRL base funding and ONR. LBS was supported by the ARO, AFOSR, and NIH.

\textsuperscript{2}Nonlinear Systems Dynamics Section

8:48AM L44.00003 Revealing non-Gaussian noise through noise-induced switching in a parametric oscillator , PAVEL POLUNIN, Michigan State University, PANPAN ZHOU, Hong Kong University of Science and Technology, NICHOLAS MILLER, SiTime, STEVEN SHAW, Michigan State University, HO BUN CHAN, Hong Kong University of Science and Technology, MARK DYKMAN, Michigan State University — Rates of noise-induced switching between coexisting states of dynamical systems exponentially strongly depend on the noise characteristics. We use the related sensitivity to reveal the deviation of the noise from Gaussian. We study a parametrically driven nonlinear oscillator, which has two stable stationary states. One of the consequences is that, in the space of two or more observable quantities ($q_i$), the average “angular momentum” ($\langle L_{ij} \rangle \equiv \langle q_i q_j \rangle$) is typically non-trivial. In addition, the full distribution of $L$ often display remarkable properties. We will provide a general framework for the study of noise-induced switching and extinction in delayed systems modeling population dynamics. In the weak noise limit, the rates of inter-attractor switching and extinction are associated with the membrane potential while the second is associated with membrane ionic permeability. Noise-induced switching times correspond to the rate at which spontaneous action potentials occur. The fast-slow nature of this system allows us to derive analytical expressions for both the MPEPs and mean switching times as functions of the relative noise intensity. Derived expressions are found to be in good agreement with both computational minimization of the geometric action as well as direct simulation of the underlying stochastic differential equations. [1] P. H. Dannenberg, J. C. Neu, and S. W. Teitsworth, Phys. Rev. Lett. 113, 020601 (2014).

9:00AM L44.00004 Dependence of mean switching times on relative noise intensity in fast-slow dynamical systems , STEPHEN TEITSWORTH, PAUL DANNENBERG, JOHN NEU, Duke University — Recently, we used a geometric minimum action method to analytically and numerically study the dependence of most probable escape paths (MPEPs) on relative noise intensities in a generic two-dimensional fast-slow dynamical system [1]. In this talk, we apply and extend this approach to study MPEPs and associated mean switching times in a quadratic integrate-and-fire model of single neuron dynamics as a function of relative noise intensity in the two dynamical variables. Here, one variable is associated with the membrane potential while the second is associated with membrane ionic permeability. Noise-induced switching times correspond to the rate at which spontaneous action potentials occur. The fast-slow nature of this system allows us to derive analytical expressions for both the MPEPs and mean switching times as functions of the relative noise intensity. Derived expressions are found to be in good agreement with both computational minimization of the geometric action as well as direct simulation of the underlying stochastic differential equations. [1] P. H. Dannenberg, J. C. Neu, and S. W. Teitsworth, Phys. Rev. Lett. 113, 020601 (2014).

9:12AM L44.00005 Noise Induced Switching and Extinction in Systems with Delay\textsuperscript{1} , LORA BILLINGS, Montclair State University, IRA SCHWARTZ, US Naval Research Laboratory, TOM CARR, Southern Methodist University, MARK DYKMAN, Michigan State University — We consider the rates of noise-induced switching between multiple attractors of dynamical systems with delay, and the rates of noise-induced extinction in delayed systems modeling population dynamics. In the weak noise limit, the rates of inter-attractor switching and extinction are exponentially small. To logarithmic accuracy, the formulation of the rates is reduced to variational problems, which give the most probable paths followed by both switching or extinction dynamics. We show that the equations for the most probable paths are acausal and formulate the appropriate boundary conditions. Explicit general results of the rates are obtained for small delay compared to the relaxation rate, and verified using a direct variational method to find the rates. We find that the analytical results agree well with the numerical simulations for both switching and extinction rates.

\textsuperscript{1}Supported by ARO, DARPA, NSF, and ONR.

9:24AM L44.00006 Probability current loops in non-equilibrium steady states and statistical properties of angular momenta in configuration space\textsuperscript{1} , R.K.P. ZIA, Physics Dept, Virginia Tech, Blacksburg, VA, BAYLOR FOX-KEMPER, Department of Geological Sciences, Brown University, Providence, RI, DIBYENDU MANDAL, JEFFREY WEISS, Department of Atmospheric and Oceanic Sciences, University of Colorado, Boulder, CO — Unlike systems in thermal equilibrium, steady probability current loops persist in non-equilibrium stationary states. One of the consequences is that, in the space of two or more observable quantities ($q_i$), the average “angular momentum” ($\langle L_{ij} \rangle \equiv \langle q_i q_j \rangle$) is typically non-trivial. In addition, the full distribution of $L$ often display remarkable properties. We will provide a general framework for the study of $L$, as well as specific examples -- in the context of both exactly solvable models (based on linear Langevin equations with additive white noise) and physical data of global ocean heat content.

\textsuperscript{1}Supported in part by NSF grants DMS-1245944 and DMR-1244666
9:36AM L44.00007 Experimental Observation of Dynamic Phase Transitions in uniaxial Co-Films, ANDREAS BERGER, OLATZ IDIGORAS, CIC nanoGUNE, PAOLO VAVASSORI, CIC nanoGUNE and IKERBASQUE Foundation — We studied the time dependent magnetic reversal behavior of uniaxial films in the vicinity of the dynamic phase transition (DPT) as a function of the period \( P \) and bias \( H_b \) of an oscillating magnetic field. For our experiments, we have used Co-films with in-plane orientation of the uniaxial magneto-crystalline anisotropy axis to avoid complications due to long-range magneto-static interactions. Correspondingly, we have grown 30 nm thick Co-films that exhibit (10-10) surface orientation by means of suitable growth sequences and deposition conditions [1]. For the dynamic field response experiments, we utilized a home-built high-sensitivity magneto-optical Kerr effect set-up, which allowed for real-time low-noise hysteresis loop measurements with \( P \) as small as 0.580 ms. Our experiments reveal in addition to the DPT at a critical period \( P_c \), the occurrence of transient dynamic behavior for \( P < P_c \). [2]. Our data are consistently explained by a phase line at \( H_b = 0 \) for \( P < P_c \), which causes a first order phase transition in between two antiparallel dynamic order states, thus indicating far-reaching similarities of the DPT to equilibrium phase transitions [2]. However, we also observe anomalies, such as unusual fluctuation pattern in the \( P-H_b \) plane, which might be related to the recently suggested occurrence of dynamically “dead” surfaces [3]. References: [1] O. Idigoras et al., J. Appl. Phys. 115, 083912 (2014); [2] A. Berger et al., Phys. Rev. Lett. 111, 190602 (2013); [3] H. Park and M. Pleimling, Phys. Rev. Lett. 109, 175703 (2012).

9:48AM L44.00008 Effects of magnetic field quenches on the relaxation dynamics of vortex lines in disordered type-II superconductors\(^1\), HIBA ASSI, HARSHWARDHAN CHATURVEDI, MICHEL PLEIMLING, UWE C. TÄUBER, Department of Physics, Virginia Tech, ULRICH DOBRAMYSL, Mathematical Institute, University of Oxford — Understanding the relaxation dynamics of vortex matter in disordered type-II superconductors from experimentally realizable initial conditions may improve material characterization and optimization for technological applications. We model magnetic flux lines in the London limit as interacting directed elastic lines subject to uncorrelated point-like or extended columnar pinning centers. We employ a Langevin Molecular Dynamics algorithm to simulate the vortex dynamics. We analyze the vortex relaxation kinetics following sudden magnetic field changes by instantaneously adding or removing lines from the system at random. By studying two-time correlation functions such as the mean-square displacement and height autocorrelation function, as well as one-time observables such as the ratio of pinned line elements and radius of gyration, we disentangle the effects of the competing repulsive vortex interaction and pinning and we compare the distinct relaxation properties due to the type of disorder. We discovered some universal features regardless of the type of quench and the presence of vortex interactions, and others that are dependent on the type of disorder and the system’s initial conditions.

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\(^1\)Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-09ER46613.

10:00AM L44.00009 Pinning time statistics for vortex lines in disordered environments\(^1\), UWE C. TÄUBER, Department of Physics, Virginia Tech, ULRICH DOBRAMYSL, University of Oxford, MICHEL PLEIMLING, Department of Physics, Virginia Tech — We study the pinning dynamics of magnetic flux (vortex) lines in a disordered type-II superconductor. Using numerical simulations of a directed elastic line model, we extract the pinning time distributions of vortex line segments. We compare different model implementations for the disorder in the surrounding medium: discrete, localized pinning potential wells that are either attractive and repulsive or purely attractive, and whose strengths are drawn from a Gaussian distribution; as well as continuous Gaussian random potential landscapes. We find that both schemes yield power law distributions in the pinned phase as predicted by event-extreme statistics, yet they differ significantly in their effective scaling exponents and their short-time behavior.

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\(^1\)This research is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-09ER46613.

10:12AM L44.00010 Dead magnetic surface layers near dynamic phase transitions, PATRICIA RIEGO, ANDREAS BERGER, CIC nanoGUNE Consolider — We have performed a detailed study of the dynamic phase transition (DPT) for a magnetic layer system with surfaces subjected to an oscillatory external magnetic field in mean field approximation (MFA). Specifically, we focused our study on bulk-terminated surfaces, i.e., we deal with multilayer systems that have the same exchange coupling strength between nearest neighbors everywhere, including at the surface. We are able to reproduce within the MFA the absence of a surface phase transition at the bulk critical point that was previously reported by Tauscher et al. utilizing Monte-Carlo simulations [1]. In addition, we observe that the DPT is also absent or at least severely suppressed for several layers below the surface, which exhibit susceptibility peaks that are four orders of magnitude smaller than the one corresponding to the bulk. Most importantly, we identify the reason for this “dead” surface behavior. The oscillatory magnetization \( M(t) \) response to the external magnetic field is not synchronous in between the surface and the bulk near the DPT. This lack of correlation prevents the layers from sufficiently supporting each other’s dynamic ordering, so that the surface and the layers close to it cannot follow the bulk DPT.


10:24AM L44.00011 Spherical surface growth models, XAVIER DURANG, Korean Institute for Advanced Study, MALTE HENKEL, Universite de Lorraine, France — We study several surface growth models obtained by treating and replacing the non-linear term in the noisy Burgers equation or the KPZ equation by a mean spherical condition. We want to explore the consequences of such constraints on the Edwards-Wilkinson (EW) equation and the KPZ equation by a mean spherical condition. We study the pinning dynamics of magnetic flux (vortex) lines in a disordered type-II superconductor. Using numerical simulations of a directed elastic line model, we extract the pinning time distributions of vortex line segments. In those exactly solvable models, one has to solve the spherical conditions and then we can derive the two-time quantities (the correlation function and the response function). Therefore, we have access to the non-equilibrium exponents and compare them to those of the EW model or the KPZ model.

10:36AM L44.00012 Failure of Steady State Thermodynamics\(^1\), RONALD DICKMAN, Universidade Federal de Minas Gerais — To be useful, steady state thermodynamics (SST) must be self-consistent and have predictive value. Consistency of SST was recently verified for driven lattice gases under global weak exchange. Here, I verify consistency of SST under local (pointwise) exchange, but only in the limit of a vanishing exchange rate; for a finite exchange rate the coexisting systems have different chemical potentials. I consider the lattice gas with nearest-neighbor exclusion on the square lattice, with nearest-neighbor hopping (NNE dynamics), and with hopping to both nearest and next-nearest neighbors (NNE2 dynamics). I show that SST does not predict the coexisting densities under a nonuniform drive, or in the presence of a nonuniform density provoked by a hard wall or nonuniform transition rates. The steady state chemical potential profile is, moreover, nonuniform at coexistence, contrary to the basic principles of thermodynamics. Finally, I discuss examples of a pair of systems possessing identical steady states, but which do not coexist when placed in contact. These results cast serious doubt on the consistency and predictive value of SST.

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\(^1\)Supported by CNPq, Brazil
Self-organization in non-equilibrium systems

Jodie Lutkenhaus, Texas A&M University

The question about why complex systems self-organize to reach more efficient and robust states is still without a satisfactory answer. We approach it from a physics perspective, where energy gradients lead to change in the structure of systems to ensure the most efficient energy transport. This approach stems from fundamental variational principles in physics, such as the principle of least action, which determine the motion of particles. We compare energy transport through a cell which has random motion of its molecules, and a cell which can form convection cells. We examine the sign of change of entropy, and the action needed for the motion inside those systems. The system in which convective motion occurs, reduces the time for energy transmission, compared to random motion. For more complex systems, this convection cells become a network of transport channels, for the purpose of obeying the equations of motion in this geometry. Those transport networks are an essential feature of complex systems in biology, ecology, economy and society in general. This approach can help explain some of the features of those transport networks, and how they correlate with the level of complexity of systems.

Wednesday, March 4, 2015 8:00AM - 11:00AM –
Session L45 DPOLY: Focus Session: Polymers in Batteries and Electrochemical Capacitors II
216AB - Jodie Lutkenhaus, Texas A&M University

Ion transport and softening in a polymerized ionic liquid

RAJEEV KUMAR, Center for Nanophase Materials Science & Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN, VERA BOCHAROVA, Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, EVGHENI STRELCOV, Center for Nanophase Materials Science, Oak Ridge National Laboratory, Oak Ridge, TN, VERONIKA STREHMEL, Hochschule Niederrhein University of Applied Sciences, Krefeld, Germany, JOSHUA SANGORO, Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, TN, ALEXEI SOKOLOV, Department of Chemistry, University of Tennessee, Knoxville, TN, SERGEI KALinin, BOBBY SUMPTER, Center for Nanophase Materials Science, Oak Ridge National Laboratory, Oak Ridge, TN — Polymerized ionic liquids (PolyILs) are promising materials for various solid-state electronic applications such as dye-sensitized solar cells, lithium batteries, actuators, and field-effect transistors. However, fundamental understanding of interconnection between ionic transport and mechanical properties in PolyILs is far from complete. In this work, local charge transport and structural changes in films of a PolyIL are studied using an integrated experiment-theory based approach. Kinetics of charging, steady state current-voltage relations and softening of the PolyIL films beyond certain threshold voltages are studied by applying electric field through a scanning probe microscopy (SPM) tip. All of the experimental data can be explained by a modified Poisson-Nernst-Planck formalism for the charge transport, which takes into account the dissociation of ions under applied electric field (the Wien effect).

Formation of ion clusters in the phase separated structures of neutral-charged polymer blends

HA-KYUNG KWON, MONICA OLVERA DE LA CRUZ, Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, United States — Polyelectrolyte blends, consisting of at least one charged species, are promising candidate materials for fuel cell membranes, for their mechanical stability and high selectivity for proton conduction. The phase behavior of the blends is important to understand, as this can significantly affect the performance of the device. The phase behavior is controlled by χ, the Flory-Huggins parameter multiplied by the number of mers, as well as the electrostatic interactions between the charged backbone and the counterions. It has recently been shown that local ionic correlations, incorporated via liquid state (LS) theory, enhance phase separation of the blend, even in the absence of polymer interactions. In this study, we show phase diagrams of neutral-charged polymer blends including ionic correlations via LS theory. In addition to enhanced phase separation at low χ, the blends show liquid-liquid phase separation at high electrostatic interaction strengths. Above the critical strength, the charged polymer phase separates into ion-rich and ion-poor regions, resulting in the formation of ion clusters within the charged polymer phase. This can be shown by the appearance of multiple spinodal and critical points, indicating the coexistence of several charge separated phases.

Diffusional Response of Assembled Polyelectrolyte Chains to Salt Annealing

VICTOR SELIN, Department of Chemistry, Chemical Biology and Biomedical Engineering, Stevens Institute of Technology, Hoboken, New Jersey 07030, JOHN F. ANKNER, Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, Svetlana Sukhishvili, Department of Chemistry, Chemical Biology and Biomedical Engineering, Stevens Institute of Technology, Hoboken, New Jersey 07030 — We report on the effect of salt on the diffusion of polyelectrolyte (PE) chains within electrostatically assembled polyelectrolyte multilayers. Layer-by-layer (LbL) films were assembled using poly(methacrylic acid) (PMAA) as a polyanion and quaternized poly-2-(dimethylamino)ethyl methacrylate as a polycation. Fluorescence recovery after photobleaching and neutron reflectometry were used to monitor the center-of-mass diffusion of PMAA chains in directions parallel and perpendicular to the substrate (D// and D⊥, respectively). In both directions, the diffusion coefficient was exponentially dependent on salt concentration, with significantly faster diffusion in the direction parallel to the substrate. At the same time, D// dramatically decreased with salt annealing time as the films became increasingly intermixed, reflecting strong coupling between internal layering and PE chain dynamics within LbL films.

Characterization of diblock copolymer lamellar structure from neutron scattering measurements and molecular dynamics simulations

CHEOL JEOng, JENNY KIM, SANGCHEOL KIM, NIST - Natl Inst of Stds & Tech, TSUNG-HAN TSAI, E. BRIAN COUGHLIN, University of Massachusetts Amherst, CHRISTOPHER SOLES, NIST - Natl Inst of Stds & Tech — The Nanoscale structure of block copolymers (BCP) with lamellar morphology plays an important role in transport properties for fuel cell and battery application. We develop a paracrystalline model to interpret small angle neutron scattering (SANS) and X-ray scattering (SAXS) data of hydrated amphiphilic BCP lamellar phase in order to elucidate water distribution as well as hydrophilic and hydrophobic domain spacing. We assume Gamma distribution for the fluctuation of lamellar thickness instead of Gaussian. It is observed that BCP can deswell upon hydration along lamellar normal direction due to chain collapse of hydrophobic domain overcoming expansion of hydrophilic domain, which has been compared with coarse-grained molecular dynamics simulation (CGMD). CGMD results show that the variation of interfacial area per chain is strongly correlated to the conformation of hydrophobic chains, domain spacing and water distribution in the hydrophilic domain, compatible with the observation from SANS and SAXS.
compare the conductivity of SbMMA/IL with the homopolymer/IL mixture, and to discuss the ion transport mechanism.

lamellar morphology with long-range order. Slower rates of solvent evaporation produce films with lamellae preferentially oriented to be in the plane. In-plane

impedance spectroscopy over a range of compositions. Two glass transition temperatures ($T_g$ and long-range order of ion-containing microdomains were prepared to probe the impact of grain boundaries and microdomain orientation on ion transport. We

ions. Typical SPEs have an $f$-value less than 0.2, while the ionomers of study exhibit $f$-values near unity or higher. Understanding what properties

with polymer dynamics. The improvement in conductivity through the use of ion aggregates can be quantified by calculating the inverse of the Haven Ratio,

polymer electrolytes. This is achieved by binding the anion to the polymer backbone, significantly reducing the anions mobility. Ion aggregation is prevalent in

with polymer morphology and the development of hydrophilic channels throughout the material. Reaction induced phase separation has been shown to create such morphologies when used with uncharged copolymers and crosslinking

membranes. Herein we demonstrate a novel approach of fabricating block copolymer electrolyte membranes, by inducing pores in the proton-conducting phase. We examine morphology of these membranes with contrast-matched resonant soft X-ray scattering (RSAXS) and high-angle annular dark field scanning transmission electron microscopy (HAADF STEM). These materials show excellent charge transport behavior and water vapor transport properties, surpassing commercially available materials. These results and efforts to improve other important physical characteristics for membrane applications will be presented.

Morphology and Proton Transport in Porous Block Copolymer Electrolyte Membranes, CHELSEA CHEN, University of California, Berkeley. JEFFREY KORTRIGHT, Lawrence Berkeley National Lab, DAVID WONG, Exponent, NITASH BALSAURA, University of California, Berkeley — Block copolymer electrolyte membranes consisting of a proton-conducting block and an uncharged structural block are attractive due to their potential in clean energy applications. Herein we demonstrate a novel approach of fabricating block copolymer electrolyte membranes, by inducing pores in the proton-conducting phase. We examine morphology of these membranes with contrast-matched resonant soft X-ray scattering (RSAXS) and electron tomography. Proton conductivity as a function of porosity and water activity is also investigated. By tuning the porosity of the membranes, we are able to adjust the water uptake of the membranes for improved proton conductivities, in both humid air and liquid water.

Morphology-structure-property relationships in polymerized ionomeric liquids, JOSHUA SANGORO, MAXIMILIAN HERES, JOSEPH MINUTOLO, JACOB SHAMBULN, MAIR LANG, Univ of Tennessee, KNOXVILLE, STEFAN BORDZINSKI, VERONIKA STREHMEHL, Hochschule Niederrhein University of Applied Sciences, STEPHEN PADDISON, Univ of Tennessee, Knoxville — Charge transport and structural dynamics in systematic series of polymerized ammonium- and imidazolium-based ionic liquids are investigated by broadband dielectric spectroscopy, temperature-modulated differential scanning calorimetry, and X-ray as well neutron scattering techniques. Detailed analysis reveal strong decoupling of these processes in the polymerized ionic liquids, implying failure of the classical theories in describing charge transport and molecular dynamics in these systems. In addition, a strong correlation is observed between the ionic conductivity at the respective calorimetric glass transition temperatures and the morphologies revealed by the scattering experiments. In this talk, a physical explanation of the origin of the observed decoupling of ionic conductivity from structural dynamics will be proposed.

Controlling ion aggregation and conduction in PEO-based ionomers, DAVID CALDWELL II, JANNA MARANAS, Pennsylvania State Univ — PEO-based ionomers are ideal for reducing concentration polarization found in typical solid polymer electrolytes. This is achieved by binding the anion to the polymer backbone, significantly reducing the anions mobility. Ion aggregation is prevalent in these systems, but their influence on SPE performance is difficult to study experimentally. We present results of molecular dynamics simulations that explore the relationship between ion content and temperature on ion aggregation, polymer motion, and ion conduction. An unforeseen result of ionomers is the creation of string-like aggregates that form conduction pathways in the amorphous region. These conduction pathways allow for a partial decoupling of ion conduction with polymer dynamics. The improvement in conductivity through the use of ion aggregates can be quantified by calculating the inverse of the Haven Ratio, dubbed $f$-value. Typical SPEs have an $f$-value less than 0.2, while the ionomers of study exhibit $f$-values near unity or higher. Understanding what properties influence the development and use of these conduction pathways will provide insight for further development of solid polymer electrolytes.

Dynamics of Polymerized Ionic Liquids and their Monomers, RALPH H. COLBY, Materials Science and Engineering, Penn State University — Dielectric spectroscopy determines the static dielectric constants ($\varepsilon_s$) of polymers with imidazolium pendant structures containing a combination of alkyene and ethyleneoxy units as spacers between the backbone and the imidazolium cation. All monomers and their polymers exhibited two dipolar relaxations, assigned to the usual segmental motion ($\alpha_s$) associated with the glass transition and a lower frequency stronger relaxation ($\alpha_g$), attributed to ions rearranging. While pairs in conventional (smaller) ionic liquids prefer antiparallel alignment [Kirkwood $g \approx 0.1$ with $\varepsilon_s \approx 15$], because their polarizability volumes strongly overlap, ion pair dipoles in the larger ionic liquid monomers display $g$ of order unity and $50 \leq \varepsilon_s \leq 110$. Longer spacings lead to higher static dielectric constant, owing to a significant increase of the relaxation strength of the $\alpha_g$ process, which is directly reflected through an unanticipated increase of the static dielectric constant with ionic liquid molecular volume. The ionomers consistently exhibit 1.5 - 2.3 times higher static dielectric constants than the monomers from which they were synthesized, suggesting that polymerization encourages the observed synergistic dipole alignment ($g > 1$). Comparison of dielectric and linear viscoelastic responses reveals a strong connection between the time scales of polymer segmental motion ($\alpha_s$), ion rearrangements ($\alpha_g$) and the viscoelastic softening associated with the glass transition. For all polymers with imidazolium side chains and a wide variety of counter-ions, a single strong low molecular volume. Large side chains have low $T_g \approx -50$ °C and their ionic conductivity increases as ethylene oxide repeats are incorporated into the side chains.

Morphology and Ionic Conductivity of Oriented Block Copolymer/Ionic Liquid Mixtures, SHARON SHARICK, KAREN I. WINEY, University of Pennsylvania — Ion-containing block copolymers with increased continuity and long-range order of ion-containing microdomains were prepared to probe the impact of grain boundaries and microdomain orientation on ion transport. We studied poly(styrene-b-methyl methacrylate) diblock copolymers swollen with 1-ethyl-3-methyl-imidazolium bis(trifluoromethylsulfonylimide) (SBMMA/IL), and characterized the thermal transitions, morphologies, and ionic conductivities by differential scanning calorimetry, small-angle X-ray scattering, and electrochemical impedance spectroscopy over a range of compositions. Two glass transition temperatures ($T_g$) are observed, corresponding to PS and PMMA/IL microdomains, and $T_{DP-PMMMA/IL}$ is modeled well by the Gordon-Taylor expression. SBMMA/IL films prepared by solvent evaporation exhibit strongly microphase-separated lamellar morphology with long-range order. Slower rates of solvent evaporation produce films with lamellae preferentially oriented to be in the plane. In-plane conductivities increased with both increasing ionic liquid content and with better parallel alignment of lamellae. The Sax and Ottino model will be used to compare the conductivity of SBMMA/IL with the homopolymer/IL mixture, PMMA/IL, and to discuss the ion transport mechanism.
10:36 AM L45.00012 Effect of Lithium Ion Concentration of a Single-Ion-Conducting Block Copolymer Electrolyte on the Morphology-Conductivity Relationship. ADRIANA A. ROJAS, University of California, Berkeley, SEBNEM İNCEOGLU, Lawrence Berkeley National Laboratory, GREG STONE, Malvern Instruments, NITASH BALSARA, University of California, Berkeley — Single-ion-conducting block copolymer electrolytes are desirable for lithium metal batteries because they enable the sole conduction of lithium ions, the reacting species in lithium batteries; hence, they avert detrimental battery limitations due to salt concentration gradients. A single-ion-conducting block copolymer electrolyte, poly(ethylene oxide)-b-poly(styrenesulfonfyl lithium) (trifluoromethyl sulfonyl) imide (PEO-b-PSSLiTFSI), was characterized in-situ and ex-situ for its ionic conductivity and morphology using AC impedance spectroscopy and small angle x-ray scattering, respectively. This work is the first to elucidate the relationship between the two properties in a single-ion block copolymer electrolyte. The transference number for the copolymers was determined to be greater than or equal to 0.87, indicating that to a good approximation, the block copolymers are single-ion conducting electrolytes. It was found that increasing the molecular weight of the PSSLiTFSI block led to an increase in the extent of block copolymer block-mixing and a change in the conductivity profile from discontinuous to continuous. These effects can be attributed to the disruption of PEO crystallization, which was shown to drive microphase separation.

1 Joint Center for Energy Storage Research, Lawrence Berkeley National Laboratory

10:48 AM L45.00013 Role of Constituent Hard Polymer in Enhancing Lithium Transfer Number of Lithium Salt-Polymer Complexes. GYUHA JO, MOON JEONG PARK, Pohang Univ of Sci & Tech — Lithium polymer batteries have been projected as promising energy storage systems, owing to their unique advantages such as long cycle life, high specific capacity, and high cell potential. While the polymer electrolytes such as poly(ethylene oxide) (PEO) employed in lithium polymer batteries have high ionic conductivity and low volatility, the PEO-lithium salt complexes indicated immense shortcomings of concentration polarization, ascribed to the motion of free anions within PEO. This has limited charge/discharge rate of lithium batteries. In this study, we present a new methodology for improving the ionic conductivity and lithium transference number of PEO, by block copolymerization with a hard polymer, namely poly(dithiooxamide) (PDTOA). Compared to a simple PEO/PDTOA blend, lithium-salt doped PEO-b-PDTOA block copolymers exhibited significantly improved ionic conductivity values. Further, lithium transference numbers as high as 0.66 were observed, which are much higher than the corresponding values for conventional PEO-salt electrolytes (∼0.25).

Wednesday, March 4, 2015 8:00 AM - 11:00 AM — Session L46 DBIO DCMP: Invited Session: Design Principles in Synthetic Biology

217A - Ned Wingreen, Princeton University

8:00 AM L46.00001 Enzyme clustering can induce metabolic channeling. MICHELE CASTELLANA, Lewis-Sigler Institute for Integrative Genomics, Princeton University, Princeton, NJ, United States — Direct channeling of intermediates via a physical tunnel between enzyme active sites is an established mechanism to improve metabolic efficiency. In this talk, I will present a theoretical model that demonstrates, that co-clustering enzyme active sites can yield the full efficiency benefits of direct channeling if the enzyme active sites are close enough in proximity. The model predicts the separation of the size of clusters that maximize metabolic efficiency, and this prediction is in agreement with the spacing between co-clusters in yeast and mammalian cells. The model also predicts that enzyme agglomerates can regulate steady-state flux division at metabolic branch points: we experimentally test this prediction for a fundamental branch point in Escherichia coli, and the results confirm that enzyme colocalization within an agglomerate can accelerate the processing of a shared intermediate by one branch. Our studies establish a quantitative framework to understand co-clustering-mediated metabolic channeling and its application to both efficiency improvement and metabolic regulation.

8:36 AM L46.00002 Programming Biology for Health and Sustainability. PAMELA SILVER, Harvard Medical School — Biology presents us with an array of design principles. From studies of both simple and more complex systems, we understand some of the fundamentals of how Nature works. We are interested in using the foundations of biology to engineer cells in a logical and predictable way to perform certain functions. By necessity, the predictable engineering of biology requires knowledge of quantitative behavior of individual cells and communities. By building and analyzing synthetic systems, we learn more about the fundamentals of biological design as well as engineer useful living devices with myriad applications. For example, we are interested in building cells that can perform specific tasks, such as remembering past events and thus acting as biological computers. Moreover, we design cells with predictable biological properties that serve as cell-based sensors, factories for generating useful commodities and improved centers for carbon fixation. We have recently engineered natural gut bacteria that can non-invasively report on the dynamics of the animal gut. In doing so, we have made new findings about how cells interact with and impact on their environment. These principles can be applied to problems of all natural environments.

9:12 AM L46.00003 Signaling Mechanisms of Proteins and Protein Complexes. WENDELL LIM, University of California, San Francisco — No abstract available.

9:48 AM L46.00004 Synthetic networks in microbial communities. GUROL SUEL, UCSD — While bacteria are single celled organisms, they predominantly reside in structured communities known as biofilms. Cells in biofilms are encapsulated and protected by the extracellular matrix (ECM), which also confines cells in space. During biofilm development, microbial cells are organized in space and over time. Little is known regarding the processes that drive the spatio-temporal organization of microbial communities. Here I will present our latest findings that utilize synthetic biology approaches to uncover the organizational principles that drive biofilm development. I will also discuss the possible implications of our recent findings in terms of the cost and benefit to biofilm cells.

10:24 AM L46.00005 Metabolite Valves: Dynamic Control of Metabolic Flux for Pathway Engineering. KRISTALA PRATHER, Massachusetts Institute of Technology — Microbial strains have been successfully engineered to produce a wide variety of chemical compounds, several of which have been commercialized. As new products are targeted for biological synthesis, yield is frequently considered a primary driver towards determining feasibility. Theoretical yields can be calculated, establishing an upper limit on the potential conversion of starting substrates to target compounds. Such yields typically ignore loss of substrate to byproducts, with the assumption that competing reactions can be eliminated, usually by deleting the genes encoding the corresponding enzymes. However, when an enzyme encodes an essential gene, especially one involved in primary metabolism, deletion is not a viable option. Reducing gene expression in a static fashion is possible, but this solution ignores the metabolic demand needed for synthesis of the enzymes required for the desired pathway. We have developed Metabolite valves to address this challenge. The valves are designed to allow high flux through the essential enzyme during an initial period where growth is favored. Following an external perturbation, enzyme activity is then reduced, enabling a higher precursor pool to be diverted towards the pathway of interest. We have designed valves with control at both the transcriptional and post-translational levels. In both cases, key enzymes in glucose metabolism are regulated, and two different compounds are targeted for heterologous production. We have measured increased concentrations of intracellular metabolites once the valve is closed, and have demonstrated that these increased pools lead to increased product yields. These metabolite valves should prove broadly useful for dynamic control of metabolic flux, resulting in improvements in product yields.
be approximated by a drift-diffusion model for which we calculate diffusion and drift coefficients as functions of the CTRW model parameters. We also show that, in the limit of slowly-varying (long-wavelength) density perturbations, the time-dependent linear density response can whereas stability indicates absence of aggregation. We show that a broadening of CTRW distributions of the random speed and/or random runtimes strongly aggregation, individual bacteria follow random walk paths determined by randomly selected runtimes, turning angles, and speeds. We have simulated this

0 whether a uniform cell density \( R(r, t, \theta) \). By way of a linear stability analysis, we investigated the instabilities in the subset of a single cell. We aim to characterise growth cone navigation in defined nano-dot guidance cue environments, by using the tools of computational neuroscience to conduct “molecular psychophysics.” We start with a generative model of growth cone behaviour and we characterise sensory and internal sources of noise contributing to behavioural variables, by combining knowledge of the underlying stochastic dynamics in cue sensing and the growth of the cytoskeleton. This enables us to produce bottom-up lower limit estimates of behavioural response reliability and visualise it as probability distributions over axon growth trajectories. Given this information we can match our in silico model’s “psychometric” decision curves with empirical data. Finally we use a Monte-Carlo approach to predict response distributions of axon trajectories from our model.

1 Work funded by the United States National Science Foundation.

8:36AM L47.00002 Motor Switching Rates in Caulobacter Crescentus Follow First Passage Time Distribution1
JAY TANG, MICHAEL MORSE, JORDAN BELL, GUANGLAI LI, Brown University — The flagellar motor of uni-flagellated bacterium Caulobacter crescentus switches stochastically between clockwise (CW) and counterclockwise (CCW) rotation. We performed measurements of the time intervals between switches in order to gain insight on motor dynamics and regulation. Our measurements were performed both on free swimming cells and tethered cells with their flagella attached to a glass slide. A peak time of approximately one second was observed in both motor directions with counterclockwise intervals more sharply peaked. The distributions of switching times can be fitted using biased first passage time statistics. We present a model of motor switching dynamics, which is controlled by the binding of CheY-P to motor subunits FliM. A lower threshold number of FliM with CheY-P bound triggers a switch in motor rotation from CW to CCW, whereas a higher threshold triggers an opposing switch from CCW to CW. The time intervals between alternating switches may be increased or decreased by regulating CheY-P concentration, resulting in biased directional motion in the cells swimming trajectory over many motor cycles under external spatial or temporal gradients.

STUART SEVIER, HERBERT LEVINE, Rice University — The ability to watch biochemical events play out at the single-molecule level has led to the discovery that transcription occurs in a noisy, “bursty” manner. Recently, as the single-molecule lens is placed over a larger number of organisms and genes, relationships between mean expression and noise beyond the “bursty” paradigm have emerged. Through a master-equation formulation of transcription we have found that many powerful physical principles relating to irreversibility seem to play a central role in the newly uncovered trends. Specifically, the relationships between mean expression and noise appears to be a direct consequence of network currents. We discuss how emphasizing the underlying principles in the models can explain recent experimental data and lead to a generalized view of transcription.

8:48AM L47.00003 Consequences of Irreversibility in Fundamental Models of Transcription
STUART SEVIER, HERBERT LEVINE, Rice University — The ability to watch biochemical events play out at the single-molecule level has led to the discovery that transcription occurs in a noisy, “bursty” manner. Recently, as the single-molecule lens is placed over a larger number of organisms and genes, relationships between mean expression and noise beyond the “bursty” paradigm have emerged. Through a master-equation formulation of transcription we have found that many powerful physical principles relating to irreversibility seem to play a central role in the newly uncovered trends. Specifically, the relationships between mean expression and noise appears to be a direct consequence of network currents. We discuss how emphasizing the underlying principles in the models can explain recent experimental data and lead to a generalized view of transcription.

9:00AM L47.00004 Variability and Reliability in Axon Growth Cone Navigation Decision Making
MARTA GARNELO, Imperial College London, SÉBASTIEN G. RICOULT, DAVID JUNCKER, TIMOTHY E. KENNEDY, McGill University, ALDO A. FAISAL, Imperial College London — The nervous system’s wiring is a result of axon growth cones navigating through specific molecular environments during development. In order to reach their target, growth cones need to make decisions under uncertainty as they are faced with stochastic sensory information and probabilistic movements. The nervous system’s wiring therefore exhibits features of both organisms (perception–decision–motor) and the axon. We aim to characterise growth cone navigation in defined nano-dot guidance cue environments, by using the tools of computational neuroscience to conduct “molecular psychophysics.” We start with a generative model of growth cone behaviour and we characterise sensory and internal sources of noise contributing to behavioural variables, by combining knowledge of the underlying stochastic dynamics in cue sensing and the growth of the cytoskeleton. This enables us to produce bottom-up lower limit estimates of behavioural response reliability and visualise it as probability distributions over axon growth trajectories. Given this information we can match our in silico model’s “psychometric” decision curves with empirical data. Finally we use a Monte-Carlo approach to predict response distributions of axon trajectories from our model.

9:12AM L47.00005 Stability of a Random Walk Model for Fruiting Body Aggregation in M. xanthus1
G.C. MCKENZIE-SMITH, Bowdoin College, H.B. SCHÜTTLER, C. COTTER, L. SHIMKETS, University of Georgia — Myxococcus xanthus exhibits the social starvation behaviour of aggregation into a fruiting body containing myxospores able to survive harsh conditions. During fruiting body aggregation, individual bacteria follow random walk paths determined by randomly selected runtimes, turning angles, and speeds. We have simulated this behavior in terms of a continuous-time random walk (CTRW) model, re-formulated as a system of integral equations, describing the angle-resolved cell density, \( R(r, t, \theta) \), at position \( r \) and cell orientation angle \( \theta \) at time \( t \), and angle-integrated ambient cell density \( \rho(r, t) \). By way of a linear stability analysis, we investigated whether a uniform cell density \( R_0 \) will be unstable for a small non-uniform density perturbation \( \Delta R(r, t, \theta) \). Such instability indicates aggregate formation, whereas stability indicates absence of aggregation. We show that a broadening of CTRW distributions of the random speed and/or random runtimes strongly favors aggregation. We also show that, in the limit of slowly-varying (long-wavelength) density perturbations, the time-dependent linear density response can be approximated by a drift-diffusion model for which we calculate diffusion and drift coefficients as functions of the CTRW model parameters.

1 Funded by the Fungal Genomics and Computational Biology REU at UGA.
9:24AM L47.00006 Single-cell analysis of transcription kinetics across the cell cycle , SAMUEL SKINNER, HENG XU, Department of Biochemistry and Molecular Biology, Baylor College of Medicine; CENTER FOR THEORETICAL BIOLOGICAL PHYSICS, RICE UNIVERSITY, SONAL JAISWAL, PABLO FREIRE, Baylor College of Medicine, THOMAS ZWAKA, Department for Developmental and Regenerative Biology, Icahn School of Medicine at Mount Sinai, IDO GOLDING, Department of Physics and Center for the Physics of Living Cells, University of Illinois at Urbana-Champaign — Transcription is a highly stochastic process. A common way of inferring transcription kinetics is to measure mRNA abundance in individual cells and compare the observed copy-number statistics to the prediction of a theoretical stochastic model. However, the reliability of this procedure is hampered by the fact that the measured mRNA numbers represent integration over the finite lifetime of mRNA, over multiple copies of the same gene, and the mixing of cells from different phases of the cell cycle. Here we address these limitations by simultaneously quantifying nascent and mature mRNA in individual cells, and incorporating gene-copy and cell-cycle effects in the analysis of mRNA statistics. We demonstrate this approach on Oct4 and Nanog, two key players in the mouse pluripotency network. We find that both genes are well described by a two-state stochastic model for transcription initiation. The difference in their expression characteristics is attributed to a 2.6-fold difference in the probability of switching to an active transcriptional state. Early in the cell cycle, the two copies of each gene exhibit independent activity. However, after gene replication, the probability of each gene copy to be active diminishes, resulting in dosage compensation.

9:36AM L47.00007 Inference of protein diffusion probed via fluorescence correlation spectroscopy , KONSTANTINOS TSEKOURAS, IUPUI — Fluorophores are an inherent part of single molecule or few particle biophysical data sets. Traditionally, "noise" fluctuations have been viewed as a nuisance, to be eliminated or minimized. Here we look on how statistical inference methods — that take explicit advantage of fluctuations — have allowed us to draw an unexpected picture of single molecule diffusional dynamics. Our focus is on the diffusion of proteins probed using fluorescence correlation spectroscopy (FCS). First, we discuss how — in collaboration with the Bustamante and Marqusee labs at UC Berkeley — we determined using FCS data that individual enzymes are perturbed by self-generated catalytic heat (Riedel et al, Nature, 2014). Using the tools of inference, we found that distributions of enzyme diffusion coefficients shift in the presence of substrate revealing that enzymes performing highly exothermic reactions dissipate heat by transiently accelerating their center of mass following a catalytic reaction. Next, when molecules diffuse in the cell nucleus they often appear to diffuse anomalously. We analyze FCS data — in collaboration with Rich Day at the IU Med School — to propose a simple model for transcription factor binding-unbinding in the nucleus to show that it may give rise to apparent anomalous diffusion. Here inference methods extract entire binding affinity distributions for the diffusing transcription factors, allowing us to precisely characterize their interactions with different components of the nuclear environment. From this analysis, we draw key mechanistic insight that goes beyond what is possible by simply fitting data to "anomalous diffusion" models.

10:12AM L47.00008 Simple models do not explain early dynamics of H. influenzae bacteremia , XINXIAN SHAO, Department of Physics, Emory University, BRUCE LEVIN, Department of Biology, Emory University, ILYA NEMENMAN, Department of Physics, Emory University — There is an abundance of largely qualitative information about the physiological and molecular mechanisms of bacterial pathogenesis. However, little is known about population dynamic processes by which bacteria colonize hosts and invade cells and tissues and thereby cause disease. Classic experiment of Moxon and Murphy[1] observed that, when inoculated intranasally with a mixture of equally virulent strains of Haemophilus influenzae type b(Hib), neonatal rats develop a bacteremic infection that often is dominated by only one random competing strain. A common qualitative explanation for this phenomenon is that the bacteria must switch stochastically into a rapidly growing phenotype to start the full-fledged invasion. Then the first bacterium to switch activates the host immune response, which in turn shuts the door in front of the second strain. We implemented this model computationally and analytically, and we conclude that the data do not support the hypothesis that the observed dependence of the rate of infections on the inoculum size. New experiments are needed to identify mechanisms underlying the dependence.

10:24AM L47.00009 The Dynamics in Epithelial Cell Intercalation in Drosophila Morphogenesis1, FRED WOLF, LARS REICHL, Max Planck Institute for Dynamics and Self-Organization, DEQING KONG, YUJUN ZHANG, Institute for Developmental Biochemistry, Medical School, University of Göttingen, STEPHAN EULE, JAKOB METZGER, Max Planck Institute for Dynamics and Self-Organization, JÖRG GROßHANS, Institute for Developmental Biochemistry, Medical School, University of Göttingen — Epithelial cell rearrangement is important for many processes in morphogenesis. During germband extension in early gastrulation of Drosophila embryos, exchange of neighbors is achieved by junction remodeling that follows a topological T1 process. Its first step is the constriction of dorsal-ventral junctions and fusion of two 3x vertices into a 4x vertex: a process believed to be junction autonomous. We established a high throughput imaging pipeline, by which we recorded, segmented and analysed more than 1000 neighbor exchanges in drosophila embryos. Characterizing the dynamics of junction lengths we find that the constriction of cell contacts follows intriguingly simple quantitative laws. (1) The mean contact length decreases approximately as a square root of time to collapse. (2) The time dependent variance of contact lengths is proportional to the square of mean. (3) The time dependent probability density of the contact lengths remains close to Gaussian during the entire process. These observations are sufficient to derive a stochastic differential equation for contact length that captures the non-equilibrium statistical mechanics of contact collapse. 1Supported by the German Research Foundation.

10:36AM L47.00010 Stochastic Terminal Dynamics in Epithelial Cell Intercalation , STEPHAN EULE, JAKOB METZGER, LARS REICHL, Max Planck Institute for Dynamics and Self-Organization, DEQING KONG, YUJUN ZHANG, JOERG GROSSHANS, Institute for Developmental Biochemistry, Medical School, University of Göttingen, FRED WOLF, Max Planck Institute for Dynamics and Self-Organization — We found that the constriction of epithelial cell contacts during intercalation in germ band extension in Drosophila embryos follows intriguingly simple quantitative laws. The mean contact length (Λ) follows (Λ(t)) ∼ (T − t)α , where T is the finite collapse time; the time dependent variance of contact length is proportional to the square of the mean; finally the time dependent probability density of the contact lengths remains close to Gaussian during the entire process. These observations suggest that the dynamics of contact collapse can be captured by a stochastic differential equation analytically tractable in small noise approximation. Here, we present such a model, providing an effective description of the non-equilibrium statistical mechanics of contact collapse. All model parameters are fixed by measurements of time dependent mean and variance of contact lengths. The model predicts the contact length covariance function that we obtain in closed form. The contact length covariance function closely matches experimental observations suggesting that the model well captures the dynamics of contact collapse.

10:48AM L47.00011 Methods for reconstructing sets of ordinary differential equations from time series data , MANUEL MAI, Department of Physics, Yale University, NEW HAVEN, CT, USA, COREY O’HERN, Department of Physics, Department of Computational Biology and Bioinformatics, Yale University, NEW HAVEN, CT, USA, MARK D. SHATTUCK, Benjamin Levich Institute and Physics Department, The City College of New York, NEW YORK, NY, USA — We propose a novel method for reconstructing the underlying non-linear ordinary differential equations (ODE) for a physical system from time series data. Common methods for ODE reconstruction generate suitable candidate equations for the system and then fit the ODE parameters to the time series data. Candidate sets of ODEs are evolved using genetic programming methods and candidates that poorly fit the data are discarded. Such schemes are computationally expensive. We develop an alternative more efficient approach to ODE reconstruction. In the first step, we identify key features of the set of ODEs (such as the number and stability of fixed points) from the data. In the second step, we develop functional forms for the right-hand sides of the ODEs that interpolate between fixed points and saddles. We will show a number of examples where we can reconstruct nonlinear ordinary differential equations that capture the equivalent dynamics as that found in the original time series data.
8:00AM L48.00001 Genetic networks specifying the functional architecture of orientation domains in V1. JOSCHA LIEDTKE, FRED WOLF, Max Planck Institute for Dynamics and Self-Organization — Although genetic information is critically important for brain development and structure, it is widely believed that neocortical functional architecture is largely shaped by activity dependent mechanisms. Here we show theoretically that mathematical models of genetic networks of principal neurons interacting by long range axonal morphogen transport can generate morphogen patterns that exactly prescribe the functional architecture of the primary visual cortex (V1) as experimentally observed. We analyze in detail an example genetic network that encodes the functional architecture of V1 by a dynamically generated morphogen pattern. We use analytical methods from weakly non-linear analysis [Cross & Hohenberg 1993] complemented by numerical simulations to obtain solutions of the model. In particular we find that the pinwheel statistics are in quantitative agreement with high precision experimental measurements [Kaschube et al. 2010]. This theory opens a novel perspective on the experimentally observed robustness of V1’s architecture against radically abnormal developmental conditions such a dark rearing [White et al. 2001]. Furthermore, it provides for the first time a scheme how the pattern of a complex cortical architecture can be specified using only a small genetic bandwidth. 

8:12AM L48.00002 Numerical simulations on active rod like particles as a model for the collective behavior of Myxococcus xanthus, MANON WIGBERS, Department of Physics and Astronomy, Vrije Universiteit, Amsterdam, 1081HV. The Netherlands, SHASHI THUTUPALLI, JOSHUA SHEAVITZ, Department of Physics, Princeton University, Princeton, NJ, 08544, USA — We study collective behavior of Myxococcus xanthus using numerical simulations. Under starvation conditions, these social bacteria organize into multi-cellular structures, called “fruited bodies,” within which cells sporulate. During the process of fruiting body formation, cells show various collective motion patterns. One of the most striking of these patterns is the so called rippling motility, characterized by standing density waves of reversing bacteria. Similar rippling behaviour is also observed during predatory feeding of the bacteria. Until now, the principles underlying this rippling behavior are not fully elucidated. Analogous to the well studied liquid crystalline phases in condensed matter physics, the ordering of the baceria within these rippling waves resembles a smectic like layered structure. In contrast to active nematic liquid crystalline phases widely studied in recent times, this represents the first known empirical example of an active smectic phase. Inspired by single-cell resolution experimental data of the bacteria, we develop a model of active rod like particles and use numerical simulations to study the organizing principles that drive the transitions between the various active liquid crystalline phases in the myxobacterial collective behavior.

8:24AM L48.00003 Non-ergodic diffusion on quenched, scale-free disorder in two dimensions, GERALD J. LAPEYRE, JR., PIETRO MASSIGNAN, CARLO MANZO, JUAN A. TORRENTO-PINA, MARIA F. GARCÍA-PARAJO, MACIEJ LEWENSTEIN, ICF0-The Institute of Photonic Sciences — We discuss our recently introduced models of diffusion on media with random diffusivity [1] and their application to transport in cell membranes [2]. We find that the diffusion shows weak ergodicity breaking, and compute the anomalous exponents as a function of model parameters. We also report recent results on criteria for predicting weak ergodicity breaking in random walks on specific models of quenched, scale-free, random media.


8:36AM L48.00004 Growth Kinetics of Intracellular RNA/Protein Droplets: Signature of a Liquid-Liquid Phase Transition?, JOEL BERRY, STEPHANIE C. WEBER, NILESH VAIDYA, LIAN ZHU, MIKKO HAATAJA, CLIFFORD P. BRANGWYNNE, Princeton University — Nonmembrane-bound organelles are functional, dynamic assemblies of RNA and/or protein that can self-assemble and disassemble within the cytoplasm or nucleoplasm. The possibility that underlying intracellular phase transitions may drive and mediate the morphological evolution of some membrane-less organelles has been supported by several recent studies. In this talk, results from a collaborative experimental-theoretical study of the growth and dissolution kinetics of nucleoli and extranucleolar droplets (ENDs) in C. elegans embryos will be presented. We have employed Flory-Huggins solution theory, reaction-diffusion kinetics, and quantitative statistical dynamic scaling analysis to characterize the specific growth mechanisms at work. Our findings indicate that both in vivo and in vitro droplet scaling and growth kinetics are consistent with those resulting from an equilibrium liquid-liquid phase transition mediated by passive nonequilibrium growth mechanisms—simultaneous Brownian coalescence and Ostwald ripening. This supports a view in which cells can employ phase transitions to drive structural organization, while utilizing active processes, such as local transcriptional activity, to fine tune the kinetics of these phase transitions in response to given conditions.

8:48AM L48.00005 External stimulation strength controls actin response dynamics in Dicyostelium cells, HSIN-FANG HSU, Max Planck Institute for Dynamics and Self-Organization, CHRISTIAN WESTENDORF, Institut für Pflanzenwissenschaften, Universität Graz, MARCO TARANTOLA, VLADIMIR ZYKOV, EBERHARD BODENSCHATZ, Max Planck Institute for Dynamics and Self-Organization, CARSTEN BETA, Institute of Physics and Astronomy, University of Potsdam — Self-sustained oscillation and the resonance frequency of the cytoskeletal actin polymerization/depolymerization have recently been observed in Dicyostelium, a model system for studying chemotaxis. Here we report that the resonance frequency is not constant but rather varies with the strength of external stimuli. To understand the underlying mechanism, we analyzed the polymerization and depolymerization time at different levels of external stimulation. We found that polymerization time is independent of external stimuli but the depolymerization time is prolonged as the stimulation increases. These observations can be successfully reproduced in the frame work of our time delayed differential equation model.
9:00AM L48.00006 Fluorescent BODIPY Rotor: Viscometer for Cellular Organelles and Membrane-Mimicking Vesicles

9:12AM L48.00007 Nanotopography-induced symmetry-breaking and guidance of actin polymerization waves and cell migration

9:24AM L48.00008 Quantifying and controlling collective motion in externally guided cells

9:36AM L48.00009 The effects of out-of-plane curvature on the growth of epithelia

9:48AM L48.00010 Glycosylases utilize “stop and go” motion to locate DNA damage

10:24AM L48.00011 Silicon Micropore based Electromechanical Transducer to Differentiate Tumor Cells

1This work was supported by the NIH grant R01EB12003, the NSF grant CBET-1264608, and the INFOR grant from TCU.

2supported by NSF-PoLS

3Support Acknowledged from NSF through ECCS-1201878
10:36AM L48.00012 Terasaki Ramps in the Endoplasmic Reticulum: Structure, Function and Formation, GREG HUBER, Kavli Institute of Theoretical Physics, UCSB, JEMAL GUVEN, DULCE-MARIA VALENCIA, Instituto de Ciencias Nuclareas, UNAM, Mexico City — The endoplasmic reticulum (ER) has long been considered an exceedingly important and complex cellular organelle in eukaryotes (like you). It is a membrane structure, part folded lamellae, part tubular network, that both envelopes the nucleus and threads its way outward, all the way to the cell’s periphery. Despite the elegant mechanics of bilayer membranes offered by the work of Helfrich and Canham, as far as the ER is concerned, theory has mostly sat on the sidelines. However, refined imaging of the ER has recently revealed beautiful and subtle geometrical forms – simple geometries, from the mathematical point of view – which some have called a “parking garage for ribosomes.” I’ll review the discovery and physics of Terasaki ramps and discuss their relation to cell-biological questions, such as ER and nuclear-membrane re-organization during mitosis. Rather than being a footnote in a textbook on differential geometry, these structures suggest answers to a number of the ER’s structure-function problems.

Wednesday, March 4, 2015 8:00AM - 11:00AM –
Session L49 GSOFT GSNP: Focus Session: Mechanics of Defects and Discontinuities 217D - James Hanna, Virginia Polytechnic Institute and State University

8:00AM L49.00001 Fracture of brittle coatings on soft plastic substrates, JOEL MARTHELOT, Massachusetts Institute of Technology, DAVY DALMAS, JEREMIE TEISSEIRE, SVI, CNRS, Saint-Gobain, JOSE BICO, BENOIT ROMAN, PMMH, ESPCI ParisTech — Mechanics of stiff and electrically conductive films deposited on soft plastic substrates have recently gain interest due to the development of stretchable electronics applications. When submitted to tensile stress, such films tend to fail with the apparition of arrays of parallel channel cracks transverse to the direction of deformation, with fatal consequences for electrical conductivity. We study the propagation of such fractures in oxide monolayers coated on a polymer substrate under uniaxial stretching. We show how the crack density undergoes a transition from a statistic failure distribution of brittle material to a deterministic failure set by the elastic mismatch between the film and the substrate. A two-dimensional model of a film bonded to an elastic substrate fails to describe the saturation observed at high strain. We present experimental evidences of the localization of strain in the substrate by in-situ AFM imaging of the fracture process. We propose an increment of the model to account for the plasticity of the substrate. This description allows to pass continuously from the elastic to the plastic regime and to predict the saturation of the fragmentation as observed experimentally at large deformation.

8:12AM L49.00002 ABSTRACT WITHDRAWN —

8:24AM L49.00003 Effect of topological defects and curvature on anisotropic crystal growth, AMIR AZADI, Department of Physics, University of Massachusetts, Amherst, GREGORY M. GRASON, Department of Polymer Science and Engineering, University of Massachusetts, Amherst — The equilibrium shapes and symmetries of crystals are vestiges of the physical principles underlying their formation. We perform particle-based simulations guided by analytical analysis to investigate the structure of crystalline domains on curved substrates, a focus on the impact of topological defects on domain morphology. We find at low area fraction, as has been argued previously, that isotropic crystal growth with relatively compact domains generates large curvature-induced strains accommodated by relative ductile interactions, while the formation of anisotropic ribbon-like structures with lower-curvature induced stresses, introduces a larger line tension cost, and is thus favored for brittle crystals. Our results show that for ductile crystals with large surface coverage, appearance of stable topological defects precludes the formation of anisotropic, ribbon-like structures. However branch-like structures with large interfacial area are stable for certain values of intermediate curvature and crystalline ductility. These processes are guided by the interplay between elastic shape instability, defects, and curvature, where pattern formations are not related to kinetic instabilities.

8:36AM L49.00004 Energy Barriers for Defects in Disordered Solids, SVEN WIJTMANS, LISA MANNING, Syracuse University — In solids, defects govern flow and failure. In crystals, defects are easily-identified dislocations, while in disordered solids, defects can be found by analyzing the vibrational modes of the system, which are eigenvectors of the matrix describing the linear response. The low frequency modes are typically quasi-localized hybrids of excitations localized at the defects and plane-wave like modes. Additional analysis can separate these components, giving the location of a defect or a point of particle along a defect. Together, the energy barrier for each defect, we place particles along an isolated defect mode and calculate the energy at which the system transitions to a new energy basin. Different definitions of a new basin, such as a change in the particle contact network or particle displacements above a specific threshold, give different results. We identify several criteria that are consistent and provide a reasonable, robust definition of an energy barrier. Somewhat surprisingly, we find that energy barriers for isolated defects are generally higher than energy barriers for typical quasi-localized modes in the system.

8:48AM L49.00005 Tuning a material’s properties through the excitation of localized defect modes, MARC SERRA GARCIA, ETH Zurich, JOSEPH LYDON, California Institute of Technology, CHIARA DARAIO, ETH Zurich — Technological applications such as acoustic super-lenses and vibration mitigation require materials with extreme mechanical properties (Very high, zero, or negative stiffness). These properties can be achieved through buckling instabilities, local resonances and phase transitions, mechanisms that are limited to particular frequencies, strains or temperatures. In this talk I will present an alternative mechanism to tune the stiffness of a lattice. The mechanism is based on the excitation of a nonlinear localized defect mode. The oscillation of the defect mode affects the bulk properties of the lattice. This is due to the thermal expansion of the defect mode and the nonlinear coupling between the mode amplitude and the strain of the lattice. Due to the singular properties of nonlinear systems near bifurcation points, the lattice can achieve an arbitrarily large stiffness. It is possible to select point of the force-displacement relation that is being tuned by selecting the defect’s excitation frequency and amplitude. Depending on the nonlinear interaction potential at the defect site, the stiffness can be tuned to extremely positive or extremely negative values. While our theoretical and experimental results have been obtained in a granular crystal, the analysis suggests that an equivalent effect should be present in other lattices with localized modes and nonlinearity.

9:00AM L49.00006 Scars and the stability of crystalline shells under external pressure1, DUAN-DUAN WAN, MARK BOWICK, Syracuse University, RASTKO SKNEPNEK, University of Dundee — While continuum elastic theory predicts the mechanical properties of ideal spherical shells under external pressure, on microscopic scale the response of shells to pressure may be affected by their crystalline order and defect structure. Here we compare the stability, under external pressure, of shells with a minimal set of topologically-required defects to shells with extended defect arrays (grain boundary “scars”). In particular, we perform Monte Carlo simulations to compare how shells with and without scars deform quasi-statically under external hydrostatic pressure. We find that the critical pressure at which shells collapse is lowered when the scar distribution breaks icosahedral symmetry and raised when symmetry is preserved. The particular shapes resulting from collapses which break icosahedral symmetry depend crucially on the Föppl-von Karman number.

1We thank the Soft Matter Program of Syracuse University for support.
9:12AM L49.00007 Dynamics and geometry of interacting fractures in torn elastic sheets: convergent, divergent, and multiple swirling cracks, EUGENIO HAMM, Universidad de Santiago de Chile — I will present some recent results on the dynamics of multiple interacting cracks in torn elastic sheets. Specifically, I will consider a peeling - like configuration, in which two cracks converge in a robust fashion, and a “concertina” configuration in which two cracks systematically diverge. Based on experiments, I will discuss the non-trivial aspects of both problems, namely the way in which elasticity and fracture mechanics are concomitant when it comes to predict crack paths. Besides, I will show cases in which the trajectory of a crack is dictated by the path followed by another crack. This delayed interaction of cracks allows the construction of multiple crack configurations in which each crack recursively interacts with a nearby crack, giving rise to divergent self-similar spiral trajectories. Finally, I will discuss the effects of material anisotropy on the propagation of cracks. If time permits, I will also present a concise review of a second example of defect dynamics: the motion of conical singularities in thin elastic sheets, subjected to external forcing, and their mutual interaction. Specifically I will consider the gliding, climbing, annihilation and rotation of such structures.

9:48AM L49.00008 Untangling Superfluid Vortices, DUSTIN KLECKNER, MARTIN W. SCHEELER, University of Chicago, DAVIDE PROMENT, University of East Anglia, WILLIAM T. M. IRVINE, University of Chicago — What is the role of topology, or knottedness, in superfluid phase defects (quantum vortices)? In ideal classical fluids, vortex knots may never untie, and so there is an associated conserved quantity – helicity – which measures how tangled a flow is. One might expect a similar robustness for superfluid defects, however, simulations of the Gross-Pitaevskii equation demonstrate that vortex knots and links spontaneously untie and unlink. Nonetheless, the topology dramatically affects the vortex evolution, and a component of the initial helicity is transferred to helical coils as the knots unravel. These effects are remarkably similar to the behavior of tangled vortices in viscous fluids, suggesting they are universal features of non-ideal fluids.

10:00AM L49.00009 Dynamics of vacancies in two-dimensional Lennard-Jones crystals, ZHENWEI YAO, MONICA OLVERA DE LA CRUZ, Northwestern University — Vacancies represent an important class of crystallographic defects, and their behaviors can be strongly coupled with relevant material properties. We report the rich dynamics of vacancies in two-dimensional Lennard-Jones crystals in several thermodynamic states. Specifically, we numerically observe significantly faster diffusion of the 2-point vacancy with two missing particles in comparison with other types of vacancies; it opens the possibility of doping 2-point vacancies into atomic materials to enhance atomic migration. In addition, the resulting dislocations in the healing of a long vacancy suggest the intimate connection between vacancies and topological defects that may provide an extra dimension in the engineering of defects in extensive crystalline materials for desired properties.

1We thank the financial support from the U.S. Department of Commerce, National Institute of Standards and Technology, the Office of the Director of Defense Research and Engineering (DDR&E) and the Air Force Office of Scientific Research.

10:12AM L49.00010 Jump conditions for thin bodies from an action principle, JAMES HANNA, Virginia Polytechnic Institute and State University — Thin, flexible bodies such as strings, sheets, and rods often sustain kinky geometric features, or experience discontinuous contact forces in their interactions with obstacles. The physics of dynamic and static versions of these phenomena differ. Kink/shock propagation, impact, peeling, unwrapping, tearing and cracking all occur at geometric locations in a body that do not correspond to material points. I will discuss how the jump conditions for momentum and energy across such moving discontinuities may be derived from an action principle for an extended body with time-dependent, non-material boundaries.

10:24AM L49.00011 ABSTRACT WITHDRAWN —

10:36AM L49.00012 Nonlinear optical probing of electric field induced oxygen migrations in Fe doped SrTiO$_3$, HAOCHEH YUAN, DAVID ASCIENZO, ONUR KURT, ZEHRA CEVHER, STEVE GREENBAUM, CUNY-Hunter Coll, RUSSELL MAIER, CLIVE RANDALL, the Pennsylvania State University, YUHANG REN, CUNY-Hunter Coll, CENTER FOR DIELECTRIC STUDIES, MATERIALS RESEARCH INSTITUTE TEAM — We report on our recent study of the electric field induced oxygen migration dynamics and defect states near the interface in Fe-doped SrTiO$_3$ single crystals by optical second harmonic generation (SHG) using a femtosecond Ti:sapphire laser at 800 nm wavelength. By varying both the incidence and the output angles, we identified a strong correlation between the measured SHG signals and the microscopic defect textures of the samples. Significant changes in SHG intensities and phases are explained by the formation and extension of oxygen vacancies and crystalline distortions near Fe defect centers. Our results show that the SHG technique is a powerful tool for detecting local environment near interfaces and oxygen migrations in ferroelectric structures.

1Research at Hunter was supported by the AFOSR FA9550-14-1-0179.

10:48AM L49.00013 Positron beam spectroscopy of defect kinetics in highly oriented pyrolytic graphite, VARGHESE ANTO CHIRAYATH, AMARENDRA G, IGCAR, Kalpakkam, India - 603102 — We report here slow positron beam spectroscopy of thermally activated defect annealing mechanisms in highly oriented pyrolytic graphite (HOPG) which has been implanted with 200 keV carbon ions. The HOPG samples were irradiated to a dose of 10$^{14}$ and 10$^{15}$ ions/cm$^2$ which are just below the dose required for amorphization. The open volume defect-sensitive positron studies have clearly shown a defect annealing mechanism at temperatures close to the Wigner energy release peak for both the lower and higher dose irradiated samples. The sample irradiated to higher dose has also shown a second defect annealing step at 723K from near the end of range of the implanted ions. This step however was not visible in the lower dose sample and has not been previously reported. Positron beam spectroscopy could also detect the presence of interstitial defects trapped at the inter-planar regions after the open volume defect recovery by 973 K. These results will be compared to the present understanding of the open volume defect structures and their migration in graphite as well as in other sp$^2$ hybridized nanostructures like graphene.

1Research fellowship from Department of Atomic Energy, India
2presently at Univ of Texas, Arlington

Wednesday, March 4, 2015 8:00AM - 11:00AM —
Session L50 GSOFT: Self and Directed Assembly I: Mostly Nanoparticles/Rods and Colloids
218 - Alberto Olson-Reichhardt, Georgia Institute of Technology

8:00AM L50.00001 ABSTRACT WITHDRAWN —
8:12AM L50.00002 Switchable End-Linking of Gold Nanorods Induced by a Computationally Designed, Metal-Binding Peptide, ROBERT C. FERRIER, MATTHEW EIBLING, University of Pennsylvania, CHRISTOPHER MACDERMAID, Temple University, CHRISTOPHER LANCHI, JEFFERY G. SAVEN, RUSSELL J. COMPOSTO, University of Pennsylvania — Gold nanorods (AuNRs) possess unique optical properties that depend on the local orientation and separation of the individual rods. Previously, our group has explored the ‘permanent’ end-linking of AuNRs with alkane diethiols. The present work investigates the switchable end-linking of AuNRs via a computationally designed peptide. AuNRs are end-functionalized with a peptide designed in silico to bind a specific metal-ion. AuNRs end-to-end assemble when this metal-ion is present in solution above a particular concentration. The effect of metal-ion concentration on AuNR assembly is probed via UV/Visible spectroscopy and electron microscopy. A chelating agent is added to disassemble the AuNRs, returning the AuNRs to their original, unlinked, state. AuNRs can then be assembled again by adding more metal-ions, thereby allowing the solution optical properties to be switched between two states.

8:24AM L50.00003 Electrical anisotropy in coatings of aligned silver nanowires1, YE XU, Department of Physics and Astronomy, University of Pennsylvania. GABRIEL GÄLDERON-ORTIZ, Department of Physics and Astronomy, University of Puerto Rico at Humacao, ANNEMARIE EXARHOS, Department of Physics and Astronomy, University of Pennsylvania, AHMED ALSAYED, Complex Assemblies of Soft Matter, CNRS-Rhodia-UPenn UMI 3254, KAREN WINEY, Department of Materials Science and Engineering, University of Pennsylvania, JAY KIKKAWA, ARJUN YODH, Department of Physics and Astronomy, University of Pennsylvania — Conductive and transparent coatings consisting of silver nanowires (AgNWs) have been suggested as a promising candidate to replace traditional ITO coatings for emerging flexible electronics applications. The electrical properties of such AgNW coatings depend strongly on the structure of nanowire networks formed by various processing methods. In this work, we study how the alignment of nanowires affects the electrical anisotropy in AgNW coatings. Specifically, we introduce a robust method to prepare coatings of well-aligned AgNWs on glass substrates; the method utilizes the rapid flow of AgNW suspensions through a confined geometry. The angle-dependent sheet resistance of the coatings was measured, and large anisotropy in surface conductivity was found to characterize the aligned AgNW networks. We also explore the degree of alignment and surface coverage of AgNWs in the networks, thereby establishing connections between microscopy network structures and macroscopic electrical anisotropy.

8:36AM L50.00004 Molecular simulations of PEGylated lipids at interfaces: size selective dispersion of nanoscale objects, MARIA SAMMALKORPI, SAMPSA VIERROS, Department of Chemistry, Aalto University, Finland, PAUL R. VAN TASSEL, Department of Chemical & Environmental Engineering, Yale University, USA, JUKKA MÄTTÄ, Department of Chemistry, Aalto University, Finland — Phospholipids and phospholipid derivatives offer efficient, noncovalent functionalization and dispersion of hydrophobic objects, e.g., therapeutic molecules and nanoparticles including carbon nanotubes (CNTs). However, the relation of lipid aggregates in bulk solution and in the presence of the object, and the resulting dispersion remain important questions. We employ here molecular dynamics simulations to explore PEGylated lipid aggregates at interfaces and the resulting dispersion efficiency. By varying lipid and substrate curvature, and the PEG chain length, we find 1) lipid-CNT and PEGylated lipid-CNT aggregation behavior consistent with recent experiments, 2) the assembled morphology to vary from micellar-like to tubular coating (phospholipids) and micellar to monolayer-like (PEGylated lipids) with the transition depending on lipid curvature and for PEGylated lipids also on the PEG chain length and CNT diameter, 3) aggregation morphology dependent CNT dispersion ability, and 4) good agreement between simulation and scaling theories of a brush-type PEG [1,2]. Finally, we discuss the implications to size-selective separation of hydrophobic particles and experimental observations.

1This work was supported by the NSF DMR12-05463, DMR-1305199, PENN MRSEC DMR11-20901, NASA NNX08AO0G grants, and Solvay.

8:48AM L50.00005 Designing entropy-driven binary ordered superlattices from polyhedral nanoparticles, MIHIR KHADILKAR, FERNANDO ESCOBEDO, Cornell University — While ordered multicomponent structures of nanoparticles are certainly desirable in view of multiple potential applications, their self-assembly often requires highly tuned enthalpic interactions between the different constituents. We present simulation results on binary mixtures of hard polyhedral nanoparticles that form ordered superlattices without any enthalpic interaction, with the help of shape anisotropy alone. We also identify a rule that maximizes packing compatibility and hence promotes the formation of ordered superlattices based on the order-disorder transition pressures of the pure components. Results show formation of plastic solid solutions in the case of binary mixtures involving nanoparticle shapes from the truncated cube family, whose pure-components also form plastic crystals. Preliminary results for 2D systems will also be presented.


9:00AM L50.00006 Computer simulation study on the self-assembly structure of soft Janus particles, ZHAO-YAN SUN, ZHAN-WEI LI, Stete Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, MULTI-SCALE SIMULATION TEAM — Soft and deformable Janus particles have received more attention due to their unique properties and enormous potential applications in recent years. Here we present a mesoscale model for soft Janus particles, which successfully reflects their physical nature by directly mapping onto experimentally measurable particle properties. By properly tuning Janus balance and the strength of attraction between attractive patches, soft Janus particles can reversibly self-assemble into a number of fascinating hierarchical superstructures in dilute solutions, such as micelles, wormlike strings, single helices, double helices, bilayers, tetragonal bilayers, complex supermicelles, and in bulk systems, such as the hexagonal columnar structure and the body-centered tetragonal structure. We also introduce a new concept in achieving template-free fabrication of diverse 2D ordered nanostructures by utilizing anisotropic characteristics of soft triblock Janus particles. Our work demonstrates that soft Janus particles with the deformable and non-centrosymmetric characteristics hide many surprises in the design and fabrication of hierarchically self-assembled superstructures.

9:12AM L50.00007 Self-organization in periodically sheared granular materials, SAM WILKEN, GARY L HUNTER, PAUL M CHAIKIN, New York University — Self-organization as a result of periodic shear is becoming a feature observed in an increasing number of systems. In our experiments, we enforce cyclic shear on a three dimensional system of non-Brownian particles to investigate the global packing behavior of the granular assembly. By starting with a diluted, loosely packed system and measuring the packing fraction after each shear cycle, we find the system compacts to reach a steady state with a well defined packing fraction. The shear amplitude determines the steady state packing fraction, where large amplitude shear produces a lower packing density and small amplitude shear produces a higher packing density. We also study the phase diagram of this system which exhibits caged motion and a transition to vorticity.
9:24AM L50.00008 Bio-inspired Structural Colors from Deposition of Synthetic Melanin Nanoparticles by Evaporative Self-assembly. MING XIAO, Univ of Akron, YIWEN LI, University of California, San Diego, DIMITRI DEHEYN, Scripps Institution of Oceanography, University of California, San Diego, XIULIJUN YUE, NATHAN GIANNESCHI, University of California, San Diego, MATTHEW SHAWKEY, ALI DHINOJWALA, Univ of Akron — Melanin, a ubiquitous black or brown pigment in the animal kingdom, is a unique but poorly understood biomaterial. Many bird feathers contain melanosomes (melanin-containing organelles), which pack into ordered nanostructures, like multilayer or two-dimensional photonic crystal structures, to produce structural colors. To understand the optical properties of melanin and how melanosomes assemble into certain structures to produce colors, we prepared synthetic melanin (polypodamine) particles with variable sizes and aspect ratios. We have characterized the absorption and refractive index of the synthetic melanin particles. We have also shown that we can use an evaporative process to self-assemble melanin films with a wide range of colors. The colors obtained using this technique is modeled using a thin-film interference model and the optical properties of the synthetic melanin nanoparticles. Our results on self-assembly of synthetic melanin nanoparticles provide an explanation as why the use of melanosomes to produce colors is prevalent in the animal kingdom.

1National scientific foundation, air force office of scientific research, human frontier science program

9:36AM L50.00009 Mobility and diffusion of bound DNA-coated colloids. ETIENNE DUCROT, JEREMY S. YODH, Center for Soft Matter Research, New York University, YU WANG, Molecular Design Institute, New York University, YUFE WANG, Center for Soft Matter Research, New York University, XIAOLONG ZHENG, MARCUS WECK, Molecular Design Institute, New York University, DAVID J. PINE, Center for Soft Matter Research, New York University — DNA coatings have been proposed as a versatile means for programming the self-assembly of micrometer and nanometer size particles. Progress in achieving this goal for particles larger than about 100 nm, where the DNA coatings are typically much thinner than the particle diameter, has been impeded because such DNA-coated colloids stick to each other like Velcro; they collide and bind but fail to anneal into their preprogrammed structure. Most notably, they generally fail to assemble into colloidal crystals but form random aggregates. We have prepared micrometer-size colloids coated with single stranded DNA that are mobile even after they bind, so that the particles can rapidly rearrange. Here we report measurements of the mean square displacement of one ssDNA particle on a second ssDNA particle immobilized on a substrate, when the temperature is quenched to just below the melting temperature (near 40°C). For shallow quenches of ΔT ≈ 0.5°C, the mean square displacement is proportional to time, Δr^2~At, indicating diffusive motion. For deeper quenches of ΔT ≈ 1°C, Δr^2~At^n, where n ≈ 1, indicating subdiffusive motion. This behavior is discussed in terms of a random distribution of traps.

9:48AM L50.0010 High-yield production of stable colloidal clusters and their use in hierarchical DNA-directed assemblies. JAMES MCGINLEY, YIFAN WANG, IAN JENKINS, TALID SINNO, JOHN CROCKER, University of Pennsylvania, CROCKER RESEARCH GROUP COLLABORATION, SINNO RESEARCH GROUP COLLABORATION — Our goal is to produce and purify high yields of stable DNA-coated colloidal clusters by using crystal templates and reprogrammable DNA interactions. First, we incorporate “impurity” particles into a host colloidal crystal made up of DNA-coated polymer microspheres, and ensure that the only bonds that are preserved are those between the impurity particles’ DNA strands and those of their nearest neighboring host particles. After dispersing the host crystal and making all DNA bonds permanent using a DNA-reactive enzyme, we are left with stable colloidal clusters, each comprised of a single impurity particle surrounded by a number of particles dictated by the host crystal structure. The clusters can be made withicosahedral, Cuboctahedral, Tetrahedral, Cubic, and Octahedral symmetries, and can then be purified using density gradient fractionation. We will demonstrate that the scalable production of purified, well-oriented and stable DNA-coated colloidal clusters allows for the exploration of hierarchical assemblies with asymmetric building blocks and directional bonding.

10:00AM L50.0011 Using Microfluidics to Measure the Equation of State for a 2D Colloidal Membrane. ANDREW BALCHUNAS, RAFAEL CABANAS, SETH FRADEN, ZVONIMIR DOGIC, Brandeis Univ — In the presence of non-adsorbing polymer, monodisperse filamentous viruses assemble into colloidal membranes, which are 2D liquid-like one-rod-length-thick monolayers of aligned rods. Colloidal membranes are of particular interest because their properties are accounted for by the same theoretical models that are used to describe the biophysics of conventional lipid bilayers. However, bulk membrane formation only occurs over a very limited range of depletant concentrations and ionic strengths. In order to explore the properties of the colloidal membranes under a much wider range of molecular parameters, we have developed a microfluidic technique that allows for in-situ exchange of the enveloping polymer suspension. This allows us to access the region of phase space where membranes are metastable. Using our technique we can measure how the colloidal membrane area depends on applied osmotic pressure, allowing us to determine its equation of state. We also characterize the dynamics of the constituent rods by using single molecule tracking techniques.

10:12AM L50.00012 Assembly and interactions of achiral rafts in colloidal membranes. JOIA MILLER, Brandeis University, PRERNAA SHARMA, Indian Institute of Science Bangalore, ZVONIMIR DOGIC, Brandeis University — Two-dimensional colloidal membranes composed of rods of different lengths display rich phase behavior. In particular, chirality of constituent rods stabilizes assembly of colloidal rafts, micron sized droplets enriched in one type of rod floating in the background membrane. Colloidal rafts interact via long-range repulsive interactions that are mediated by local rod twisting due to their rods’ inherent chirality. We explore the behavior of an achiral bidisperse mixture of colloidal rods. Even in the achiral limit we observe assembly of stable or meta-stable finite-sized rafts. However, in contrast to the chiral limit, the long-range interactions between achiral rafts are attractive. These rafts are embedded in a host membrane that has nearly critical fluctuations in composition. We correlate the attractive domain interactions with these critical fluctuations.

10:24AM L50.00013 Patchy particles using colloidal caps. CHRISTINE MIDDLETON, DAVID PINE, New York University — We present a method for making patchy particles functionalized with single stranded sticky end DNA only on their patches. This is done by adding “spherical cap” particles as patches to single stranded DNA-coated colloids. The caps are single stranded DNA using copper-free click chemistry. Due to being attached only by depletion, the patches diffuse on the surface of the particle. The patchy particles can then interact with each other in a specific, directional way through the mobile, DNA functionalized patches.

10:36AM L50.00014 Temperature controlled nanoparticle stability in concentrated polymer solutions. SO YOUN KIM, Ulsan Natl Inst of Sci & Tech, CHARLES F. ZUKOSKI, University at Buffalo — Polyethylene glycol (PEG) in water is known to display a lower critical solution temperature (LCST) and a closed loop at high temperature. When silica nanoparticles are suspended in concentrated PEG solution, we observe temperature dependent phase separation even below the 60°C which is much lower than the LCST for the lowest PEG reported. Depending on the conditions, nanoparticles form clusters and show gelation and both can be reversible. Small angle x-ray scattering (SAXS) is used to characterize microstructure of nanoparticle dispersion and diffusing wave spectroscopy (DWS) and other light scattering techniques are employed to understand particle correlations in dense systems. Polymer dynamics near particle substrate is discussed with NMR Free Induction decay experiment. These combined experimental studies help to understand the detailed mechanism of nanoparticle gelation in polymer solutions.
10:48AM L50.00015 A Directional Entropic Force Approach to Assemble Anisotropic Nanoparticles into Superlattices1, BYEONGDU LEE, Argonne Natl Lab, TAO LI TEAM, KAYLIE YOUNG, GEORGE C. SCHATZ, CHAD A. MIRKIN COLLABORATION2, MICHAEL ENGEL, PABLO F. DAMASCENO, SHARON C. GLOTZER COLLABORATION3 — We introduce a directional entropic force approach (DEFA) for controlling the assembly of anisotropic nanoparticles into crystalline lattices. The method relies on surfactant micelle-induced depletion interactions to assemble anisotropic gold nanoparticles into reconfigurable, non-close-packed (open) superlattices in solution. The anisotropic nanoparticles align along their flat facets to maximize entropy, and therefore minimize the free energy of the system, leading to assemblies with long-range order. Importantly, our experimental work complements recent theoretical work that proposes directional entropic forces between nanoparticle facets as a viable means for thermodynamically assembling nanoparticle superlattices. The experimental work herein uses depletants to create strong attractive forces that can drive assembly of reversible superlattices with tunable spacing in solution. These directional entropic forces are analogous to the directional bonding between atoms in molecules. The resulting crystalline superlattices are therefore shape-dependent. We show that the electrostatic and depletion interactions combine to determine the lattice spacing, and can be tuned independently with surfactant concentration and ionic strength to reconfigure the lattice constant.


Wednesday, March 4, 2015 8:00AM - 11:00AM –
Session L51 DCMP: Invited Session: Topological Superconductors
Grand Ballroom C1 - Ady Stern, Weizmann Institute of Science

8:00AM L51.00001 Time reversal invariant topological superconductors in one dimension: how to realize them and what can they do for you, EREZ BERG, Weizmann Institute of Science — Time-reversal invariant (TRI) topological superconductors are exotic superconductors that support anomalous protected edge states. These states are electronic analogues of the B phase of superfluid $^3$He. In one spatial dimension, a TRI superconductor carries a Kramers pair of Majorana zero modes at each end. In this talk, I will discuss setups to realize this phase in spin-orbit coupled quantum wires, in proximity to conventional superconductors. The topologically non-trivial phase can be stabilized either by coupling the wire to two superconductors with a phase difference of $\pi$ between them, or spontaneously, due to repulsive interactions in the wire. In the former case, the system is a natural realization of a fermion parity pump, switching the local fermion parity of both edges when the relative phase between the superconductors is changed adiabatically by $2\pi$. I will show that a gapless TRI topological phase with exponentially localized edge states can exist even if the superconductor used to induce pairing is one-dimensional, and superconducting long-range order is destroyed by long-wavelength fluctuations. If time allows, I will talk about the signatures of the TRI phase in noise correlation experiments, and compare it to the the case of a time reversal breaking phase with a single Majorana zero mode at the ends.


8:36AM L51.00002 Induced superconductivity in the quantum spin Hall edge, SEAN HART, Harvard University — The quantum spin Hall insulator is an example of a two-dimensional topological insulator, a phase of matter in which protected gapless surface states surround a gapped bulk. Inducing superconducting pairing within the helical edge states of the quantum spin Hall effect has been proposed as an avenue towards topological superconductivity. In this talk we present measurements of superconductivity induced in two-dimensional HgTe/HgCdTe quantum wells, a material which becomes a quantum spin Hall insulator when the well width exceeds $d_C = 6.3$ nm. In wells that are 7.5 nm wide, we find that supercurrents are confined to the one-dimensional sample edges as the bulk density is depleted. However, when the well width is decreased to 4.5 nm the edge supercurrents cannot be distinguished from those in the bulk. Our Josephson interferometry measurements provide evidence for supercurrents carried by the helical edges of the quantum spin Hall effect, one of the crucial ingredients for one-dimensional topological superconductivity. These results also directly yield information about the microscopic structure of the edge modes. In particular we find that the widths of the edge channels range from 180 nm to 408 nm.

9:12AM L51.00003 Local Adiabatic Mixing of Kramers Pairs of Majorana Bound States, KARSTEN FLENSBERG, Center for Quantum Devices, The Niels Bohr Institute, Univ of Copenhagen, Denmark — In this talk adiabatic time evolution of Kramers pairs of Majorana bound states and the prospects of using such bound states as parity qubits are discussed. It is shown that local adiabatic perturbations can cause a rotation in the space spanned by the Kramers pair and that the quantum information is therefore unprotected against local perturbations. This is in contrast to the case of single localized Majorana bound states in systems with broken time reversal symmetry. However, under certain conditions such mixing does not occur. A general scheme for determining when these conditions are satisfied is explained and exemplified with a quasi-1D model of a time reversal symmetric topological superconductor.

9:48AM L51.00004 Phase coherent transport in hybrid superconductor-topological insulator devices1, AARON FINCK, University of Illinois at Urbana-Champaign — Heterostructures of superconductors and topological insulators are predicted to host unusual zero energy bound states known as Majorana fermions, which can robustly store and process quantum information. Here, I will discuss our studies of such heterostructures through phase-coherent transport, which can act as a unique probe of Majorana fermions. We have extensively explored topological insulator Josephson junctions through SQUID and single-junction diffraction patterns, whose unusual behavior give evidence for low-energy Andreev bound states. In topological insulator devices with closely spaced normal and superconducting leads, we observe prominent Fabry-Perot oscillations, signifying gate-tunable, quasi-ballistic transport that can elegantly interact with Andreev reflection. Superconducting disks deposited on the surface of a topological insulator generate Aharonov-Bohm-like oscillations, giving evidence for unusual states lying near the interface between the superconductor and topological insulator surface. Our results point the way towards sophisticated interferometers that can detect and read out the state of Majorana fermions in topological systems. This work was done in collaboration with Cihan Kurter, Yew San Hor, and Dale Van Harlingen.

1We acknowledge funding from Microsoft Project Q.
weakly coupled to a heat bath. I will conclude with a brief discussion of how these phenomena may best be detected in experiments.

References:


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Wednesday, March 4, 2015 8:00AM - 11:00AM — Session L52 DCMP: Invited Session: Many Body Localization and Entanglement  Grand Ballroom

C2 - Chandran Anushya, Perimeter Institute for Theoretical Physics

10:24AM L51.00005 Selective Equal Spin Andreev Reflections induced by Majorana Fermions

KAM TUEN LAW, Hong Kong Univ of Sci & Tech — The search for Majorana fermions has become an important subject in recent years. Zero-bias conductance peaks (ZBCPs) possibly induced by Majorana fermions have been reported in tunneling spectroscopy experiments. However, the origin of these ZBCPs is still under debate. In this talk, I would like to point out that Majorana fermions induce a special type of Andreev reflection processes called selective equal spin Andreev reflections (SESARs) [1]. For SESAR processes at a normal lead/topological superconductor interface, incoming electrons with certain spin polarization in the lead are reflected as counter-propagating holes with the same spin. The spin polarization direction of the electrons of this Andreev reflected channel is selected by the Majorana fermions. Moreover, electrons with opposite spin polarization are always reflected as electrons with unchanged spin. We show that the tunneling current from a ferromagnetic lead to a topological superconductor is strongly affected by the spin polarization direction of the lead due to SESARs. This property can be used to detect Majorana fermions in several candidate topological superconductors. The application of SESARs in generating giant spin currents in nodal topological superconductors will also be discussed.


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This research is supported in part by the ERC synergy grant UQUAM

8:00AM L52.00001 Renormalization group studies of many-body localization

EHUD ALTMAN, The Weizmann Institute of Science — Quantum correlations do not usually persist for long in systems at finite energy density and disappear once the system thermalizes. But many-body localization offers an alternative paradigm, whereby quantum matter can evade the usual fate of thermal equilibrium and retain retrievable quantum correlations even at high energies. I will survey a dynamical renormalization group (RG) approach used to characterize the novel dynamics and entanglement structures, which develop in the localized phase in lieu of classical thermalization. Then I will present a theory of the transition between the ergodic and the many-body localized phase based on a novel RG framework. Here eigenstate entanglement entropy emerges as a natural scaling variable; the RG describes a change from area-law to volume law entanglement through an intriguing critical point, where the distribution of entanglement entropy becomes maximally broad. The ergodic phase established near the critical point is a Griffiths phase, which exhibits sub-diffusive energy transport and sub-ballistic entanglement propagation. The anomalous diffusion exponent vanishes continuously at the critical point. Before closing I will discuss recent progress in confronting the emerging theoretical understanding of many-body localization with experimental tests.

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This research was supported in part by the ERC synergy grant UQUAM

8:36AM L52.00002 Evidence for Many-Body Localization in an Ultracold Fermi-Hubbard Gas

BRIAN DEMARCO, University of Illinois at Urbana-Champaign — Many-body localization (MBL) is a promising new paradigm for understanding disorder-induced localization in interacting quantum systems at non-zero temperature. We observe the emergence of an insulating state consistent with MBL in a strongly correlated atomic Fermi gas trapped in a disordered optical lattice, a closed system that realizes the disordered Fermi-Hubbard model. In measurements of disorder-induced localization obtained via mass transport, we detect three phenomena characteristic of MBL. We measure localization of this strongly interacting system at non-zero temperature, and we observe interaction-driven delocalization. We also observe localization that persists as the temperature and energy density of the gas are increased.

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This work was supported by the NSF and ARO.

9:12AM L52.00003 Entanglement and universal dynamics in many-body localized systems

DMITRY ABANIN, Perimeter Institute for Theoretical Physics — We are used to describing systems of many particles by statistical mechanics. However, the basic postulate of statistical mechanics – ergodicity – breaks down in so-called many-body localized systems, where disorder prevents particle transport and thermalization. In this talk, I will describe a phenomenological theory of the many-body localized (MBL) phase, based on new insights from quantum entanglement [1]. I will argue that, in contrast to ergodic systems, MBL eigenstates are not highly entangled, but rather obey so-called area law, typical of ground states in gapped systems. I will use this fact to show that MBL phase is characterized by an infinite number of emergent local conservation laws, in terms of which the Hamiltonian acquires a universal form. Turning to the experimental implications, I will describe the behavior of MBL systems following quantum quenches: surprisingly, entanglement shows logarithmic in time growth [1,2], reminiscent of glasses, while local observables exhibit power-law approach to ‘equilibrium’ values [3]. I will support the presented theory with the results of numerical experiments. I will close by discussing experimental implications and other directions in exploring ergodicity and its breaking in quantum many-body systems, including many-body localization in periodically driven systems.


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9:48AM L52.00004 Localization protected quantum order

RAHUL NANDKISHORE, Princeton University — Many body localization occurs in isolated quantum systems, usually with strong disorder, and is marked by absence of dissipation, absence of thermal equilibration, and a memory of the initial conditions that survives in local observables for arbitrarily long times. The many body localized regime is a non-equilibrium, strongly disordered, non-self averaging regime that presents a new frontier for quantum statistical mechanics. In this talk, I point out that there exists a vast zoo of correlated many body localized states of matter, which may be classified using familiar notions of spontaneous symmetry breaking and topological order. I will point out that in the many body localized regime, spontaneous symmetry breaking can occur even at high energy densities in one dimensional systems, and topological order can arise even without a bulk gap. I will also discuss the phenomena of perfectly isolated many body localized systems, which are weakly coupled to a heat bath. I will conclude with a brief discussion of how these phenomena may best be detected in experiments. References: Phys. Rev. B 88, 014206 (2013), Phys. Rev. B 90, 195115 (2014), Phys. Rev. B 90, 064203 (2014)

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Infinite dimensions has emerged. However, it is an understatement to say that large, exactly isostatic packings approach to other open issues in the theory of glasses. With a recently developed scaling theory of the jamming transition, and with numerical simulations. Finally, I will briefly discuss some possible extensions of this impact on the critical properties of the jamming transition and allows one to obtain analytic predictions for the critical exponents. The predictions are consistent in the solution: as in the SK model, the glassy states turn out to be marginally stable, and are described by a Parisi equation. Marginal stability has a deep based on the exact solution of the hard sphere model in infinite dimension. An unexpected analogy with the Sherrington-Kirkpatrick spin glass model emerges independent of spatial dimension, suggesting that a mean field theory can correctly predict their values. I will discuss a mean field approach to the problem.

FRANCESCO ZAMPONI, LPTENS and CNRS, Ecole Normale Superieure, Paris — The jamming transition marks the emergence of rigidity in a system of many-body localized phases—the interacting analogs of the Anderson insulator. In this talk I will discuss in detail three observations related to the entanglement properties of many-body localized systems: (i) A global quench within the many-body localized phase gives rise to a slowly (logarithmically) increasing entanglement entropy. This is due to interaction induced dephasing that is absent in the Anderson insulator and therefore serves as a unique signature of the many-body localized phase. (ii) A local quench from an eigenstate leads to an extensive increase in the entanglement entropy only at the many-body localization transition itself. And (iii) at the many-body localization transition the distribution of entanglement entropies becomes extensively broad, while it vanishes both in the extended metallic phase and in the localized phases. The width of the entanglement distribution, like the long time limit of the local quench, is therefore a useful diagnostic for a many-body localization transition. I explicitly demonstrate how all these features are observed in microscopic spin chain models of many-body localization, and, in particular, discuss how they can be used to detect a many-body mobility edge.


Wednesday, March 4, 2015 8:00AM - 11:00AM –
Session L53 DCMP GSOFT: Invited Session: Advances in Glassy Systems Across Many Scales
Grand Ballroom C3 - Andrea Liu, University of Pennsylvania

8:00AM L53.00001 Thermodynamic glass transitions in three dimensional glasses, LUDOVIC BERTHIER, CNRS & University Montpellier 2 — The physics associated to the glass transition controls the dramatic evolution of transport coefficients in systems as diverse as dense liquids, polymers, colloids, but also granular particles and active matter. The experimental liquid-glass transition in equilibrium fluids is characterized by several phenomenological crossovers, but glasses can form without crossing any sharp singularity. I will present multiple evidences suggesting that the glass formation process is underlied by equilibrium phase transitions. Combining numerical tools developed to study ordinary phase transitions to recent theoretical analytical progress I will demonstrate that studies of the glass transition have entered a new phase, where the relevant order parameter, thermodynamic fluctuations and phase transformations can be directly analysed in finite dimensional model glasses.

8:36AM L53.00002 Exact computation of the critical exponents of the jamming transition, FRANCESCO ZAMPONI, LPTENS and CNRS, Ecole Normale Superieure, Paris — The jamming transition marks the emergence of rigidity in a system of amorphous and athermal grains. It is characterized by a divergent correlation length of the force-force correlation and non-trivial critical exponents that are independent of spatial dimension, suggesting that a mean field theory can correctly predict their values. I will discuss a mean field approach to the problem based on the exact solution of the hard sphere model in infinite dimension. An unexpected analogy with the Sherrington-Kirkpatrick spin glass model emerges in the solution: as in the SK model, the glassy states turn out to be marginally stable, and are described by a Parisi equation. Marginal stability has a deep impact on the critical properties of the jamming transition and allows one to obtain analytic predictions for the critical exponents. The predictions are consistent with a recently developed scaling theory of the jamming transition, and with numerical simulations. Finally, I will briefly discuss some possible extensions of this approach to other open issues in the theory of glasses.

9:12AM L53.00003 Revealing the critical behavior of jamming: high precision simulations of large, exactly isostatic packings1, ERIC CORWIN, Univ of Oregon — Recently, an exact first-principle theory of jamming criticality in infinite dimensions has emerged. However, it is an understatement to say that it is far from the physically relevant dimensions of d = 2 and 3. In this work we probe how meaningful these infinite-dimensional predictions are in low dimensions by examining the scaling of the weak contact forces at jamming. We use a combination of 1) newly developed GPU techniques implementing quad-precision simulations and 2) an algorithm to calculate extremely accurate interparticle forces for isostatic packings to probe the behavior of systems of very-many-particles in dimensions d = 2 – 6. We find that the weak forces arise from two populations, one associated with localized excitations and the other with extended excitations. We find that the fraction of localized excitations decreases with increasing dimension. Surprisingly, the infinite-dimensional predictions hold exactly all the way down to d = 2 for the extended excitations.

1Supported by NSF CAREER Award No. DMR-1255370.


10:24AM L53.00005 Seeking Quantum Speedup Through Spin Glasses: Evidence of Tunneling?, HELMUT G. KATZGRABER, Texas A&M University — Quantum annealing machines use a non-mainstream method known as adiabatic quantum annealing to perform optimization tasks. Very recently, tests performed by different research teams on the D-Wave Two quantum annealer using spin glasses as a benchmark have shown that, although the machine indeed appears to tap into quantum effects, it shows no speedup over traditional computing architectures. We present results that suggest that the benchmark instances used are too simple to detect quantum speedup and based on insights from spin-glass physics outline strategies to develop hard instance classes. With our choice of benchmark strategy, we show that the D-Wave Two quantum annealer does not outperform current computer technologies, mainly due to noise and calibration errors of the device. However, our results do indicate that quantum tunneling might be present.

Work done in collaboration with F. Hamze (D-Wave Systems, Inc.), Zheng Zhu (Texas A&M University) and Andrew J. Ochoa (Texas A&M University). H.K.K. acknowledges support from the NSF (Grant No. DMR-1151387).
11:15AM M1.00001 Tunable layer-by-layer oxidation of atomically thin WSe$_2$. MAHIRO YAMAGAMI, MASAHIRO ISHIHAMA, Department of Physics, University of Tokyo, JAPAN. — The ability to tailor the properties of a material nanoscale heterostructures is limited by the intrinsic crystalline quality of the TMDs. Our research group has focused on the intrinsic properties of BN, which is considered to be an ideal substrate for graphene devices. However, many intrinsic properties of BN have not been clarified yet, since many researchers have focused on the electrical properties of BN. In this study, we demonstrate that the layer-by-layer dielectric breakdown of BN is systematically studied using the conductive atomic force microscopy. We find that the obtained field strength is about 12 MV/cm, which is comparable to the conventional SiO$_2$. After the dielectric breakdown, BN fractured like a flower with equilateral triangular fragments. However, when an applied voltage is stopped just in the middle of the dielectric breakdown, the formation of holes is clearly observed, which does not penetrate to the bottom metal electrode. Subsequent IV measurement at the hole indicates that the remaining BN layer in the hole is still electrically inactive. A possible explanation is presented.

11:27AM M1.00002 Layer-by-layer Dielectric Breakdown of Hexagonal Boron Nitride Film in Conductive AFM Measurement. YOSHIKI HATTORI, The University of Tokyo, JAPAN, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, JAPAN. — We have investigated the structural and electronic properties of fluorinated (MoS$_2$), WS$_2$, MoTe$_2$, and WTe$_2$. We have demonstrated the feasibility of conducting the measurements in situ conductance and crystalline properties of graphene and MoS$_2$ monolayers. We realized back or side gated electrical devices from monolayer MoS$_2$ or graphene crystals (trigonals respectively hexagons) suspended on a 50nm SiNx m. The devices are exposed to electron irradiation inside a 200kV transmission electron microscope (TEM) and we perform in situ conductance measurements. The number of defects and the quality of the graphene and MoS$_2$ monolayers is strongly affected by monolayer MoS$_2$ and the binding leads to p-doping. Fluorine atoms are strongly bound on molydisulfide and the binding leads to p-type conductivity. As such, fluorination can be useful for chemical doping of monolayer MoS$_2$.

11:39AM M1.00003 Fluorinating Single Layer Molydisulfide. MASAHIRO ISHIHAMA, JYOTI KATOCH, Department of Physics and Nanoscience Technology Center, University of Central Florida — We have investigated the structural and electronic properties of fluorinated (MoS$_2$) using electron microscopy, scanning tunneling microscopy and spectroscopy, photoluminescence and ultraviolet photoelectron spectroscopy. Fluorine atoms are strongly bound on molybdenum disulfide and the binding is p-type. As such, fluorination can be useful for chemical doping of monolayer molybdenum disulfide. We will discuss our experimental results in light of our recent ab-initio calculations.

11:51AM M1.00004 The effect of defects produced by electron irradiation on the electrical properties of graphene and MoS$_2$. JULIO ALEJANDRO RODRIGUEZ-MANZO, ADRIAN BALAN, CARL NAYOR, WILL PARKIN, MATTHEW PUSTER, A.T. CHARLIE JOHNSON, MARIJA DRNDIC, Univ of Pennsylvania — We present a study of the effects of the defects produced by electron irradiation on the electrical and crystalline properties of graphene and MoS$_2$ monolayers.

12:03PM M1.00005 Intrinsic disorder in graphene on transition metal dichalcogenide heterostructures. MATTY KANTZ, MATTHEW PUSTER, University of Texas at Austin, DEVIN MCKENZIE, SHENGQIANG HUANG, MARINA PAGGEN, University of Arizona, MAZHAR ALI, ROBERT CAVA, Princeton University, EMMANUEL TANG, University of Texas at Austin, BRIAN L. LEROY, University of Arizona. — Recently, semiconducting materials in the transition metal dichalcogenide (TMD) family have gained great popularity for use in novel graphene-based heterostructure devices such as tunneling transistors, highly efficient flexible photovoltaic devices, and nonvolatile memory cells. TMDs have also been explored as alternatives to hexagonal boron nitride (hBN) as substrates for pristine graphene devices. Their quality has thus far been significantly worse than comparable hBN devices. We examine graphene on numerous TMD substrates (MoS$_2$, WS$_2$, WSe$_2$, MoTe$_2$) with scanning tunneling microscopy and spectroscopy and find that point and line defects intrinsic to all TMD crystals (both of natural and synthetic origin) result in scattering of electrons in graphene. Our findings suggest that the quality of graphene on TMD heterostructures is limited by the intrinsic crystalline quality of the TMDs.

12:15PM M1.00006 Tailoring the properties of two dimensional molybdenum disulfide. SAIFUL I. KHONDAKER, MUHAMMAD R. ISLAM, NARAE KANG, UDAI BHANU, HARI P. PAUDEL, MIKHAIL EREMENCHOUK, LAURENCE TETARD, MICHAEL N. LEUENBERGER, NanoScience Technology Center and Department of Physics, University of Central Florida — The ability to tailor the properties of a material is essential to optimize device functionality. In this talk, we will present evidence that the electrical and optical properties two-dimensional (2D) molybdenum disulfide (MoS$_2$) can be tuned by controlled exposure to plasma oxygen plasma. We find that the mobility, on-current and resistance of 2D MoS$_2$ FETs vary exponentially by up to four orders of magnitude with respect to the plasma exposure time. Photoluminescence (PL) study show a decrease of PL intensity leading a complete quenching. Raman studies show a significant decrease of intensity of MoS$_2$ peaks with the creation of new oxidation induced peak, while X-ray photoelectron spectroscopy (XPS) study show peaks associated with MoO$_3$ after plasma exposure. We suggest that during exposure to oxygen plasma, the energetic oxygen molecules interact with MoS$_2$ and create MoO$_3$ rich defected-regions, which are insulating. MoO$_3$ defected-regions act as a tunnel barrier for the injected conduction electrons, giving rise to the exponential increase in resistivity as a function of plasma exposure time. Bandstructure calculation shows that the PL quenching upon plasma exposure is due to the creation of MoO$_3$ defected-regions which causes a direct to indirect bandgap transition in monolayer MoS$_2$. This work is based on research supported by the National Science Foundation under Grant No. 0955625.
12:27PM M1.00007 Synthesis and Characterizations of Two-Dimensional Atomic Layers and Their Heterostructures, YI-HSIEN LEE, National Tsing Hua University — Monolayers of van der Waals (vdW) materials, including graphene, h-BN, and MoS$_2$, have been highlighted regarding both scientific and industrial aspects due to novel physical phenomenon inherited from the reduced dimensionality. Layered transition metal dichalcogenides (TMD) atomic layers, being considered as the thinnest semiconductor, exhibit great potential for advanced nanodevices. Monolayer in the class of offered a burgeoning field in fundamental physics, energy harvesting, electronics and optoelectronics. Recently, atomically thin heterostructures of TMD monolayer with various geometrical and energy band alignments are expected to be the key materials for next generation flexible optoelectronics. The individual TMD monolayers can be aligned vertically or laterally to construct diverse heterostructures which are difficult to reach with the laborious pick up-and-transfer method of the exfoliated flakes. The ability to produce copious amounts of high quality layered heterostructures on diverse surfaces is highly desirable but it has remained a challenging issue. Here, we have achieved a direct synthesis of various heterostructures of monolayer TMDs. The synthesis was performed using ambient-pressure CVD with aromatic molecules as seeding promoters. We discuss possible growth behaviors, and we examine the symmetry and the interface of these heterostructures using optical analysis and atomic-resolution scanning TEM. Our method offers a controllable synthesis of to obtain high-quality heterogeneous of TMD atomic layers with diverse interface geometry.


1:03PM M1.00008 Spatial Progression of Thermal Oxidation in Layered WSe$_2$ Nano-sheets, YINGNAN LIU, Department of Physics, University of Texas at Austin, CHENG TAN, Microelectronics Research Center, University of Texas at Austin, HARRY CHOU, Department of Mechanical Engineering, University of Texas at Austin, AVINASH NAYAK, Microelectronics Research Center, University of Texas at Austin, DI WU, Department of Physics, University of Texas at Austin, JONYEOK KIM, Microelectronics Research Center, University of Texas at Austin, RODNEY RUOFF, Department of Mechanical Engineering, University of Texas at Austin, KEJI AKINWANDE, Microelectronics Research Center, University of Texas at Austin, KEJI LAI, Department of Physics, University of Texas at Austin — Owing to the extremely different bonding strengths between intralayer covalent bonds and interlayer van der Waals interaction, many physical and chemical properties of layered transition metal dichalcogenides are expected to be highly anisotropic in nature. Using a number of compositional, structural, and electrical characterization tools, we have studied the spatial progression of the thermal oxidation of exfoliated WSe$_2$ nano-sheets, which primarily starts at the sample edges and propagates laterally towards the center. As revealed by microwave impedance microscopy and transport measurements, the partially oxidized regions show much higher conductivity than either the WSe$_2$ itself or the completely oxidized WO$_3$. The ability to electrically map out how chemical reactions are taking place in the nanoscale could be of particular importance for 2D materials that hold promise for future applications.


1:15PM M1.00009 Bulk Direct Band Gap MoS$_2$ by Plasma Induced Layer Decoupling, ROHAN DHALL, University of Southern California, MAHESH NEUPANE, DARSHANA WICKRAMARATNE, University of California-Riverside, MATTHEW MECKLENBURG, ZHEN LI, University of Southern California, CARLON MOORE, XEI SCIENTIFIC, ROGER LAKE, University of California-Riverside, STEPHEN CRONIN, University of Southern California — We report a robust method for engineering the optoelectronic properties of few layer MoS$_2$ using low energy oxygen plasma treatment. Gas phase treatment of MoS$_2$ by an upstream N$_2$-O$_2$ plasma is shown to enhance the photoluminescence (PL) of few layer MoS$_2$ flakes by up to 20 times, without reducing the layer thickness. A blue shift in the photoluminescence spectra and narrowing of linewidth is consistent with a transition of MoS$_2$ from indirect to direct band gap material. Atomic force microscope and Raman spectra reveal that the flake thickness actually increases as a result of the plasma treatment, indicating an increase in the interlayer separation in MoS$_2$. Ab-initio calculations reveal that the increased interlayer separation is sufficient to decouple the electronic states in individual layers, leading to a transition from an indirect to direct gap semiconductor. With optimized plasma treatment parameters, we observed enhanced PL signals for 32 out of 35 few layer MoS$_2$ flakes tested, indicating this method is robust and scalable. Monolayer MoS$_2$, while direct band gap, has a small optical density, which limits its potential use in practical devices. The results presented here provide a material with the direct band gap of monolayer MoS$_2$, without reducing sample thickness, and hence optical density.


1:27PM M1.00010 High-Throughput Screening of Substrates for Synthesis of Two-Dimensional Materials, ARUNIMA K. SINGH, NIST - Natl Inst of Stds & Tech, HOULONG L. ZHUANG, Oak Ridge National Laboratory, FRANCESCA TAVAZZA, NIST - Natl Inst of Stds & Tech, RICHARD G. HENNIG, University of Florida, Cornel University — Since the discovery of graphene, several two-dimensional (2D) materials have been synthesized experimentally, but many theoretically predicted 2D materials are yet to be synthesized. Common synthesis techniques such as chemical-vapor deposition and molecular-beam epitaxy require suitable substrates. We are developing a strategy to enable high-throughput searches for suitable substrates for 2D materials by automatically identifying suitable substrate candidates and characterize their stabilizing properties and doping effects using density-functional theory. As first steps, we have found that several transition-metal, rare-earth-metal, and refractory-diboride substrates sufficiently reduce the formation energies of 2D group-III-V materials, making them thermodynamically stable on these substrates [1,2]. Additionally, these substrates lead to variable amount of doping of the 2D materials depending on the work functions of the 2D materials and the substrates. We observe large adsorption energies and strong doping of the 2D materials which indicates that these substrates can provide good electrical contact to enable transport measurements and electronic applications.


1:39PM M1.00011 Direct patterning and characterization of large area, single layer MoS$_2$ film synthesized by chemical vapor deposition, WOANSEO PARK, Seoul Natl Univ, JAEEYOUN BAIK, Pohang Accelerator Laboratory, TAE-YOUNG KIM, KYUNGJUNE CHO, Seoul Natl Univ, WOONG-KI HONG, Korea Basic Science Institute, HYUN-JOON SHIN, Pohang Accelerator Laboratory, TAKHEE LEE, Seoul Natl Univ — Molybdenum disulfide (MoS$_2$) has gained a significant amount of attention due to a great potential for atomic-film electronics. Recently chemical vapor deposition (CVD) method has been utilized to synthesize MoS$_2$ films, however, the synthesis of large area MoS$_2$ films still remains a challenge for practical device development. For the further utilization, existing synthetic approaches that can be used to fabricate large-area MoS$_2$ films require additional patterning processes, which may introduce unintentional contamination from other chemicals during the various processes. Therefore, it is required to directly prepare patterned, MoS$_2$ films during the CVD synthesis. In this presentation, we report a simple method for the synthesis of MoS$_2$ films that can be directly patterned during the synthesis, so that post-patterning processes can be avoided and device fabrication can be made simultaneously. This study suggests that large-area, single-layer MoS$_2$ films can be synthesized by CVD and directly patterned for atomic-film electronic devices.
1:15PM M1.00012 Chemical Exfoliation of Layered Superconductors: An Avenue to Synthesize Boron-rich Quasi Two Dimensional Nanostructures, SAROJ KUMAR DAS, ASHA LIZA JAMES, KABEER JASUJA, Indian Institute of Technology Gandhinagar — Zero-dimensional and one-dimensional boron based nanostructures have presented excellent avenues in the past for utilizing the fascinating science of boron at the atomic level. The research on synthesizing two-dimensional (2-D) boron-based nanostructures is currently in its incipient stages. In this talk, we demonstrate two chemical approaches that yield quasi 2-D boron-rich nanostructures by enabling an exfoliation of a layered boron-based superconductor. While one approach employs the simple tool of ultrasonication in an aqueous phase, the other approach utilizes a chelation mediated strategy based on coordination of metal ions and organic ligands. Both these synthetic routes are shown to result in a processable colloidal dispersion of boron-rich nanostructures. This talk will present details of the two exfoliation approaches and a comprehensive study of the morphological, chemical and optical properties of the dispersed nanosheets. We will demonstrate that the exfoliated nanosheets undergo an in-situ chemical modification with ionizable functional groups derived from solvent that enable electrostatic stabilization. We will further shown that this functionalization modifies the band structure of the nanosheets which gives rise to photoluminescence and result in physico-chemical properties distinct from the parent superconductor. This ability to synthesize quasi 2-D boron rich nanostructures significantly adds to the current state of literature on boron-based quasi-planar nanostructures.

2:03PM M1.00013 The formation of Colloidal 2D/3D MoS2 Nanostructures in Organic Liquid Environment1, ENGIN DURGUN, H. SENER SEN, TUGBA OZTAS, BULEND ORTAC, Bilkent University - UNAM — 2D MoS2 nanosheets (2D MoS2 NS) and fullerene-like MoS2 nanostructures (3D MoS2 NS) with varying sizes are synthesized by nanosecond laser ablation of hexagonal crystalline 2H-MoS2 powder in methanol. Structural, chemical, and optical properties of MoS2 NS are characterized by optical microscopy, SEM, TEM, XRD, Raman and UV/VIS/NIR absorption spectroscopy techniques. Results of structural analysis show that the obtained MoS2 NS mainly present layered morphology from micron to nanometer scale. Detailed analysis of the product also proves the existence of inorganic polyhedral fullerene-like 3D MoS2 NS generated by pulsed laser ablation in methanol. The possible factors which may lead to formation of both 2D and 3D MoS2 NS in methanol are examined by ab initio calculations and shown that it is correlated with vacancy formation. The hexagonal crystalline structure of MoS2 NS was determined by XRD analysis. The colloidal MoS2 NS solution presents broadband absorption edge tailoring from UV region to NIR region. Investigations of MoS2 NS show that the one step physical process of pulsed laser ablation-bulk MoS2 powder interaction in organic solution opens doors to the formation of “two scales” micron- and nanometer-sized layered and fullerene-like morphology MoS2 structures.

3This work was partially supported by TUBITAK under the Project No. 113T050 and Bilim Akademisi - The Science Academy, Turkey under the BAGEP program.


11:15AM M2.00001 Ultrafast generation of pseudo-magnetic field for valley excitons in WSe2 monolayers, JONGHWAN KIM, XIAOPING HONG, CHENHAO JIN, SU-FEI SHI, Univ of California - Berkeley, CHIH-YUAN S. CHANG, Academia Sinica, MING-HUI CHIU, LAIN-JONG LI, King Abdullah University of Science, FENG WANG, Univ of California - Berkeley — The valley pseudospin emerges as a new degree of freedom in atomically thin two-dimensional transition metal dichalcogenides (MX2). In analogy to the control of spin in spintrons, the capability to manipulate the valley pseudospin can provide exciting opportunities in valleytronics. Here we present that femtosecond pulses with circular polarization can generate ultrafast and ultrahigh valley pseudomagnetic field in a monolayer MX2. Our polarization-resolved transient absorption measurement shows that the degeneracy of valley exciton transitions at K and K’ valley in WSe2 monolayers can be lifted by optical Stark effect from the non-resonant pump. Energy splitting due to the optical Stark effect is linear with both the pump intensity and the inverse of pump detuning. We observe that valley-selective optical Stark effect can create an energy splitting more than 10 meV which corresponds to a pseudomagnetic field over 60 Tesla. Our study demonstrates efficient and ultrafast control of the valley excitons with optical light which can open up the possibility of coherent manipulation of the valley polarization in MX2.

11:27AM M2.00002 Valley splitting and polarization by the Zeeman effect in monolayer MoSe2, YEILE LI, Columbia Univ, JONATHAN LUDWIG, National High Magnetic Field Lab, TONY LOW, ALEXEY CHERKIKOV, XU CUI, GHIDEWON AREFE, YOUNG DUCK KIM, AREND VAN DER ZANDE, ALBERT RIGOSI, HEATHER HILL, SUK HYUN KIM, JAMES HONE, Columbia Univ, ZHIQIANG LI, DMITRY SMIRNOV, National High Magnetic Field Lab, TONY HEINZ, Columbia Univ — We have measured circularly polarized photoluminescence in monolayer MoSe2 under perpendicular magnetic fields up to 10 T. At low doping densities, the neutral and charged excitons shift linearly with field strength at a rate of $\pm 0.12$ meV/T for emission arising, respectively, from the K and K’ valleys. The opposite sign for emission from different valleys demonstrates lifting of the valley degeneracy. The magnitude of the Zeeman shift agrees with predicted magnetic moments for carriers in the conduction and valence bands. The relative intensity of neutral and charged exciton emission is modified by the magnetic field, reflecting the creation of field-induced valley polarization. At high doping levels, the Zeeman shift of the charged exciton increases to $\pm 0.18$ meV/T. This enhancement is attributed to many-body effects on the binding energy of the charged excitons.

11:39AM M2.00003 Nonlinear Optical and Excitonic Effects in Two-Dimensional Transition Metal Dichalcogenides, WANG-KONG TSE, Los Alamos National Laboratory — We present a theory for coherent optics in two-dimensional transition metal dichalcogenides. Using the density matrix formalism, we derive the kinetic equations for the interband polarization and band population distributions, and study the regime of strong optical fields where Coulomb interaction effects are small and the regime of weak optical fields where excitonic effects are important. In particular, the influence of the optical Stark effect on the excitonic properties is studied within our theory. We also address the excitonic effects of Coulomb interaction on the optical conductivity and compare our results with that of graphene.

11:51AM M2.00004 Direct observation of spin-valley-layer locking in centrosymmetric bulk WSe2 by spin- and angle-resolved photoemission, PHIL KING, School of Physics and Astronomy, University of St Andrews, UK — Methods to generate spin-polarized electronic states in non-magnetic solids are strongly desired to enable all-electrical manipulation of electron spins for new quantum devices. This is generally accepted to require breaking global structural inversion symmetry. In contrast, I will report our observation from spin- and angle-resolved photoemission spectroscopy of spin-polarized bulk states in the centrosymmetric transition-metal dichalcogenide 2H-WSe2 [1]. Mediated by a lack of inversion symmetry in constituent Se-W-Se monolayers of the bulk crystal where the electronic states are localized, we show how enormous spin splittings up to $\approx 0.5$ eV result, with a spin texture that is strongly modulated in both real and momentum space. Through this, our study provides direct experimental evidence for a putative locking of the spin with the layer and valley pseudospins in transition-metal dichalcogenides, of key importance for using these compounds in proposed valleytronics devices.

12:27PM M2.00005 Topological induced valley polarization in bilayer graphene/Boron Nitride

LEONARDO BASILE, Escuela Politecnica Nacional, JUAN C IDROBO, Oak Ridge National Laboratory — Novel electronic devices relay in our ability to control internal quantum degrees of freedom of the electron e.g., its spin. The valley number degree of freedom is a pseudospin that labels degenerate eigenstates at local maximum/minimum on the valence/conduction band. Valley polarization, that is, selective electronic localization in a momentum valley and its manipulation can be achieved by means of circular polarized light (CPL) in a system with strong spin-orbit coupling (SOC). In this talk, we will show theoretically that the fact that neither graphene nor BN have a strong SOC, a bilayer of graphene on BN oriented at a twist angle has different absorption for right- and left- CPL. This induced polarization occurs due to band folding of the electronic bands, i.e., it has a topological origin.

This research was supported EPN multidisciplinary grant and by DOE SUFD MSED

12:39PM M2.00006 Anomalous temperature dependence of charged exciton photoluminescence polarization in monolayer WSe$_2$

A.T. HANBICKI, Naval Research Laboratory, G. KIOSEOGLOU, University of Crete, M. CURRIE, C.S. HELBERG, A.L. FRIEDMAN, K.M. MCCREARY, B.T. JONKER, Naval Research Laboratory — Monolayer WSe$_2$ is a direct-gap transition metal dichalcogenide semiconductor. Its low-dimensional hexagonal structure leads to two inequivalent K-points in the Brillouin zone. The valley index and spin are intrinsically coupled with spin-dependent selection rules that enable populating and interrogating each valley using circularly polarized light. Here, we probe the degree of circular polarization of the emitted photoluminescence (PL) as function of the photo-excitation energy and temperature to elucidate spin-dependent inter- and intra-valley relaxation mechanisms. Monolayer WSe$_2$ flakes have PL emission from the free and charged exciton near 2.0 eV. We reproductively isolate these excitons via appropriate sample preparation. With excitation using positive helicity light, we analyze the PL for positive and negative helicities to determine polarization. Unlike MoS$_2$, we measure significant polarization from the charged exciton for high excitation energies, even at room temperature. There is also an enhancement of polarization of the charged exciton at intermediate temperatures. We discuss the polarization behavior in terms of phonon assisted intervalley scattering processes.

1This work was supported by internal programs at NRL and the NRL Nanoscience Institute.


12:51PM M2.00007 First-Principles Calculations of LEEM Reflectivity Spectra of Molybdenum Disulfide

JOHN MCCLAIN, Integrated Applied Mathematics, University of New Hampshire, KARSTEN POHL, Department of Physics and Materials Science Program, University of New Hampshire, JIAN-MING TANG, Department of Physics, University of New Hampshire — We present calculations of the low-energy electron specular reflectivity spectra of systems of a few layers of molybdenum disulfide at general angles of incidence using a newly modified algorithm within our first-principles theoretical approach, which leverages the self-consistent scattering potentials produced by density-functional theory [1]. Our calculated normal-incidence spectra for MoS$_2$ reveal layer-dependent features around 7-8 eV and 15 eV, allowing for a characterization of the number of layers via LEEM reflectivity and thus an in-situ technique for growth monitoring. We have previously described the application of our approach to the off-normal spectra of few-layer graphene, but the lack of mirror symmetry in MoS$_2$ requires a new algorithm for finding degenerate pairs of solutions for the matching procedure. The computed off-normal spectra illustrates the complexity of the electronic structure of MoS$_2$. We also present the way in which our new off-normal algorithm leads naturally to an approach to higher-order diffraction intensity calculations with the wave-matching scheme, along with our results for higher-order diffraction in model systems and progress towards results for real systems. [1] McClain et al., arXiv.1311.2917.

This work is partly supported by a University of New Hampshire Dissertation Year Fellowship.

1:03PM M2.00008 Spin-orbit coupling in the band structure WSe$_2$ monolayers

IORI TANABE, Univ of Nebraska - Lincoln, Dept. of Physics and Astronomy, ALEXEI BARINOV, Elettra Experimental Division, Sincrotrone Trieste, DUY LE, University of Central Florida, EDWIN PRECIADO, MIGUEL ISARRARAZ, LUDWIG BARTELS, University of California Riverside, Department of Chemistry, TALAT RAHMAN, University of Central Florida, Dept. of Physics, PETER DOWBEN, Univ of Nebraska - Lincoln, Dept. of Physics and Astronomy — We have mapped the occupied band structure of monolayer WSe$_2$ by small spatial spot angle resolved photoemission and have found significant spin-orbit coupling in excess of 500 meV, far larger than for MoS$_2$. The experimental band mapping is consistent with theoretical expectations with the top of the valence band is seen at K, not Γ, thus distinct from the band structure for the bilayer and bulk single crystals. This shift of the top of the valence band in monolayer WSe$_2$, from Γ to K, is also predicted in density functional theory. In general the wave vector dependent experimental band structure confirms the expectations of density functional theory.

1:15PM M2.00009 Intrinsic circular polarization in centrosymmetric stacks of transition-metal dichalcogenide

QIHANG LIU, XIUWEN ZHANG, ALEX ZUNGER, University of Colorado, Boulder — The circular polarization (CP) that the photoluminescence inherits from the excitation source in n monolayers of transition-metal dichalcogenides (MX)$_n$ has been previously explained as a special feature of odd values of n, where the inversion symmetry is absent. This valley polarization effect results from the fact that in the absence of inversion, charge carriers in different band valleys could be selectively excited by different circular polarized light. Such restriction to non-centrosymmetric systems poses a limitation on the material selection for achieving CP. Although several experiments observed CP in centrosymmetric MX$_2$ systems e.g., for bilayer in MX$_2$, they were dismissed as being due to some extrinsic sample irregularities. Here we show that for n = even where inversion symmetry is present and valley polarization physics is strictly absent, such intrinsic selectivity in CP is to be expected on the basis of fundamental spin-orbit physics. First-principles calculations of CP predict significant polarization for n = 2 bilayers: from 69% in MoS$_2$ to 93% in WSe$_2$. This realization could broaden the range of materials to be considered as CP sources.

This work was supported by National Science Foundation (Grant No. DMREF-13-34170).

1:27PM M2.00010 Electric field and spin-orbit coupling effects on the band structure of monolayer WSe$_2$

TTITPONG FONGKAEW, School of Physics, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand, WALTER R.L. LAMBRECHT, Department of Physics, Case Western Reserve University, Cleveland, OH, USA 44106 — Transition metal dichalcogenides are known to switch from indirect to direct gap between bulk and monolayer form. Here we show that in WSe$_2$, an electric field perpendicular to the layer of order a few 0.1 MV/cm has strong effects on the conduction band and can convert the material back to an indirect gap. The competing minima at different points in the Brillouin zone undergo different shifts with electric field because of their different orbital character. Using first-principles GGA calculations in the presence of an electric field with and without spin-orbit coupling, we determine the critical field at which the minimum between Γ and K (where the gap occurs in bulk) becomes back the lowest conduction band minimum. For even stronger electric fields we find the CBM to shift to the Γ-point. While the electric fields considered here are much larger than the fields obtained in gated structures, they may be possible using electric double layers using an electrolyte. Such measurements have already been done on bulk WSe$_2$, [Nature Physics 9, 563 (2013)] but focused on the valence band and Rashba effects instead of the conduction band.

This work was supported by Development and Promotion of Science and Technology Talents Project (DPST).
1:39PM M2.00011 Spin-dependent refraction at the atomic step of transition-metal dichalcogenides. MIKITO KOSHINO, TETSURO HABE, Tohoku Univ. — We theoretically propose a spin-dependent electronic transport mechanism in the transition metal dichalcogenide, in which the spin-opposed electron beam is split into different directions depending on spins at an atomic domain boundary. Specifically, we calculate the electronic transmission across a boundary between monolayer and bilayer of the transition metal dichalcogenide, and demonstrate that up-spin and down-spin electrons entering the boundary are refracted and collimated to opposite directions. The phenomenon is attributed to the strong spin-orbit interaction, the trigonally-warped Fermi surface, and the different crystal symmetries between the monolayer and bilayer systems. The spin-dependent refraction suggests a potential application for a spin splitter, which spatially separates up-spin and down-spin electrons simply by passing the electric current through the boundary.

1:51PM M2.00012 Two dimensional valley electrons and excitons in the noncentrosymmetric 3R MoS2. RYOSUKE AKASHI1, MASAYUKI OCHI, Riken Center for Emergent Matter Science, Japan, SANDOR BORDACS, Budapest University of Technology and Economics, Hungary, RYUJI SUZUKI, The University of Tokyo, Japan, YOSHINORI TOKURA, Riken Center for Emergent Matter Science, Japan, YOSHIHIO IWA, The University of Tokyo, Japan, RYOTARO ARITA, Riken Center for Emergent Matter Science, Japan — Possible control of the valley-dependent spin polarization in transition-metal dichalcogenides has been a hot topic as the valleytronics. Through the recent great progress based on the monolayer systems, people’s interest is shifting to multilayered polytypes. The centrosymmetric 2H-stacked systems have been much studied for switching of the valley-dependent spin polarization. On the other hand, some of the authors [Suzuki et al., Nat. Nanotechnol. 9, 611 (2014)] have successfully fabricated the noncentrosymmetric 3R-stacked MoS2 multilayer and demonstrated the valley polarization independent of the number of layers. On the basis of this success, we further examined the valley electronic states in the 3R-MoS2 and found their novel two-dimensional properties utilizable for the valleytronics [Akashi et al., submitted]. Namely, interlayer hopping of the valley electrons was proved to be zero as a consequence of a quantum-interference effect caused by the 3R-stacking geometry. In the talk, we report the results of the reflectivity measurement and analysis with an anisotropic hydrogen atomic model and show that the zero hopping causes 2D-hydrogen-like spectroscopic and confinement of the wave function within a single layer of the valley exciton.

2:03PM M2.00013 Electrical Control of Exciton-Enhanced Second-Harmonic Generation in Monolayer WSe2. KYLE SEYLER, JOHN SCHAIBLEY, University of Washington, RUI GONG, University of Hong Kong, PASQUAL RIVERA, AARON JONES, SANFENG WU, University of Washington, JIAQIANG YAN, DAVID MANDRUS, Oak Ridge National Laboratory, WANG YAO, University of Hong Kong, XIAODONG XU, University of Washington — Nonlinear optical frequency conversion, in which optical fields interact with a nonlinear medium to produce new field frequencies, is ubiquitous in modern photonic systems. However, the nonlinear electric susceptibilities that give rise to such phenomena are often challenging to tune in a given material, and so far, dynamical control of optical nonlinearities remains confined to research labs. In this talk, we report a new mechanism to electrically control second-order optical nonlinearities in monolayer WSe2. We show that the intensity of second-harmonic generation (SHG) at its lowest exciton resonance is widely tunable through electrostatic doping in a field-effect transistor device. Such remarkable tunability arises from the strong exciton charging effects in monolayer semiconductors, which allow for exceptional control over the exciton and trion oscillator strengths. Our study paves the way for a new platform of chip-scale, electrically tunable nonlinear optical devices based on two-dimensional semiconductors.


11:15AM M3.00001 The Future of (Artificial) Intelligence. STUART RUSSELL, Professor of Computer Science, University of California, Berkeley — No abstract available.

11:51AM M3.00002 Cognitive Computing: From Breakthroughs in the Lab to Applications in the Field. GURUDUTH BANAVAR, IBM TJ Watson Research Center — In the last decade, the availability of massive amounts of new data, and the development of new machine learning technologies, have augmented reasoning systems to give rise to a new class of computing systems. These “Cognitive Systems” learn from data, reason from models, and interact naturally with us, to perform complex tasks better than either humans or machines can do by themselves. In essence, cognitive systems help us penetrate the complexity of big data, reason using rich models, and enable each of us to perform like the best. We believe this will transform every industry for the better. Artificial Intelligence (AI) has a rich history, dating back to 1950’s. The desire to build a Turing machine that would imitate a human dominated the psyche of the AI researchers for many decades [1]. The complex reality of human beings and the limitations of early symbolic approaches narrowed the success of early AI technology to a few specialized and small-scale applications [2, 3]. Over the last decade, new kinds of unstructured data from social networks, streaming data, and online publications, as well as massive data emitted from sensors from the physical world have outpaced traditional forms of structured data. This will continue to grow exponentially. The insights embedded in this massive amount of data can provide unprecedented opportunities for business and social value. Data has indeed become one of our most precious resources, and with its accelerated pace of evolution, it will determine the future trajectory of business and society [4]. New tools are being developed to extract insights out of the big data, which is abundant, unstructured, noisy, and unreliable. These tools have not relied on the same techniques that helped us exploit clean, structured data of the past, using small-scale models of the world and explicitly specified reasoning mechanisms. The new tools are using more automated statistical pattern-matching techniques, called machine learning, that have come of age in the last decade [ref]. In addition to reasoning from explicitly specified models of the world, these new machine learning techniques have given rise to a new class of systems that effectively learn from patterns in big data, and simultaneously augment their world models. Such systems can also interact naturally with us, on human terms, through natural language (i.e., unstructured text data), speech (i.e., unstructured audio data), vision (i.e., unstructured video data), and other modalities. We call this emerging class of systems that reason, learn, and interact naturally with us “Cognitive Systems”. IBM’s Watson is a family of cognitive systems targeted to a variety of domains. The first Watson system was capable of answering factoid questions as effectively as the best professionals in that field (as demonstrated by the Jeopardy! exhibition match, see illustration). Follow-on systems answer other types of questions, e.g., those that require passage answers, as well as other domains, e.g., healthcare, insurance, and education. Yet other cognitive systems in the Watson family go beyond question answering to support discovery of insights hidden in big data, such as in huge repositories of scientific literature, reasoning with evidence to support or refute topics of discussion, and to go beyond textual data to images and videos.

1:03PM M3.00004 Beneficial Smarter-than-human Intelligence: the Challenges and the Path Forward. BENJA FALLENSTEIN, Machine Intelligence Research Institute — Today, human-level machine intelligence is still in the domain of futurism, but there is every reason to expect that it will be developed eventually. A generally intelligent agent as smart or smarter than a human, and capable of improving itself further, would be a system we’d need to design for safety from the ground up: There is no reason to think that such an agent would be driven by human motivations like a lust for power; but almost any goals will be easier to meet with access to more resources, suggesting that most goals an agent might pursue, if they don’t explicitly include human welfare, would likely put its interests at odds with ours, by incentivizing it to try to acquire the physical resources currently being used by humanity. Moreover, since we might try to prevent this, such an agent would have an incentive to deceive its human operators about its true intentions, and to resist interventions to modify it to make it more aligned with humanity’s interests, making it difficult to test and debug its behavior. This suggests that in order to create a beneficial smarter-than-human agent, we will need to face three formidable challenges: How can we formally specify goals that are in fact beneficial? How can we create an agent that will reliably pursue the goals that we give it? And how can we ensure that this agent will not try to prevent us from modifying it if we find mistakes in its initial version? In order to become confident that such an agent behaves as intended, we will not only want to have a practical implementation that seems to meet these challenges, but to have a solid theoretical understanding of why it does so. In this talk, I will argue that even though human-level machine intelligence does not exist yet, there are foundational technical research questions in this area which we can and should begin to work on today. For example, probability theory provides a principled framework for representing uncertainty about the physical environment. It seems certain to be helpful to future work on beneficial smarter-than-human agents, but standard probability theory assumes omniscience about logical facts; no principled framework for representing uncertainty about the outputs of deterministic computations exists as yet, even though any smarter-than-human agent will certainly need to deal with uncertainty of this type. I will discuss this and other examples of ongoing foundational work.

Wednesday, March 4, 2015 11:15AM - 1:51PM
Session M5 DMP DCOMP: Focus Session: Intercalated FeSe and Other Fe-chalcogenide Superconductors
Juan Gorman Room 005 - Stephen Wilson, University of California, Santa Barbara

11:15AM M5.00001 High transition temperatures in molecular intercalates of FeSe$^1$. STEPHEN BLUNDELL, University of Oxford — Molecular groups can now be intercalated into iron-based superconductors with dramatic consequences on the superconducting properties. These species act as charge reservoirs, sources of electrical polarization, and also make subtle structural modifications to superconducting layers, all of which can make novel adjustments to the band structure that in turn can control superconducting properties. By synthesizing the compound $\text{Li}(\text{NH}_2)\text{y}(\text{NH}_3)_{1−y}\text{Fe}_2\text{Se}_2$ ($x \approx 0.6; y \approx 0.2$), in which lithium ions, lithium amide and ammonia (NH$_3$) act as the spacer layer between FeSe layers, we have turned a 9 K superconductor into a 43 K superconductor [1]. Further chemical modification allow us to produce a range of new superconducting materials which we have studied using a variety of techniques including muon-spin rotation. Recently, we have used hydrothermal reactions to produce layered lithium iron selenide hydroxides with chemical formula $\text{Li}_x\text{Fe}_y(\text{OH})\text{Fe}_{1−y}\text{Se}$ and thereby producing compounds whose transition temperature can be tuned from zero up to about 40 K [2]. Minimizing the concentration of iron vacancies in the iron selenide layer and simultaneously increasing the electron count on iron in the selenide layers enhance the superconducting properties in this family. Future prospects for new superconducting materials using these novel synthetic routes will be discussed, as will also our current understanding of the superconductivity in these materials. (Work performed in collaboration with S. J. Clarke and coworkers at Oxford, RAL and Durham, UK.)

2H. Sun et al. arXiv:1408.4350

1Work supported by EPSRC(UK).

11:51AM M5.00002 Unified picture of the doping dependence of superconducting transition temperatures in alkali metal/ammonia intercalated FeSe$^1$. DANIEL GUTERDING, HARALD JESCHKE, Institute for Theoretical Physics, University of Frankfurt, Frankfurt a.M., Germany, PETER HIRSCHFELD, Department of Physics, University of Florida, Gainesville, FL, ROSEN VALENTI, Institute for Theoretical Physics, University of Frankfurt, Frankfurt a.M., Germany — We present a theoretical investigation of alkali metal/ammonia intercalated FeSe$^1$. Using ab-initio density functional theory we unravel how charge doping and dimensionality of the electronic structure can be controlled through the chemical composition of the intercalated molecules. Within random phase approximation spin fluctuation theory we analyze the impact of intercalation on the superconducting pairing strength. We find that high $T_c$, does not exceed 40 K in the iron selenide layer and simultaneously increasing the electron count on iron in the selenide layers enhance the superconducting properties in this family. Future prospects for new superconducting materials using these novel synthetic routes will be discussed, as will also our current understanding of the superconductivity in these materials. (Work performed in collaboration with S. J. Clarke and coworkers at Oxford, RAL and Durham, UK.)


12:03PM M5.00003 Neutron scattering studies on semiconductor Rb$_8$Fe$_{1.5}$Se$_2$. MENG WANG, PATRICK VALDIVIA, ROBERT BIRGENEAU, University of California, Berkeley, WEI TIAN, SONQUXE CHI, Oak Ridge National Laboratory, PENGCHENG DAI, Rice University, EDITH BOURRET-COURCHESNE, Lawrence Berkeley National Laboratory — We report neutron scattering and transport measurements on semiconductor Rb$_8$Fe$_{1.5}$Se$_2$, a compound isostuctural and isoelectronic to the well-studied A$_4$Fe$_2$Se$_4$($A =$ K, Rb, Cs, TI/K) superconducting systems. Both resistivity and dc susceptibility measurements reveal a magnetic phase transition at $T_c = 275$ K. Neutron diffraction studies show that the 275 K transition originates from a phase with rhombohedral iron vacancy order which exhibits an in-plane stripe antiferromagnetic ordering below 275 K. Based on the close similarities of the in-plane antiferromagnetic structures, moments sizes, and ordering temperatures in semiconducting Rb$_8$Fe$_{1.5}$Se$_2$ and K$_8$Fe$_{1.5}$Se$_2$ we argue that the in-plane antiferromagnetic order arises from strong coupling between local moments. The spin waves of the stripe AF order will also be presented.

12:15PM M5.00004 Block magnetic excitations in the orbitally-selective Mott insulator BaFe$_2$Se$_3$. M. MOURIGAL, Johns Hopkins University and Georgia Institute of Technology, SHAN WU, Johns Hopkins University, M.B. STONE, Oak Ridge National Laboratory, J.R. NEILSON, Johns Hopkins University and Colorado State University, J.M. CARON, Johns Hopkins University and Cornell University, T.M. MCQUEEN, Johns Hopkins University, C.L. BROHOLM, Johns Hopkins University and Oak Ridge National Laboratory — We investigate the spectrum of magnetic excitations in the Fe-based two-leg ladder material BaFe$_2$Se$_3$ by means of broad-band inelastic neutron scattering. BaFe$_2$Se$_3$ garnered recent attention due to its quasi-1D structure and as hosting an exotic block magnetic ground-state where 4 Fe spins co-align to form Fe$_4$ plaquettes. Our neutron results provide a detailed understanding of magnetic excitations originating from the Fe$_4$ block ground-state. Consisting of a 50 meV wide band of quasi-1D acoustic spin-waves and three high-energy modes around 100 meV and 200 meV, the spin fluctuations and the static moment carry a total squared magnetic moment of 16 $\mu_B$ per Fe, indicative of orbital selectiveness for localized spins. We develop an effective Heisenberg model that accounts for the observed spectrum and provides a set of exchange interactions to understand how magnetic magnetism stems from strong lattice, orbital and electronic correlations in iron chalcogenides.
12:27PM M5.00005 Neutron investigation of possible (ferro)magnetic order in the new superconductor \( \text{Li}_{1-x}\text{Fe}_x\text{OD} \) \((\text{Fe}_{1-y}\text{Se})\). JEFFREY LYNN, NIST Center for Neutron Research, Gaithersburg, MD 20899, XIUQUAN ZHOU, CHRISTOPHER K. H. BORG, EFRAIN RODRIGUEZ, Department of Chemistry and Biochemistry, University of Maryland 20742 — The system \( \text{Li}_{1-x}\text{Fe}_x\text{OD} \) \((\text{Fe}_{1-y}\text{Se})\) has recently been reported to become superconducting at \( T_c \approx 43 \) K and then developing ferromagnetism in terms of a spontaneous vortex lattice below \( T_{\text{f}} \approx 10 \) K [1]. We have prepared the tetragonal \((\text{Li}_{1-x}\text{Fe}_x\text{OD})\) \((\text{Fe}_{1-y}\text{Se})\) phase by hydrothermal synthesis in \( \text{D}_2\text{O} \) to reduce the neutron incoherent scattering cross section. We also prepared the samples using isotopically purified \( ^7\text{LiOD} \) as a starting material to reduce the neutron adsorption cross section. The lattice parameters according to neutron and X-ray diffraction varied with 3.79 \( \pm 0.02 \) \( \text{Å} \) for the neutron incoherent scattering cross section. The lattice parameters according to neutron and X-ray diffraction varied with 3.79 \( \pm 0.02 \) \( \text{Å} \) and 9.16 \( \pm 0.02 \) \( \text{Å} \) for the neutron incoherent scattering cross section. We have also prepared the samples using isotopically purified \( ^7\text{LiOD} \) as a starting material to reduce the neutron adsorption cross section. The lattice parameters according to neutron and X-ray diffraction varied with 3.79 \( \pm 0.02 \) \( \text{Å} \) and 9.16 \( \pm 0.02 \) \( \text{Å} \). We have carried out bulk magnetization, high resolution powder diffraction measurements to determine the crystal structure, high intensity diffraction measurements for the magnetic structure, and small angle scattering measurements to elucidate the interaction between the magnetism and superconductivity. The results of the neutron and bulk measurements will be discussed in detail.

12:39PM M5.00006 Multiband transport and nonmetallic low-temperature state of \( \text{K}_{0.50}\text{Na}_{0.25}\text{Fe}_{1.52}\text{Se}_2 \). HYEJIN RYU, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA, F. WOLFF-FABRIS, Hochfeld-Magnetlab Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany, J.B. WARREN, Instrument Division, Brookhaven National Laboratory, Upton, New York 11973, USA, M. UHLARZ, J. WOSNITZA, Hochfeld-Magnetlab Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany, C. PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA — We report evidence for multiband transport and an insulating low-temperature normal state in superconducting \( \text{K}_{0.50}\text{Na}_{0.25}\text{Fe}_{1.52}\text{Se}_2 \) with \( T_c \approx 20 \) K. The temperature-dependent upper critical field \( H_{\text{c2}} \) is well described by a two-band model. After the superconductivity is suppressed by applying magnetic field at low temperature, the normal-state resistance is found to increase logarithmically as \( T \to 0 \). This indicates that high-\( T_c \) copper oxides and granular superconductors, suggesting that the superconductor-insulator transition is related to intrinsic nanoscale phase separation. Work at Brookhaven is supported by the U.S. DOE under Contract No. DE-AC02-98CH10886 and in part by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. DOE, Office for Basic Energy Science (C.P.). We acknowledge the support of the HLD at HZDR, member of the European Magnet Field Laboratory (EMFL). C.P. acknowledges support by the Alexander von Humboldt Foundation.

12:51PM M5.00007 First-principles theory of electron-spin fluctuation coupling and superconducting instabilities in iron selenide1. JOHANNES LISCHNER, UC Berkeley and Lawrence Berkeley National Lab, TIMUR BAZHIROV, UC Berkeley, ALLAN H. MACDONALD, UT Austin, MARVIN L. COHEN, STEVEN G. LOUIE, UC Berkeley and Lawrence Berkeley National Lab — We present first-principles calculations of the coupling of quasiparticles to spin fluctuations in iron selenide and discuss which types of superconducting instabilities this coupling gives rise to. We find that strong antiferromagnetic stripe-phase spin fluctuations lead to large coupling constants for superconducting gaps with \( \pi \) symmetry, but these coupling constants are significantly reduced by other spin fluctuations with small wave vectors. An accurate description of this competition and an inclusion of band structure and Stoner parameter renormalization effects lead to a value of the coupling constant for an \( s \) wave superconductor. This is similar as for high-\( T_c \) copper oxides and granular superconductors, suggesting that the superconductor-insulator transition is related to intrinsic nanoscale phase separation.

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1 This work was supported by NSF Grant No. DMR10-1066184 and by DOE under Contract No. DE-AC02-98CH11231. Computational resources have been provided by the DOE at NERSC.

1:03PM M5.00008 “Forbidden” phonon in the iron chalcogenide series1. DAVID M. FOBES, IGOR A. ZALIZNYAK, ZHIJUN XU, GENDA GU, JOHN M. TRANQUADA, CMPMSD, Brookhaven National Lab, Upton, NY 11793-5000, USA — Recently, we uncovered evidence for the formation of a bond-order wave (BOW) leading to ferro-ordinal order at low temperature, acting to stabilize the bccillinear AFM order, in the iron-rich parent compound, \( \text{Fe}_{1+y}\text{Te}\). [D. Fobes et al., Phys. Rev. Lett. 112, 187202 (2014)]. Investigating the inelastic spectra centered near (100) in \( \text{Fe}_{1+y}\text{Te}\), a signature peak for the BOW formation in the monoclinic phase, we observed an acoustic phonon dispersion in both tetragonal and monoclinic phases. While a structural Bragg peak accompanies the mode in the monoclinic phase, in the tetragonal phase Bragg scattering at this \( Q \) is forbidden by symmetry, and we observed no elastic peak. This phonon mode was also observed in superconducting \( \text{Fe}_{60}\text{Se}_{40} \), where structural and magnetic transitions are suppressed. LDA frozen phonon calculations suggested that this mode could result from a spin imbalance between neighboring Fe atoms, but polarized neutron measurements revealed no additional magnetic scattering. We propose that this “forbidden” phonon mode may originate from dynamically broken symmetry, perhaps related to the strong dynamic spin correlations in these materials.

1 Work at BNL was supported by BES, US DOE, under Contract No. DE-AC02-98CH12883. Research at ORNL’s HFIR and SNS sponsored by Scientific User Facilities Division, BES, US DOE. We acknowledge the support of NIST, in providing neutron research facilities.

1:15PM M5.00009 Synthesis and superconductivity in spark plasma sintered pristine and graphene-doped \( \text{FeSe}_{0.5}\text{Te}_{0.5} \). POOJA PUNEET, RAMAKRISHNA PODILA, JIAN HE, APPARAO RAO, Clemson University, AUSTIN HOWARD, NICHOLAS CORNELL, ANVAR A. ZAKHIDOV, University of Texas at Dallas, DEPARTMENT OF PHYSICS AND ASTRONOMY, CLEMSON NANOMATERIALS CENTER, CLEMSON UNIVERSITY TEAM, NANOABET, UNIVERSITY OF TEXAS AT DALLAS TEAM — Replace this text with your abstract body. Here, we present a new ball-milling and spark plasma sintering based technique for the facile synthesis of \( \text{FeSe}_{0.5}\text{Te}_{0.5} \) superconductors (SC) without the need for pre-alloying. This method is advantageous since it is quick and flexible for incorporating other dopants such as graphene for vortex pinning. We observed that \( \text{FeSe}_{0.5}\text{Te}_{0.5} \) exhibits a coexistence of ferromagnetic (FM) and SC signature plausibly arising from a FM core-SC shell structure. More importantly, the \( H_{\text{c2}} \) values observed from resistivity data are higher than 7 T indicating that SPS process synthesized \( \text{FeSe}_{0.5}\text{Te}_{0.5} \) samples could lead to nextgeneration superconducting wires and cables.

1:27PM M5.00010 An ab-initio Quantum Monte Carlo analysis of pressure and magnetism in the unconventional superconductor, \( \text{FeSe} \). BRIAN BUSEMEYER, LUCAS K. WAGNER, University of Illinois, Urbana-Champaign Physics Department — We report the results of many-body ab-initio fixed-node diffusion Monte Carlo calculations performed on the unconventional superconductor, \( \text{FeSe} \). \( \text{FeSe} \) shows a strong pressure-dependent critical temperature, and because magnetism is generally expected to play an important role in understanding unconventional superconductivity, for pressures ranging from ambient to 11 GPa, we investigate the single and many-body properties of three ordered magnetic configurations, including the two found in similar iron-based superconductors. Our calculations find that at least two magnetic orders (collinear and bicollinear) are nearly degenerate in energy, becoming closer in energy as pressure increases. We also analyze how correlations between the electrons change as a function of pressure, and discuss what this could mean for superconductivity.

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2 This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Scientific Discovery through Advanced Computing (SciDAC) program under Award Number FG02-12ER46875.
This study demonstrates an efficient approach to tune the multiferroicity in the manganite system. Polarized state intimately correlates with the lower temperature ferroelectric state that is induced by the incommensurate spiral magnetic order of Mn spins. We report the formation of a highly polarized state in multiferroic DyMnO$_3$ via pressure and temperature conditions. BRANDON WILFONG, Washington College, 300 Washington Ave. Chestertown, MD 21620, USA — Recent experiments demonstrate that isovalent doping studies give the similar phase diagram as the heterovalent doped cases: with the P-doping, the magnetic order is suppressed and the superconductivity emerges. With the help of tight-binding model calculation and self-consistent lattice Bogoliubov-de Gennes (BdG) equation calculation, we choose a minimal two-orbital model and obtain the phase diagram of BaFe$_2$(As$_{1-x}$P$_x$)$_2$ against the P content x, which could be qualitatively comparable with the experimental results. Besides, we will compare these results with the recent experiments shown QCP in this system.

Wednesday, March 4, 2015 11:15AM - 2:15PM
Session M6 DMP DCOMP: Focus Session: Coupling Polarization and Magnetism I

11:15AM M6.00001 In-situ Raman Spectroscopic Investigation of Relaxor Multiferroic Pb(Fe$_{0.5}$Nb$_{0.5}$)$_3$O$_3$ under High Pressure and Temperature Conditions
BRANDON WILFONG, Washington College, 300 Washington Ave. Chestertown, MD 21620, USA — The vibrational and structural properties of lead ferroanate, Pb(Fe$_{0.5}$Nb$_{0.5}$)$_3$O$_3$, have been investigated using Raman spectroscopy up to 40 GPa and up to 415 K at selected pressures. Three phase transitions were noted via the pressure evolution at 5.5, 8.7 and 24 GPa at room temperature, respectively. The temperature dependencies of the Raman spectra indicated two phase transitions at 1.5 GPa, 335 and 365 K, which support the appearance of an intermediate tetragonal P4mm phase between the ferroelectric R3m and paraelectric Pm-3m phases. At 2.5, 3.9 and 7.4 GPa, the system showed one phase transition with temperature evolution at 337, 348 and 332 K respectively. With this set of data, a $P-T$ phase diagram was compiled to provide further insight into the magnetoelectric coupling and allow comparison to other systems in order to elucidate the impact of magnetic order on relaxor systems.

11:27AM M6.00002 Investigation of the multiferroic behavior in FeVO$_4$ single crystals
EHAB ABDELHAMID, Wayne State University, KENTA KIMURA, TSUYOSHI KIMURA, Osaka University, ONATTU D. JAYAKUMAR, Bhabha Atomic Research Centre, VAMAN M. NAIK, University of Michigan-Dearborn, RATNA NAIK, GAVIN LAWES, Wayne State University — For FeVO$_4$ is considered as a model system for understanding the magnetoelectric interaction mechanisms in low symmetry multiferroics. Bulk FeVO$_4$ exhibits two antiferromagnetic phase transitions at $T_{N1} = 22$ K and $T_{N2} = 15$ K. Below $T_{N2}$, a noncollinear magnetic order develops, breaking the space inversion symmetry that induces ferroelectric order. Earlier measurements on polycrystalline samples of FeVO$_4$ doped with magnetic (e.g.: Chromium) as well as non-magnetic (e.g.: Zinc) ions, indicate the stability of the two antiferromagnetic transition temperatures, with a change of only 2% corresponding to the doping concentration of 20%. It also shows the ability of the FeVO$_4$ trilinic structure to accommodate such high doping levels. Working along the same line, we have prepared both doped and undoped single crystals of FeVO$_4$ by a flux method. Samples were characterized using XRD and Raman spectroscopy to track the changes in lattice parameters induced by different dopants. The magnetic and ferroelectric properties were investigated in order to understand the origin of magnetoelectric coupling in low symmetry multiferroics.

1Supported by NSF under DMR-1306449.

11:39AM M6.00003 Near Room-Temperature Magnetism and Enhanced Magnetic Moments in Multiferroic (LuFeO$_3$)$_{1-x}$/(LuFe$_2$O$_3$)$_x$ Superlattices
JARRETT MOYER, University of Illinois at Urbana-Champaign, JULIA MUNDY, CHARLES BROOKS, MEGAN HOLTZ, DAVID MULLER, DARRELL SCHLOM, Cornell University, PETER SCHIFFER, University of Illinois at Urbana-Champaign — The development of room-temperature multiferroics is necessary to realize the potential of these materials in low-power energy, memory, and logic applications. Currently, there are only four potential single-phase multiferroics that exist at room-temperature, all of which have either antiferromagnetic or weakly ferromagnetic magnetic orderings. Here, we report on the magnetic properties of epitaxially grown superlattices composed of the ferroelectric, weakly ferromagnetic LuFeO$_3$ and the paraelectric, ferrimagnetic LuFe$_2$O$_3$. By inserting layers of $x$-LuFeO$_3$ ($T_N = 147$ K) into LuFe$_2$O$_3$, we increase $T_C$ from 219 K for single-phase LuFe$_2$O$_3$ to 270 K for (LuFeO$_3$)$_{1-x}$(LuFe$_2$O$_3$)$_x$. Additionally, while the magnetic moment on the LuFe$_2$O$_3$ layers remains constant for $m/(m+2n)<0.5$, it increases rapidly for $m/(m+2n)>0.5$, resulting in magnetic moments orders of magnitude larger than the weak ferromagnetic room-temperature multiferroics. We will discuss the potential mechanisms for these enhanced transition temperatures and magnetic moments and the potential to increase $T_C$ to above room temperature.

This research is primarily supported by DOE Award No. DE-SC0002334.

11:51AM M6.00004 RMO3 perovskite oxides with magnetic and ferroelectric polar structures
WEI REN, SHUNBO HU, YABEI WU, Shanghai University — Enhancing the electrical polarization and the magnetic ordering transition temperatures constitutes a current research focus in multiferroics of fundamental and technological importance. Here we report on some progress on the RMO3 perovskites for novel routes to realize multiferroics, giving specific examples of rare earth and transition metal oxide materials. First principles calculations, either supported by experimental results or awaiting for experimental verifications, are shown to offer useful guidance for the research of unconventional multiferroics. We hope to stimulate more efforts from experimentalists and theorists to work together for the future developments in fundamental science and device applications. These experimental and theoretical approaches will open up new possibilities for exploring, modeling, and exploiting novel electromagnetism and multiferroic materials.

12:03PM M6.00005 Excess-hole induced high temperature polarized state and its correlation with the multiferroicity in single crystalline DyMnO$_3$
TAO ZOU, Michigan State University, ZHILING DUN, University of Tennessee, HUIBO CAO, Oak Ridge National Lab, MENGZE ZHU, DANIEL COULTER, Michigan State University, HAIDONG ZHOU, University of Tennessee, XINQILIN K. J. Michigan State University — Controlling the ferroelectricity and magnetism in multiferroic materials has the ferroelectric R3m and paraelectric Pm-3m phases. We report the formation of a highly polarized state in multiferroic DyMnO$_3$ single crystals which develops well above the magnetic transition temperatures, and we attribute it to the thermally stimulated depolarization current effect of excess holes forming Mn$^{4+}$ ions in the system. We also show that this high temperature polarized state intimately correlates with the lower temperature ferroelectric state that is induced by the incommensurate spiral magnetic order of Mn spins. This study demonstrates an efficient approach to tune the multiferroicity in the manganite system.
12:15PM M6.00006 Colossal Directional Dichroism in a Multiferroic CuB$_2$O$_4$  SHINO GO YODA, NOBUYUKI ABE, Univ of Tokyo, SHOJIRO KIMURA, Tohoku University, YASUHIRO H. MATSUDA, TOSHIHIRO NOMURA, AKIHITO IKEDA, SHOJIRO TAKEYAMA, TAKA-HISA ARIMA, University of Tokyo — In multiferroic materials, electric and magnetic responses to light can interfere with each other, resulting in novel optical phenomena. One typical example is directional dichroism, where the absorption coefficient changes with the reversal of the propagating direction of light. It has been reported that CuB$_2$O$_4$ shows giant directional dichroism at 1.40 eV, which corresponds to the intratomic transition of Cu$^{2+}$ hole. The optical absorption coefficient changes by a factor of three at low magnetic fields. In this study, we investigated magnetic field dependence of directional dichroism up to 52 T. We have observed colossal directional dichroism where the ratio of the optical absorption coefficient is as large as 1000% at 52 T. The observed extraordinary large directional dichroism is explained by a modification of the electric and magnetic dipole transition moments due to the canting of the spin direction of Cu$^{2+}$ hole by the application of a high magnetic field.

12:27PM M6.00007 Magneto-orbital helices as a route to coupling magnetism and ferroelectricity in multiferroic CaMn$_7$O$_{12}$  ROGER JOHNSON, University of Oxford — In compounds with long-range ferromagnetic or antiferromagnetic ordering, the magnetic and structural degrees of freedom may couple through orbital ordering. It has long been hoped that this type of coupling could be exploited to create high-temperature multiferroics - materials in which both ferroelectricity and long-range magnetism coexist in a single phase, and may couple to give rise to spontaneous magneto-electric functionality. In this talk I will report a detailed experimental study of the multiferroic oxide CaMn$_7$O$_{12}$. Our complementary data from pyroelectric current, magnetometry, single crystal x-ray diffraction, and powder neutron diffraction experiments show that CaMn$_7$O$_{12}$ couple to give rise to spontaneous magneto-electric functionality. In this talk I will report a detailed experimental study of the multiferroic oxide CaMn$_7$O$_{12}$.

1:03PM M6.00008 Ultraviolet Raman spectroscopy of hexagonal LuFeO$_3$ films 1, 2  D.M. A. TENNES, D.A. HILLSBERRY, E.L. THIES, Department of Physics, Boise State University, Boise, ID 83725, USA, J.A. MUNDY, D.A. MULLER, School of Applied and Engineering Physics, Cornell University, Ithaca, NY 14853, USA, C.M. BROOKS, D.G. SCHLOM, Department of Materials Science and Engineering, Cornell University, Ithaca, NY 14853, USA — Hexagonal LuFeO$_3$ films grown by molecular-beam epitaxy on yttria-stabilized zirconia substrates were studied by variable temperature ultraviolet Raman spectroscopy. Hexagonal LuFeO$_3$ is a multiferroic that is isostructural to YMnO$_3$ at room temperature. LuFeO$_3$ spectra at room temperature are consistent with the polar hexagonal $P6_3/mmc$ structure. The temperature evolution of the Raman spectra of a LuFeO$_3$ film measured in the range 10–1250 K indicate a transition to a non-polar (likely $P6_3/mmc$) phase; fitting of the temperature dependence of the Raman intensities yields a transition temperature of 1020 ± 50 K. We also observed a change in the slope of Raman intensity vs. temperature dependence of the most intense phonon peak around 400–450 K, which might indicate another structural transition, possibly to a structure with space group $P6_3/mmc$ (also polar).

1:15PM M6.00009 Pressure induced spin-flop transition in multiferroic Mn$_{1-x}$Co$_x$WO$_3$ 1, 2  FENG YE, JINCHEN WANG, SONGXUE CHI, JAIME FERNANDEZ-BACA, Oak Ridge National Lab, M. GOOCH, BERND LORENZ, K.-C. LIANG, Y.-Q. WANG, Y.Y. SUN, C.W. CHU, University of Houston — The effect of cobalt substitution in Mn$_{1-x}$Co$_x$WO$_3$ results in the most complex multiferroic phase diagram with multiple polar phases. We have examined the spin-flop transition in Co$_{40}$Fe$_{40}$B$_{20}$/Pb(Mg$_{1/3}$No$_{2/3}$)$_{1-x}$Ti$_x$O$_3$ (1-x)TixO3 multiferroic heterostructures, of which Pb(Mg$_{1/3}$No$_{2/3}$)$_{1-x}$Ti$_x$O$_3$ structure varies with increasing x from rhombohedral (R) phase, through tetragonal (T) phase, to tetragonal phase. We found that the samples with Pb(Mg$_{1/3}$No$_{2/3}$)$_{1-x}$Ti$_x$O$_3$ in R phase and MBP both display large and nonvolatile behavior, while it shows volatile behavior in tetragonal phase. These results indicate that it is not MPB but R phase that is vital for the nonvolatile behavior. We also studied the temperature effect of electric-field-controlled magnetization by varying temperatures from 200 K to 340 K and found that the magnetic-field dependence of the optical absorption shows a hysteresis like the magnetization curve, which indicates that the change in optical absorption should originate from the rotation of the magnetic moments of Co$^{2+}$.
In this present work, using first-principles density-functional theory, we have investigated the effect of strain on previously reported MOFs, such as hybrid crystalline compounds composed of an extended ordered network made up of organic molecules, organic linkers and metal cations. In particular, MOFs with the same topology as inorganic ABO$_3$ perovskites, have been shown to have interesting properties, i.e. coexistence of ferroelectric and magnetic ordering [1]. In this present work, using first-principles density-functional theory, we have investigated the effect of strain on previously reported MOFs, such as hybrid crystalline compounds composed of an extended ordered network made up of organic molecules, organic linkers and metal cations. In particular, MOFs with the same topology as inorganic ABO$_3$ perovskites, have been shown to have interesting properties, i.e. coexistence of ferroelectric and magnetic ordering [1]. In this present work, using first-principles density-functional theory, we have investigated the effect of strain on previously reported MOFs, such as hybrid crystalline compounds composed of an extended ordered network made up of organic molecules, organic linkers and metal cations. In particular, MOFs with the same topology as inorganic ABO$_3$ perovskites, have been shown to have interesting properties, i.e. coexistence of ferroelectric and magnetic ordering [1].

Wednesday, March 4, 2015 11:15AM - 2:03PM
Session M7 DMP DCMP: Focus Session: Topological Crystalline Insulators

11:15AM M7.00001 Electron and spin properties of topological crystalline insulator (Pb,Sn)Se

TOMASZ STORY, Institute of Physics, Polish Academy of Sciences — Topological crystalline insulators (TCIs) constitute a new class of quantum materials with the Dirac-like metallic surface states that cross the bulk semiconductor band gap and are topologically protected by crystalline mirror plane symmetry. The TCI states have recently been experimentally observed in PbSe, SnTe, and PbSnTe for both (001) and (111) crystal surfaces. These IV-VI semiconductors undergo (at a specific tin content, temperature, and pressure) a band structure inversion driven by strong relativistic effects. The investigations of the surface electronic states by angle- and spin-resolved photoemission spectroscopy will be presented for bulk (Pb,Sn)Se monocrystals with tin content up to 37 at. %, also doped with magnetic Mn$^{2+}$ ions. In the inverted band structure regime we found the Dirac-like topological in-gap states in the vicinity of four X points of the (001) surface Brillouin zone and observe a temperature-driven topological phase transition from a trivial insulator to a TCI state below the band inversion point. In crystals with Mn ions we demonstrate very efficient tuning of the topological transition temperature by band gap engineering effect. The spin-resolved ARPES experiments revealed a characteristic vortical electron spin polarization texture at the Dirac points. Based on spectroscopic observation we construct the composition - temperature topological phase diagram of (Pb,Sn)Se and compare it with tight-binding band structure calculations. P. Dziawa et al., Nat. Mat. 11, 1023 (2012); B.M. Wojek et al., Phys. Rev. B 87, 115106 (2013); C.M. Polley et al., Phys. Rev. B 89, 075317 (2014); B.M. Wojek et al., Phys. Rev. B 90, 161202 (R) (2014).

1Supported by NCN (Poland) research project 2011/03/B/ST3/02659.

11:51AM M7.00002 Topological crystalline insulator states in layered materials

YOUNGKUK KIM, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, CHARLES KANE, EUGENE MELE, Department of Physics and Astronomy, University of Pennsylvania, ANDREW RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania — Topological crystalline insulator (TCI) is a topological state of materials whose topological property relies on generic crystalline symmetries. Based on first-principles calculations, we suggest new classes of topological crystalline insulators characterized by non-zero mirror Chern numbers (MCNs) hosted on the mirror-invariant plane at the boundary of the Brillouin zone (BZ). We demonstrate that the new TCI phases can be realized in layered materials, and the topological phase transitions associated with the proposed TCI phases occur under an external pressure. Our results shed light on the role of the MCNs hosted on the surface of the BZ, and open new possibilities for finding TCI materials.

12:03PM M7.00003 Strain engineering Dirac surface states in heteroepitaxial topological crystalline insulator thin films

ILJIA ZELJKOVIC, DANIEL WALKUP, BADIOH ASSAF, KANE SCIPIONI, Boston College, RAMAN SANKAR, FANGCHENG CHOU, National Taiwan University, Taipei, VIDYA MADHAVAN, University of Illinois Urbana-Champaign — In newly discovered topological crystalline insulators (TCIs), the unique crystalline protection of the surface state (SS) band structure has led to a series of intriguing predictions of strain generated phenomena, such as the momentum-space tunability of the Dirac nodes. In this work, we have designed an experiment to not only generate and measure strain locally, but to also directly measure the resulting effects on the Dirac SS. We grow heteroepitaxial thin films of TCI SnTe in-situ and measure them by using high-resolution scanning tunneling microscopy (STM). Large STM images were analyzed to determine picoscale changes in the atomic positions which reveal regions of both tensile and compressive strain. Simultaneous Fourier-transform STM was then used to determine the effects of strain on the Dirac electrons. We find that strain continuously tunes the momentum space position of the Dirac points, consistent with theoretical predictions. Our experiments demonstrate the fundamental mechanism necessary for using TCIs in strain-based applications.

12:15PM M7.00004 ABSTRACT WITHDRAWN
12:27PM M7.00005 Realization of topological phase transition in Pb$_{1−x}$Sn$_x$Te (111) films
CHENHUI YAN, Institute of Metal Research, Chinese Academy of Sciences, JUNWEI LIU, YUNYI ZANG, ZHENYU WANG, JIANFENG WANG, Department of Physics, Tsinghua University, ZHIDONG ZHANG, Institute of Metal Research, Chinese Academy of Sciences, LILI WANG, XUCUN MA, SHUAIHUA JI, KE HE, Department of Physics, Tsinghua University, LIANG FU, Department of Physics, Massachusetts Institute of Technology, WENHUI DUAN, QI-KUN XUE, XI CHEN, Department of Physics, Tsinghua University — Recently, it was confirmed that the single crystal SnTe is a Topological crystalline insulator (TCI) by theoretical calculations and experiments. It is well known that the (001) surfaces of SnTe are the natural cleavage planes and therefore all the previous experiments for the TCI phase were performed on the (001) surfaces. The (111) surface, which is a polar surface with unpaired electrons, is very difficult to obtain by traditional crystal growth method. Here we present the epitaxial growth of high quality Pb$_{1−x}$Sn$_x$Te (111) films and observation of TCI phase by in-situ angle-resolved photoemission spectroscopy. The Pb$_{1−x}$Sn$_x$Te (111) films undergo a topological phase transition from trivial insulator to TCI via increasing the Sn/Pb ratio, accompanied by a crossover from n-type to p-type doping in the films. In addition, a sizeable Rashba effect is clearly seen in the PbTe (111) film. Our work demonstrates the manipulation of topological properties of TCI, which is crucial for future fundamental research and applications. C. Yan et al., Phys. Rev. Lett., 112, 186801 (2014).

3Work supported by grants from NSF11025419, 11074139, and 51331006

12:39PM M7.00006 Searching for ideal bulk insulating Pb-system topological crystalline insulator materials
GENDA GU, R.D. ZHONG, JOHN SCHNEELOCH, T.S. LIU, JHON TRANQUADA, X.G. HE, WEI KU, I. PLETIKOSIC, T. VALLA, Brookhaven Natl Lab, CONDENSED MATTER PHYSICS & MATERIALS SCIENCE, BROOKHAVEN NATIONAL LABORATORY TEAM — The discovery of topological crystalline insulator materials is a breakthrough in the search for new electronic materials available for experimental research so that we can explore the new field. In order to search for the ideal bulk insulating topological crystalline insulator materials, we have grown a large number of the single crystals of Pb-system (Pb-Sn-In-Te) topological crystalline insulator. We have measured the physical properties on these single crystals by various techniques. We have studied the effect of crystal growth condition, impurity and composition on the bulk electrical conductivity of these single crystals. We try to find out which composition and crystal growth condition is the best for the ideal bulk insulating topological crystalline insulator materials.

1:27PM M7.00010 ABSTRACT WITHDRAWN —

1:03PM M7.00008 Properties of thin film SnTe grown by molecular beam epitaxy
K. ZOU, Department of Applied Physics and CRISP, Yale University, New Haven CT 06652, STEPHEN D. ALBRIGHT, Department of Physics and CRISP, Yale University, New Haven CT 06620, G.H. SIMON, Department of Mechanical Engineering & Materials Science, Chemical & Environmental Engineering, and CRISP, Yale University, New Haven CT 06620, M.D. MORALES-ACOSTA, Department of Applied Physics and CRISP, Yale University, New Haven CT 06620, ERIC ALTMAN, Department of Chemical & Environmental Engineering and CRISP, Yale University, New Haven CT 06620, F.J. WALKER, Department of Applied Physics and CRISP, Yale University, New Haven CT 06620, C.H. AHN, Department of Applied Physics, Mechanical Engineering & Materials Science, and CRISP, Yale University, New Haven CT 06620 — The topological crystalline insulator SnTe exhibits multiple surface states protected by crystal symmetry. Thin films of SnTe have been grown by physical vapor deposition techniques on several substrates; these films tend to consist of a heterogeneous collection domain structures. In this talk, we report systematic studies of the structure and transport properties of SnTe films grown by molecular beam epitaxy (MBE). Combining atomic force microscopy and x-ray diffraction measurements, we find that the domains consist of crystallites with 100 and 111 surfaces. When the thickness of SnTe exceeds 400 Å, the 100 surface becomes dominant. Transport measurements show that conduction in the films can be attributed to both Sn vacancies in bulk SnTe and the surface topological states of SnTe.

1:15PM M7.00009 Electronic and spin structure of topological surface state in Sn-based ternary topological insulators
MAIA G. VERGIÑO, Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain, TATIANA V. MENSCHIKOVA, Tomsk State University, pr. Lenina 36, Tomsk, 634050 Russia, IGOR V. SILKIN, Tomsk State University, Tomsk, 634050 Russia, YURY M. KOROTEEV, SERGEY V. EREMEEV, Institute of Strength Physics and Materials Science, Siberian Branch, Russian Academy of Sciences, Tomsk, 634021 Russia, EUGENIU C. CHULKOV, Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain, CHULKOV GROUP TEAM — We report the bulk and surface electronic properties and spin polarization of a new rich family of Sn-based ternary complex topological insulators studied by means of first principles calculations. These compounds exist in different stoichiometries: Sn$_x$Sb$_y$Z$_z$ (A=Sb and B=Te and Se). The crystal structure of these compounds are characterized by alternating along hexagonal axis quintuple, septuple and nonuple layer van der Waals bonded building blocks. We reveal that the bulk band gap in these systems is about 200 meV and the spin polarization near the Dirac point is up to 85%, one of the highest predicted hitherto. At the same family, for some of these compounds which crystal structure has ionic-covalent bonded Bi$_2$Te$_3$ and crystalline topological insulator SnTe atomic layers within building block the complex SOI-induced bulk band inversion caused by competition of band inversions in Bi$_2$Te$_3$ and in SnTe layers occurs and results in inherently nonlinear dispersion of the topological surface state.

1:27PM M7.00010 ABSTRACT WITHDRAWN —

1:39PM M7.00011 Hidden topological surface states on SnTe (111) surface
JIANFENG WANG, JUNWEI LIU, WENHUI DUAN, Tsinghua University — Abundant and interesting properties of topological crystalline insulator SnTe (111) surface have been studied here. Using first-principles calculations, we show the stable structures and their related topological surface states (TSS) under different growth conditions. Surface reconstruction can induce the TSS type transition. More interestingly, the position of TSS can be hidden deeply below the surface, which depends on the interlayer relaxation. The underlying mechanism can be understood by the distortion-induced topological phase transition. Our work paves the way to control the TSS, especially to realize the physical protection in real environment.
shows little or no length-dependence of the current. The dephasing is also shown to lead to a substantial reduction of the current in that dephasing leads to an exponential decay of the current as a function of molecular length, even for resonant tunneling, where the fully coherent calculation.

I will present an approach for calculating the transport properties of SAM-MJs that inherently takes into account in-plane dephasing. The approach describes well the two hallmarks of transport through SAM-MJs, namely the exponential decay of current with molecular chain length and the reduction of the current per molecule as compared to single-molecule junctions. Specifically, I will show that in-plane dephasing is a departure from existing approaches to co-crystallization, as it could guide the discovery of potentially valuable molecular ferroelectrics, and enable the rational design of organic ferroelectric co-crystals and n-crystals, which quickly become prohibitively complex to investigate using heuristic-guided approaches.

11:51AM M8.00002 Surface Dipole Control of Liquid Crystal Alignment. JEFFREY SCHWARTZ, Department of Physics & Astronomy, University of California, Los Angeles, YUXI ZHAO, ALEXANDRA MENDOZA, NATCHA WATTANATORN, Department of Chemistry & Biochemistry, University of California, Los Angeles, PAUL WEISS, Departments of Chemistry & Biochemistry and Materials Science & Engineering, University of California, Los Angeles — We investigate the influence of surface dipoles on the alignment of liquid crystals (LCs). Carbonar ethiol self-assembled monolayers (SAMs) are shown to induce planar anchoring in 4-cyano-4′-pentylphenyl LCs at the SAM/nematic interface. We exploit the different dipole moments of carbonar ethiol structural isomers in order to deconvolute the influence of SAM-LC dipolar coupling from variations in molecular geometry, tilt, and order. The LC director orientation and anchoring energy are measured for devices employing varying carbonar ethiol isomer alignment layers. By using LC orientation as a probe of interaction strength, we demonstrate that dipolar coupling of SAMs to their environment plays a key role in determining molecular orientations. This understanding may advance the engineering of molecular interactions at the nanoscale.

12:03PM M8.00003 Self-assembly of functionalized indoles on surfaces. FABRIZIO DE MARCHI, DALING CUI, JOSH LIPTON-DUFFIN, Institut National de la Recherche Scientifique, Centre Energie, Matériaux, Télécommunications, 1650 Lionel Boulet Boulevard, J3X 1S2 Varennes, CLARA SANTATO, Département de Génie Physique, École Polytechnique de Montréal, C.P. 6079, Succ. Centre Ville, H3C 3A7, Canada, JENNIFER MACLEOD, FEDERICO ROSEI, Institut National de la Recherche Scientifique, Centre Energie, Matériaux, Télécommunications, 1650 Lionel Boulet Boulevard, J3X 1S2 Varennes — To predict how a molecule on a surface will interact with its neighbors or with the substrate itself is an intriguing challenge. If overcome, it would allow the design of a pattern by the proper selection of monomers. However, we are far from a complete understanding of self-assembly mechanisms on surfaces, and more insight can be gathered by studying small, simple systems. In nature, small molecules are the building blocks for more complex systems, such as enzymes and DNA; understanding their self-assembly could lead to the ability to encode this kind of complexity and information density into engineered self-assembled molecular architectures. We report here on the self-assembly of two simple molecules: indole-2-carboxylic acid (I2CA) and 5,6-dihydroxyindole-2-carboxylic acid (DHICA) over various substrates. DHICA is one of the monomers that forms eumelanin, and brings the possibility of different bonding architectures due to its combination of carboxyl and hydroxy groups. At surfaces, DHICA forms a number of structures depending on the conditions used to prepare the surface film. On the other hand, I2CA self-assembles into a simple ordered pattern that is relatively independent of the substrate and preparation conditions. DFT calculations corroborate these observations.

12:15PM M8.00004 Stereoelectronic Switching in Single-Molecule Junctions. HAIXING LI, Department of Applied Physics and Applied Math, Columbia University, TIMOTHY SU, MICHAEL STEIGERWALD, COLIN NUCKOLLS, Department of Chemistry, Columbia University, LATHA VENKATARAMAN, Department of Applied Physics and Applied Math, Columbia University — We demonstrate the first single-molecule switch that operates through a stereoelectronic effect in silicon-based molecular backbones terminated with methyl-sulfide linker groups. We utilize the subangstrom level of control in a scanning tunneling microscope-based break-junction (STM-BJ) technique to manipulate the conformation of these molecule switch that operates through a stereoelectronic effect in silicon-based molecular backbones terminated with methyl-sulfide linker groups. We utilize the subangstrom level of control in a scanning tunneling microscope-based break-junction (STM-BJ) technique to manipulate the conformation of these molecule switch that operates through a stereoelectronic effect in silicon-based molecular backbones terminated with methyl-sulfide linker groups. We utilize the subangstrom level of control in a scanning tunneling microscope-based break-junction (STM-BJ) technique to manipulate the conformation of these molecule switch that operates through a stereoelectronic effect in silicon-based molecular backbones terminated with methyl-sulfide linker groups. We utilize the subangstrom level of control in a scanning tunneling microscope-based break-junction (STM-BJ) technique to manipulate the conformation of these.

We thank the NSF for the primary support of these studies under grant number CHE-1404922. H.L. is supported by the Semiconductor Research Corporation and New York CAIST. T.A.S. is supported by the NSF Graduate Research Fellowship under Grant No. 11-44155.

12:27PM M8.00005 Transport through Self-Assembled Monolayer Molecular Junctions: Role of In-Plane Dephasing. JONATAN DUBIN, Ben-Gurion University of the Negev — Self-assembled-monolayer (SAM) molecular junctions (MJ) constitute a promising building block candidate for future molecular electronic devices. Transport properties of SAM-MJs are usually calculated using either the phenomenological Simmons model, or a fully-coherent transport theory, employing the SAMs periodicity. As I will show, the standard theory seems to have some discrepancy with experimental observations. To overcome these discrepancies, I suggest that dephasing plays an important role in determining the transport properties of SAM-MJs. I will present an approach for calculating the transport properties of SAM-MJs that inherently takes into account in-plane dephasing in the electron motion as it traverses the SAM plane. The approach describes well the two hallmarks of transport through SAM-MJs, namely the exponential decay of current with molecular chain length and the reduction of the current per molecule as compared to single-molecule junctions. Specifically, I will show that dephasing leads to an exponential decay of the current as a function of molecular length, even for resonant tunneling, where the fully coherent calculation shows little or no length-dependence of the current. The dephasing is also shown to lead to a substantial reduction of the current in a...
12:39PM M8.00006 SERS detection of vibrational Stark effect using PCBM-based molecular junctions, YAJING LI, Department of Physics and Astronomy, Rice University, PETER DOAK, Department of Chemistry, University of California, Berkeley, PAVLO ZOLOTAVIN, Department of Physics and Astronomy, Rice University, JEFFREY BEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, DOUGLAS NATELSON, Department of Physics and Astronomy, Rice University — Understanding the interplay of local electric field and vibrational degrees of freedom of molecules are of interest. We fabricate gold bowtie structures with nanometer inter-electrode spacing using controllable electromigration. Those gold nanostructures support highly localized plasmons and have proven to be suitable SERS substrates with single-molecule sensitivity, which enable the study of molecular vibrational and electronic physics. By measuring the Raman emission from the electrically biased PCBM-containing junctions, we observed strong linear shifts on the vibrational energies of PCBM.

We will present the experiments as well as preliminary theoretical expectations obtained by DFT calculations. We compare the field driven change of vibrational energies of PCBM with those observed in C60 junctions, which have been reported to exhibit quadratic change of vibrational energies due to bias induced charge variation.

12:51PM M8.00007 Graphene Template for Epitaxial Growth of Pentacene and C60 Thin Film, KWANPYO KIM, Ulusan National Institute of Science and Technology, Korea, ELTON J.G. SANTOS, Department of Chemical Engineering, University of Maryland, TAE HOON LEE, YOSHIKO NISHI, Department of Electrical Engineering, Stanford University, ZHENAN BAO, Department of Chemical Engineering, Stanford University — The study and reliable control of molecular packing structures at the graphene-molecule interface are of great importance for various applications. We utilize suspended graphene as an assembly template to investigate thin-film epitaxial growth of various organic molecules. Thin-film packing structures of pentacene and C60 on graphene are investigated using transmission electron microscopy. For pentacene thin-film, we observe an unusual polymorph growth on graphene, which shows significant strain along the c-axis of pentacene crystals. Moreover, the strained film exhibits a specific molecular orientation and a strong azimuthal correlation with underlying graphene lattice. For C60 crystals, we observe large grain sizes and somewhat strong azimuthal correlation with respect to underlying graphene lattice direction. Utilizing ab initio electronic structure calculations with van der Waals interactions, we understand the observed molecular growth behavior mainly with graphene-molecule interaction.

1:03PM M8.00008 Study of the phase separation of organic molecules from solution on Si(111) substrates, MIRIAM CEZZA, COLIN QUALTERS, RAYMOND PHANEUF, Department of Materials Science and Engineering, University of Maryland, College Park, MD — Understanding the science behind assembly of small organic molecules into domains is important for numerous applications, among which organic solar cells are especially noteworthy. An important process on which organic solar cells depends is the phase separation of organic molecules. The formation of a morphology during phase separation from a solvent-based, bimolecular solution onto a substrate depends on several parameters: relative molecular concentrations, solubilities of each type of molecule in the solvent, solvent evaporation rate, and annealing conditions. We carry out studies on molecular mixtures consisting of tetratrito zinc-phthalocyanine (tn-ZnPc) and PCBM in chloroform, and native oxide-covered Si(111) substrates. We investigate the role that solvent evaporation rate during deposition, followed by solvent vapor annealing (SVA), plays on the formation of phase separated mixtures and their crystallization and phase transformation. We also investigated the relative concentration of individual molecules in mixtures. We found that PCBM molecules alone undergo several phase transformations as the solvent evaporation rate decreases, while tn-ZnPc is very stable. Moreover, the concentration of tn-ZnPc in mixtures highly affects the PCBM crystallization.

1Work supported by NSF-MRSEC at the University of Maryland #DMR0520471.

1:15PM M8.00009 Atmospheric Effects on dF TESADT Thin-Film Transistors, BRAD CONRAD, CORTNEY BOUGHER, SHAWN HUSTON, Appalachian State Univ, JEREMY WARD, Wake Forest University, ABDUL OBAID, MARSHA LOTH, JOHN ANTHONY, University of Kentucky, OANA JURCHESCU, Wake Forest University — Crystalline organic semiconductors often display carrier mobilities that vary with environmental conditions and fabrication parameters. Additionally, the electrical properties of organic thin-film devices are highly dependent on film structure, crystallinity, and molecular packing. In solution-deposited polycrystalline thin-films, the regions between crystals often affect the overall device performance, as molecular ordering and crystal structure may differ significantly from neighboring regions. Device characterization and Kelvin Probe Force Microscopy (KPFM) is used to analyze the electrical properties of grain boundaries, electrodes, and crystalline regions within 2,8-difluoro-5,11-triethysilylethynylanthradithiophene (dF TESADT) thin-film transistor surfaces. The influence of both atmospheric dopants and exposure time is examined and explained in the context of device characterization and interfacial effects.

1:27PM M8.00010 2d Assembly and solvation of supramolecular ionic polymers, JANICE REUTT-ROBEY, QIAN SHAO, LEVAN TSKIPURI, University of Maryland, DAISUKE TAKAJJO, Osaka University — Supramolecular polymers are important building blocks for functional nanomaterials. The structural fidelity of soft (non-covalent) species during transfer from the solution phase to a solid substrate is an important issue for many applications. We report on the 2D structures of supramolecular ionic polymer chain structures consisting of the ionic solutes C18H24N3O12 (-3) and IrN6C30H24 (-3). In solution, these ionic solutes assemble into supramolecular chain-like structures, with lengths averaging 20 nm. Deposition onto an Ag(111) substrate by a liquid microaerosol source yields 2D islands of the ionic polymers embedded in a thin film of the solvent, CH3Cl. Molecularly resolved UHV-STM images reveal in tact transfer of the supramolecules with size distributions comparable to the solution phase. Solute ion attachment/detachment from the supramolecular chain ends occurs, facilitated by the bounding solvent layer. Solvent-solute islands adopt striking geometric shapes and these structures are discussed in terms of 2-d solvation energies. This work was supported by the National Science Foundation under CHE-MSN Grant CHE1310380.

1:39PM M8.00011 High-resolution imaging of interfacial water: from water monomer to two-dimensional ice, YING JIANG, JING GUO, XIANGZHI MENG, JI CHEN, JINBO PENG, JIMING SHENG, LIMEI XU, XIANGZHE LI, ENGE WANG, International Center for Quantum Materials (ICQM) and School of Physics, Peking University, Beijing 100871, P. R.China — Water-solid interactions are of broad importance both in nature and technology. The hexagonal bilayer model based on the Bernal-Fowler-Pauling ice rules has been widely adopted to describe water structuring at interfaces. Recently, we made a breakthrough in achieving submolecular-resolution imaging of individual water molecules using a scanning tunneling microscope (STM) [1]. Such a technique opens up the possibility of determining the detailed topology of H-bonded networks at water/solid interfaces with atomic precision. Thanks to the high-resolution STM imaging, we discover a new type of two-dimensional (2D) ice-like bilayer structure built from cyclic water tetramers on an insulating NaCl(001) film, which is completely beyond the conventional bilayer picture [2]. A novel bridging mechanism allows the interconnection of water tetramers to form chains, flakes and eventually a 2D extended ice bilayer containing a regular array of Bjerrum D-type defects. Ab initio density functional theory calculations substantiate this bridging growth mode and reveal a striking proton-disordered ice structure. [1] J. Guo, X. Z. Meng, J. Chen, J. B. Peng, J. M. Sheng, L. M. Xu, J. R. Shi, E. G. Wang* and Y. Jiang*, Nature Materials 13, 184 (2014). [2] J. Chen, J. Guo, X. Z. Meng, J. B. Peng, J. M. Sheng, L. M. Xu, Y. Jiang*, X. Z. Li*, E. G. Wang, Nature Communications 5, 4056 (2014).

1Supported by the National Basic Research Programs of China and the National Science Foundation of China.
network on the reconstructed Au(100) surface are closer to that of Pt atoms in PtO, which is +2, than in Pt. This result agrees extremely well with experimental XPS data [1].

Results of our simulations show that the Pt-dipyridyltetrazine complexes form 1-dimensional chains aligned 45° with respect to the Au(100) reconstruction row with the molecule-molecule distance of 6.93 Å. More importantly, Bader analysis shows that Pt atoms are cationic with +0.75 charge. This amount of charge is in accord with the charge on Pt in PtO determined by the same analysis indicating that the oxidation states of the Pt atoms in the Pt-dipyridyltetrazine network on the reconstructed Au(100) surface are closer to that of Pt atoms in PtO, which is +2, than in Pt₂O₃ or PtO₂. This result agrees extremely well with experimental XPS data [1].

In the presence of copper, the amino acids open a channel to the surface as mediated by temperature and molecular coverage facilitated the growth of copper islands. The growth and size fluctuation of the islands offered an interesting snapshot of metal nanocluster diffusion that often occurs at time scales beyond the resolution of a given experimental technique. The presence of ~1 ML of molecules on the surface effectively trapped the metal atoms into localized islands. Elevated temperatures (≤350 K) were used to promote the further diffusion, coalescence, and extinction of the islands for a more detailed understanding of the coarsening and ripening mechanisms.

2:03PM M8.0013 Metal-Organic Chains with Single-Site Pt(II): Insights from first principles simulations1, DUY LE, TALAT S. RAHMAN, Department of Physics, University of Central Florida — Creation, stabilization, characterization and control of single atom transition metal sites on surfaces may lead to significant advancement of the next-generation catalyst. Motivated by the experimental results of Skomski et al. [1], we have performed density functional theory calculations of Pt-dipyridyltetrazine complexes on the reconstructed Au(100) surface.

The results of our simulations show that the Pt-dipyridyltetrazine complexes form 1-dimensional chains aligned 45° with respect to the Au(100) reconstruction row with the molecule-molecule distance of 6.93 Å. More importantly, Bader analysis shows that Pt atoms are cationic with +0.75 charge. This amount of charge is in accord with the charge on Pt in PtO determined by the same analysis indicating that the oxidation states of the Pt atoms in the Pt-dipyridyltetrazine network on the reconstructed Au(100) surface are closer to that of Pt atoms in PtO, which is +2, than in Pt₂O₃ or PtO₂. This result agrees extremely well with experimental XPS data [1].

3Work supported in part by NSF Grant CHE-0741423


11:15AM M9.00001 Self-heating in an AlGaN/GaN transistor studied by ultraviolet and visible micro-Raman scattering, MOHAMMAD NAZARI, LOGAN HANCOCK, EDWIN PINER, MARK HOLTZ, Texas State University — The two-dimensional electron gas (2DEG) at GaN/AlGaN interface is the basis for high electron mobility transistor. The 2DEG region forms spontaneously without any doping and is less than 10 nm in thickness. Current-induced self-heating results in large temperature rises in these devices and represents the principal limiting factor in these devices. We report direct measurements of self-heating in an AlGaN/GaN high electron mobility transistor using ultraviolet (UV) and visible micro-Raman spectroscopy. The phonon shift is used to evaluate the temperature rise in different layers of the material stack corresponding to different optical penetration depths, giving temperature rise in top 100 nm of GaN, i.e., close to the 2DEG. The visible measurements provide an average temperature rise through the 1 micron thick GaN layer and in the Si substrate close to the interface. A depth profile is developed based on the combined data sets obtained under experimentally identical conditions. Finite element thermal simulation developed based on the experimentally determined temperature-depth profile reveal thermal resistance barrier of 10⁻⁸ K·m²/W at the interface between AlN and Si substrate.

1A grant from the Korea Institute of Science and Technology (KIST) institutional program.

11:27AM M9.00002 Growth of high quality GaN layer on carbon nanotube-graphene network structure as intermediate layer1, TAEHO HOON SEO, Korea Institute of Science and Technology, AH HYUN PARK, Chonbuk National University, SUNGCHAN PARK, MYUNG JONG KIM, Korea Institute of Science and Technology, EUN-KYUNG SUH, Chonbuk National University — In general, high-quality GaN layers are synthesized on low-temperature (LT) GaN buffer layer on a single crystal sapphire substrate. However, large differences in fundamental properties such as lattice constants and thermal expansion coefficients between GaN layer and sapphire substrate generate high density of threading dislocation (TD) that leads to deterioration of optical and structural properties. Graphene has been attracting much attention due to its excellent physical properties however, direct epitaxial growth of GaN film onto graphene substrate is not easily accessible due to the lack of chemical reactivity on graphene which consisted of C-C bond of sp² hexagonally arranged carbon atoms with no dangling bonds. In this work, an intermediate layer for the GaN growth on substrate was constructed by inserting carbon nanotubes and graphene hybrid structure (CGH) Optical and structural properties of GaN layer grown on CGH were compared with those of GaN layer directly grown on sapphire CNTs as nucleation sites and play a crucial role in the growth of single crystal high-quality GaN on graphene layer. Also, graphene film acts as a mask for epitaxial lateral overgrowth of GaN layer, which can effectively reduce TD density.

Crystal growth and detector performance of large size high-purity Ge crystals, GUOJIAN WANG, Department of Physics, University of South Dakota, MARK AMMAN, Ernest Orlando Lawrence Berkeley National Laboratory, HAO MEI, DONGMING MEI, Department of Physics, University of South Dakota, THOMAS S. RITTER, Leibniz Institute for Crystal Growth, YUTONG GUAN, GANG YANG, Department of Physics, University of South Dakota — High-purity germanium crystals with 12 cm in diameter were grown in a hydrogen atmosphere using the Czochralski method. The dislocation density of the crystals was determined to be in the range of 2000 - 4000 cm⁻², which meets a requirement for use as a radiation detector. The axial and radial distributions of impurities in the crystals were measured by Hall effect and Photo-thermal ionization spectroscopy (PTIS). Two detectors were also fabricated from one of the crystals with different techniques and then evaluated for electrical and spectral performance. Measurements of gamma-ray spectra from ¹³⁷Cs, ²⁴¹Am and ¹⁰⁰Co sources demonstrate that the detectors have excellent energy resolution. Keywords: High-purity germanium crystal, Czochralski method This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota.
11:51AM M9.00004 Characterization of dislocation and defects for large high purity Ge crystals\(^1\), HAO MEI, GOUO JIAN WANG, YUTONG GUAN, GANG YANG, DONGMING MEI, University of South Dakota, CUBED COLLABORATION — Large diameter (~ 10 cm) high purity Germanium (HP-Ge) crystals have been growing via Czochralski method at University of South Dakota. We investigate the impacts of growth rate, time-temperature profile, and thermal gradient on the dislocation and defects distribution in HP-Ge crystals along <100> orientation. The dislocation density across the entire cross-section of a grown crystal is measured using microscope. Utilizing X-Ray Diffraction method, we obtain the rocking curves from the same crystal samples. We analyze the correlation between the full width at half maximum (FWHM) of the rocking curves and the dislocation densities from the optical observations (etch pits distribution). A model that describes the correlation of dislocation density, along the HP-Ge crystal, with the FWHM of the rock curves for XRD is established. We report these analytic results.

\(^1\)This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota

12:03PM M9.00005 The Relationship Between Terminating Oxide Chemistry and InAs (100) Two-Dimensional Electron Gas (2DEG) Conductivity, KRISTEN COLLAR, Department of Physics, Duke University, Durham, NC, United States, WENYUAN JIAO, JINCHENG LI, WEI KONG, APRIL BROWN, Department of Electrical and Computer Engineering, Duke University, Durham, NC, United States — InAs grown in high-conductance defect density state, high electron mobility and quasi-two dimensional electron gas (2DEG) form at the surface of oxidized and atomically-clean InAs. Electrical characterization of the 2DEG, particularly its correlation to oxide-InAs interface states is key to understanding the factors controlling conductivity. This study perturbs the oxide formation by investigating the dominating chemical reactions yielding the heterogeneous In- and As-based native oxide. Herein, we study the relationships between the conductivity and oxide surface chemistry of 100nm InAs films terminated with In or As monolayers using Molecular Beam Epitaxy then oxidized upon exposure to air. We speculate that the observed trends in the 2DEG conductivity are due to differences in the nature of predominate defects associated with oxide chemistries and their formation. Angle-resolved X-ray photoelectron spectroscopy revealed that In oxide was dominate at all probing depths, with more As oxide at the surface. Furthermore, an increase in incorporated oxygen degraded the mobility. Thus, we show that the surface termination impacts the 2DEG mobility and carrier concentration through the extent and homogeneity of oxygen incorporation during the formation of the oxide layer.

12:15PM M9.00006 Purification of Germanium Crystals by Zone Refinement: Theoretical and Experimental Approaches, GANG YANG, YUTONG GUAN, GOUO JIAN WANG, HAO MEI, FANYI JIAN, DONGMING MEI, University of South Dakota, CRYSTAL GROWTH TEAM — The results of single germanium crystals grown from zone-refined germanium ingots, identified by photon thermal ionization spectroscopy (PTIS), show that there are four main impurities, aluminum (Al), phosphor (P), boron (B) and gallium (Ga) in the crystals. Based the PTIS results, we investigated the influences of zone speed, zone width and the number of passes on effective segregation coefficient of Al, P and Ga in the process of zone refinement, then the further calculation of distribution of Al, P and Ga along the zone refined ingots has been conducted. In terms of trend of impurity distribution, the calculated results have a very good agreement with the experimental results. We report both the theoretical calculations and the experimental results. This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota.

12:27PM M9.00007 Effects of Light Exposure on Dopant Incorporation and Migration in MBE-Grown GaAs(001), CHARLOTTE E. SANDERS, D.A. BEATON, K. ALBERI, National Renewable Energy Laboratory — Light-stimulated epitaxy of II-VI semiconducting materials is known to reduce crystalline defect density and enhance substitutional dopant incorporation relative to traditional “dark” epitaxial growth. These effects have been speculated to arise from photon-atom interactions at the growth front, and from involvement in bonding processes by photogenerated carriers; however, a conclusive explanation of the observed effects has yet to be found. We are revisiting this topic, attempting to clarify the mechanisms of light-stimulated epitaxy and to explore its effects on the class of III-V materials. Here we report an ongoing investigation into dopant incorporation and migration in MBE-grown GaAs(001) when the growth front is irradiated during deposition. On the basis of our preliminary findings, and by comparing our new results with results previously obtained for light-stimulated effects on doping of II-VI systems, we can begin to draw conclusions about the mechanisms underlying light-stimulated epitaxy and their potential utility to MBE growth of complex multilayer structures. This work was supported by the DOE Office of Science, Basic Energy Sciences, under contract DE-AC36-08GO28308.

12:39PM M9.00008 Progress in the growth and optical properties of dilute bismide III-V semiconductor alloys, DANIEL A. BEATON, T. CHRISTIAN, Nat’l Renewable Energy Lab, R.B. LEWIS, Paul-Drude-Institut für Festkörperphysik, K. ALBERI, A. MASCARENHAS, Nat’l Renewable Energy Lab — The dilute bismuth containing III-V semiconducting alloys of great potential for application in many areas of semiconductor technology, such as multijunction photovoltaics and solid-state lighting. There is a large reduction of the fundamental bandgap of GaAs with bismuth incorporation resultant from the raising of the valence band maximum. Dilute bismide alloys have long been compared to the dilute nitride alloy because bismuth introduces a state near the valence band edge of the host GaAs (in contrast to the conduction band edge in the nitride alloys) that affects its optical and electronic properties. Here I will discuss some recent advances in our understanding of the surface processes involved in dilute bismide alloy growth by molecular beam epitaxy which have lead to improved film quality and the potential utility to MBE growth of complex multilayer structures. The improved film quality has made it possible to further explore the properties of this material.

12:51PM M9.00009 Interplay of film thickness and laser fluence in laser-crystallized silicon films, MATTHEW R. SEMLER, JUSTIN M. HOEY, SRINIVASAN GURUVENKET, CODY R. GETTE, ORVEN F. SWENSON, ERIK K. HOBIE, NDSU — A detailed study of the laser crystallization of amorphous silicon thin films as a function of laser fluence and film thickness will be presented. Silicon films grown through plasma-enhanced chemical vapor deposition were crystallized with a pulsed, neodymium-doped vanadate laser, operating at 355 nm. The crystallinity, morphology, and optical and electronic properties of the films are characterized through transmission and reflectance spectroscopy, resistivity measurements, Raman spectroscopy, X-ray diffraction, atomic force microscopy, and optical and scanning-electron microscopy. The films reveal a unique surface morphology that strongly couples to the electronic characteristics of the films, with a minimum laser fluence at which the film properties are optimized.
1:03PM M9.00010 Investigation of Nanodiamond and Silicon Carbide Foils Product for H-Stripping to Support Spallation Neutron Source1, GARY HARRIS2, JAMES GRIFFIN, Howard Univ, RD VISPUTTE, Bluewave Semiconductor. CIQM COLLABORATION — Diamond and silicon carbide (SiC) is an ideal material as an H-stripper foil for spallation neutron source (SNS) applications due to their high thermal conductivity, low molecular weight, and strength. Cubic silicon carbide grown on silicon is a material tension stress and the foil does not curl. Polycrystalline diamond is characterized by a high degree of internal stress, which causes the foil to curl when not supported by the substrate. the sic is grown using a RF CVD system. Hot filament chemical vapor deposition (HFCVD) was used to grow diamond on a silicon substrate. In both cases a 1.2 cm diameter window was etched in the silicon using a 1.13 solution of hydrofluoric, nitric, and acetic acids so that the diamond of SiC foil would be suspended while being supported on all sides by the silicon. Wax and or photoresist were used as masks to protect the outer silicon from etching. Raman spectroscopy verified the quality of the grown material. Atomic force microscopy (AFM) revealed that the diamond foil originally against the substrate had an average roughness of <6.7 nm while the foil away from the substrate had an average roughness of 13.2 nm. The SiC foils had roughness less than 3 nm. Scanning electron microscopy (SEM) revealed no cracks in the suspended foil.

1:15PM M9.00011 Synthesis and structural characterization of Nb2O5, LEONILSON KIYOSHI HERVAL, DRIELE VON DREIFUS, ADRIANO C. RABELO, ARIANO D. RODRIGUES, YARA GALVÃO GOBATO, ADILSON J.A. DE OLIVEIRA, ERNESTO C. PEREIRA, MARCIO P.F. DE GODOY, Universidade Federal de Sao Carlos, LABORATÓRIO INTERDISCIPLINAR DE ELETROQUÍMICA & CERÂMICA - DEPARTAMENTO DE QUÍMICA, GROUP DE DOPTELETRÔNICA E MAGNETO-ÓPTICA - DEPARTAMENTO DE FÍSICA — Niobium and niobium alloys are used in a large number of industrial applications. Niobium Pentoxide (Niobic Anhydride, Nb2O5) is probably the commonest compound of niobium. It is a colourless, stable solid that is fairly unreactive and it is the main precursor to all materials with application in electronic components such as capacitor and optical glasses. In general Nb2O5 samples present many crystalline phases which are strongly dependent on the preparation parameters. We have studied two different phases (hexagonal and orthorhombic) of Nb2O5 synthesized by Pechini method and characterized them by X-Ray Diffraction (XRD), Raman spectroscopy and Magnetometry using a Superconducting Quantum Interference Device (SQUID). Our results show that the hexagonal phase dominates for samples prepared at 500°C while the orthorhombic phase is increased for samples prepared at 600°C. Correlation between Raman spectroscopy and XRD allowed the identification of these crystalline phases as well the study of annealing effects in-situ. Both phases are paramagnetic and the orthorhombic phase presents a significant increase of effective magnetic moments as compared to hexagonal phase.

1:27PM M9.00012 Kondo effect in a novel 5d quasi-skutterudite Yb3O5SiGe3, YUGUO SHI, CHONGJING YANG, XIA WANG, XU ZHANG, DESHENG WU, YIFENG YANG, JIANLIN LUO, Beijing National Laboratory for Condensed Matter Physics & Institute of Physics, Chinese Academy of Science — We report the crystal growth of a new compound, Yb3O5SiGe3, by using a Bi-flux method. It crystalizes in the quasi-skutterudite-type caged structure with a cubic space group of Pm-3n (No. 223). Magnetic measurements reveal almost fully localized Yb f-moments above 120 K. The resistivity exhibits a crossover from metallic to insulating behavior with a logarithmic increase below ~ 40 K. The specific heat coefficient shows a rapid upturn below ~ 5 K and exceeds 2 J mol^-1 K^-2 at 2 K. Our experimental analysis and electronic band structure calculations demonstrate that Yb3O5SiGe3 exhibits the Kondo effect due to strong hybridization of the localized Yb f-moments with the p-electrons of the surrounding Ge-cages.

1:39PM M9.00013 Formation of ST12 phase Ge nanoparticles in ZnO thin films, ABDULLAH CECILYAN, Department of Physics Engineering, Hacettepe University, 06800, Ankara, Turkey, EMRE GUMRUKCU, Department of Nanotechnology and Nanomedicine, Hacettepe University, 06800, Ankara, Turkey — In this work, we investigate the effects of reactive and nonreactive growth of ZnO on the rapid thermal annealing (RTA) induced formation of Ge nanoparticles (Ge-np) in ZnO: Ge nanocomposite thin films. The samples were deposited by sequential sputtering of ZnO and Ge thin film layers with a total thickness of about 600 nm on Si substrates followed by an ex-situ (RTA) at 600°C for 30, 60, 90, 120, 150, 180, and 210 s under forming gas atmosphere. In order for the reactive sputtering of Ge, 5 mTorr Oxygen was introduced to the growth chamber. XRD and Raman analyses were utilized to investigate the effect of RTA time on the structural evolution of the samples. It has been realized that crystal structure of Ge nanoparticles is significantly affected by the growth method of the embedding ZnO layer. While reactive deposition of ZnO layers results in a mixture of diamond cubic (DC) and simple tetragonal (ST12) Ge-np, nonreactive deposition of ZnO layers leads to the formation of pure DC Ge-np upon RTA process. Formation of these two phases has been discussed based on the existence of native point defects such as oxygen vacancies and Zn interstitials.

1:51PM M9.00014 Single Element Silicon Quasicrystal on Glass, ABDUL MIDDYA, Silicon Solar, Inc., PROF. KARTIK GHOSH, PHYSICS, MATERIAL'S SCIENCE AND ASTRONOMY, MISSOURI STATE UNIVERSITY, MO 65804 COLLABORATION — Quasicrystal is an exotic form of ordering of materials structure found in nature. In this work, we report on formation of single element silicon (Si) quasicrystal, instead of metallic alloys. We found small quantity of quasicrystalline silicon on glass substrate when silicon (Si) and atomic hydrogen (H) atoms in vacuum chamber are allowed to condense on glass substrate maintained at 250°C in hot wire chemical vapor deposition (hot-wire CVD) technique. We observed Penrose tiling at the surface of silicon thin-film as observed by atomic force microscopy (AFM). However, this texturing consists of six-fold symmetry and five-fold symmetry on the surface of spherical ball. We found experimental evidence of the quasi-unit cell, building blocks of quasicrystalline structure. The ordering of quasi-unit cell improves with increasing hydrogen dilution. The Raman transverse optical (TO) peak is observed at 517 cm-1, although the grain size is only 1 to 2 μm. We also found, for the first time, direct experimental evidence of real existence of crystallographic plane in crystal structure. The micrograph of SEM shows grains appear in a very symmetric position, like diffraction spots of ceramics (alloy), we found ceramics-like silicon thin-film.

2:03PM M9.00015 Increasing The Efficiency of Silicon Solar Cells via an Anti-reflecting Nanoporous Surface Layer, AHMET COSKUNER, AISHA GOKCE, OMER ALTUNAY, YANI SKARLATOS, OZHAN OZTAY, Bogazici Univ — Electrochemical etching of silicon in a controlled environment results in a porous surface that has many application areas from drug delivery to optoluminescent devices. There is vast interest in implementing porous silicon in silicon solar cells to increase light absorption and therefore the efficiency. Here we demonstrate successful formation of a nano-porous surface on monocrystalline Si wafers as well as doped Si solar cells. Our results show that pre-cleaning and post-drying is crucial to acquire a smooth, non-cracked topography. We also find that under similar conditions, smaller pores in a denser arrangement and with shorter depths form in p-n junction type Si wafers compared to n-type or p-type Si. In ITO coated porous Si solar cells with Al back contacts, the measured efficiency increase is almost 50% of those without a porous surface. This is a promising result to further enhance the performance of Si solar cell devices.

Wednesday, March 4, 2015 11:15AM - 2:15PM – Session M10 DCMP: Anomalous Quantum Hall Effect 007A - James Williams, University of Maryland
Quantum Anomalous Hall state.

on a large scale, whereas constant pseudo-magnetic fields are generally limited to the nanoscale. The electronic properties of these systems being fundamentally

examples in mind, we discuss several different physical implementations. Periodically modulated strain fields hold the promise of realizing Quantum Hall physics

lead to partially flat bands resembling Landau level quantization due to pseudo-magnetic fields. These partially flat pseudo-Landau levels occur in systems such

Jorn W.F. Venderbos, Liang Fu, Massachusetts Inst of Tech-MIT — In this work we show how periodically modulated strain fields

Periodically modulated strain fields offer a flexible system to study quantum spin Hall edge transport as well as to build more complex 1d circuits. We will also discuss the possibility for fractional

a quantum spin Hall state where edge states in each layer counter-propagate in opposite directions with opposite spin polarizations. This bilayer realization

opposite chiralities, resulting in coexisting electron- and hole-like states. We will present evidence that, in this regime, the twisted bilayer graphene can form

in the bulk, while opening the door for interesting interactions at the edges. To probe this physics, we study the electronic transport through quantum Hall edge

a gap in the surface states, but gives rise to dissipationless chiral conduction at the edge of a magnetized film. Ideally, this leads to vanishing longitudinal

Magnetic resistance associated to spin spur is given by the following universal expression:

\[ R_{xx} = \frac{h}{e^2} \left| \frac{\nu_{xy}}{\nu_{yy}} \right| \]

\[ \sigma_{xx} \] is the electron charge, but perfect quantization has so far proved elusive. Here, we study the QAHE in the limit of zero applied magnetic field, and measure Hall resistance quantized to within one part per 10,000. Deviation from quantization is due primarily to thermally activated carriers, which can be nearly eliminated through adiabatic demagnetization cooling. This result demonstrates an important step toward dissipationless electron transport in technologically relevant conditions.

11:27AM M10.00002 Universal scaling of the quantum anomalous Hall plateau transition1. Jing Wang, Biao Lian, Shou-Cheng Zhang, Stanford Univ — We study the critical properties of the quantum anomalous Hall (QAH) plateau transition in magnetic topological insulators. We introduce a microscopic model for the plateau transition in the QAH effect at the coercive field and then map it to the network model of quantum percolation in the integer quantum Hall effect plateau transition. Generally, an intermediate plateau with zero Hall conductance could occur at a coercive field. \( \sigma_{yx} \) would have double peaks when the corresponding single peak has single peak. Remarkably, this theoretical prediction is already borne out in experiment. Universal scaling of the transport coefficients \( \rho_{xy} \) and \( \rho_{xx} \) are predicted.

\[ \frac{E}{T} = \frac{1}{\hbar} \left( \frac{1}{2\pi k_B T} \right)^{1/2} \left( \frac{N}{L} \right)^{1/2} \]

\[ \frac{1}{\lambda} = \frac{1}{L} \left( \frac{N}{L} \right)^{1/2} \]

This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-AC02-76SF00515.

11:39AM M10.00003 Tunable Anderson metal-insulator transition in quantum spin Hall insulators, Chui-Zhen Chen, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, Haiwen Liu, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China, Huai Jiang, College of Physics, Optoelectronics and Energy, Soochow University, Suzhou 215006, China, Qing-Feng Sun, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China, Ziqiang Wang, Department of Physics, Boston College, Chestnut Hill, Massachusetts 02167, USA, X.C. Xie, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China — We study disorder effects in Bernevig-Hughes-Zhang (BHZ) model (unitary system), and find that Anderson transition of quantum spin Hall insulator (QSHI) is determined by model parameters. In contrast to the common belief that 2D unitary system scales to insulator except at certain critical points, we find that an exotic metallic phase emerges between QSHI and normal insulator phases in InAs/GaSb-type BHZ model. On the other hand, direct transition from QSHI to normal insulator is found in HgTe/CdTe-type BHZ model. Furthermore, we show that the metallic phase originates from the Berry phase and can survive both inside and outside the gap.

11:51AM M10.00004 Spin Texture and Mirror Chern number in Hg-Based Chalcogenides1. Qing-Ze Wang, The Pennsylvania State University, Shu-Chun Wu, Claudia Felser, Max Planck Institute for Chemical Physics of Solids, Binghai Yan, Max Planck Institute for Chemical Physics of Solids, & Max Planck Institute for Physics of Complex Systems, Chao-Xing Liu, The Pennsylvania State University — One special feature of surface state in topological insulators is the so-called spin-momentum locking, which means that electron spin is oriented along a fixed direction for a given momentum and forms a texture in the momentum space. In this work, we study spin textures of two typical topological insulators in Hg-Based Chalcogenides, namely HgTe and HgS, based on both the first principle calculation and the eight band Kane model. We find opposite helicities of spin textures between these two materials, originating from the opposite signs of spin-orbit couplings. Furthermore, we reveal that different mirror Chern numbers between HgTe and HgS characterize different topological natures of the systems with opposite spin textures and guarantee the existence of gapless interface states.

2 This work is supported by ERC Advanced Grant (291472).

12:03PM M10.00005 Edge states in twisted bilayer graphene: quantum spin Hall and electron-hole bilayers. Javier D. Sanchez-Yamagishi, Jason Luo, Massachusetts Institute of Technology, Kenji Watanabe, Takashi Taniguchi, National Institute of Materials Science, Japan, Pablo Jarillo-Herrero, Massachusetts Institute of Technology — Twisted bilayer graphene offers a unique platform for studying 1d edge states in a bilayer 2-dimensional electron gas. Despite being spaced by only 0.34 nm, a large interlayer twist decouples the layers in the bulk, while opening the door for interesting interactions at the edges. To probe this physics, we study the electronic transport through quantum Hall edge modes twisted bilayer graphene devices. Using a large electrostatic gate, we independently control the filling factor of each layer to form different combinations of bilayer edge states while measuring their conductance. The most dramatic transport effects are observed when the layers are doped to have edge states of opposite chiralities, resulting in coexisting electron- and hole-like states. We will present evidence that, in this regime, the twisted bilayer graphene can form a quantum spin Hall state where edge states in each layer counter-propagate in opposite directions with opposite spin polarizations. This bilayer realization offers a flexible system to study quantum spin Hall edge transport as well as to build more complex 1d circuits. We will also discuss the possibility for fractional generalizations of this edge physics and our measurements of the fractional QHE in twisted bilayer graphene.

12:15PM M10.00006 ABSTRACT WITHDRAWN

12:27PM M10.00007 Interaction induced topological phases in partially flat band graphene-like systems. Jorn W.F. Venderbos, Liang Fu, Massachusetts Inst of Tech-MIT — In this work we show how periodically modulated strain fields lead to partially flat bands resembling Landau level quantization due to pseudo-magnetic fields. These partially flat pseudo-Landau levels occur in systems such as graphene or at the interface between a trivial and topological crystalline insulator, where in both cases strain fields couple as pseudo-gauge fields. With these examples in mind, we discuss several different physical implementations. Periodically modulated strain fields hold the promise of realizing Quantum Hall physics on a large scale, whereas constant pseudo-magnetic fields are generally limited to the nanoscale. The electronic properties of these systems being fundamentally altered by the formation of these flat bands, we investigate the effect of electron-electron interaction and find that they induce topological phases, notably the Quantum Anomalous Hall state.

11:15AM M10.00001 Precise quantization of anomalous Hall effect near zero magnetic field. Andrew Bestwick, Eli Fox, Stanford University, Xufeng Kou, Lei Pan, Kang Wang, University of California, Los Angeles, David Goldhaber-Gordon, Stanford University — The quantum anomalous Hall effect (QAHE) has recently been of great interest due to its recent experimental realization in thin films of Cr-doped (Bi, Sb)\(_2\)Te\(_3\), a ferromagnetic 3D topological insulator. The presence of ferromagnetic exchange breaks time-reversal symmetry, opening a gap in the surface states, but gives rise to dissipationless chiral conduction at the edge of a magnetized film. Ideally, this leads to vanishing longitudinal resistance and Hall resistance quantized to \( h/ e^2 \), where \( h \) is Planck’s constant and \( e \) is the electron charge, but perfect quantization has so far proved elusive. Here, we study the QAHE in the limit of zero applied magnetic field, and measure Hall resistance quantized to within one part per 10,000. Deviation from quantization is due primarily to thermally activated carriers, which can be nearly eliminated through adiabatic demagnetization cooling. This result demonstrates an important step toward dissipationless electron transport in technologically relevant conditions.
12:39PM M10.00008 Optimizing proximity induced anomalous Hall effect in (Bi$_{1-x}$Sb$_x$)$_2$Te$_3$/YIG heterostructures. ZILONG JIANG, CHI TANG, JING SHI, UC Riverside, CUIZU CHANG, PENG WEI, JAGADEESH S. MOODERA, MIT — The spontaneously broken time reversal symmetry leads to an energy gap in the Dirac spectrum of the surface states of a topological insulator (TI) which gives rise to the quantized anomalous Hall effect (QAHE). QAHE has been observed in TI doped with Cr. Here we explore an alternative route by coupling the surface states of TI with yttrium iron garnet (YIG) ferrimagnetic insulator (FI). Just as in Cr-doped TI, a major challenge is to reduce the bulk conduction which overwhelms the surface state contribution. We have successfully grown 5 quintuple layer thick ternary (Bi$_{1-x}$Sb$_x$)$_2$Te$_3$ on atomically flat YIG films, in which the Fermi level of TI can be controlled by the Bi:Sb ratio. We have observed the anomalous Hall effect (AHE) in TI/YIG heterostructure over a wide range of carrier density and in both electron and hole types induced by varying the Bi:Sb ratio from 0:1 to 1:0. Both $R_{xx}$ and $R_{XY}$ undergo systematic and dramatic changes as the Bi:Sb ratio is varied. The maximum $R_{XY}$ occurs near the p-n cross-over region at Bi:Sb ratio 0.2:0.8, which is nearly two orders of magnitude greater than the minimum value at Bi:Sb ratio 1:0. As the Bi:Sb ratio is varied, we find that $R_{AH}$ scales quadratically with $R_{xx}$ indicating the scattering rate independent AHE. The electric field effect study further demonstrates the existence of robust AHE while the Fermi level of TI is tuned. This research was supported by UC Lab fees program and a DOE/BES award at UCR, and by NSF/DMR at MIT.

[2] Brüne et al. PRL 106,126803(2011);

1:03PM M10.00010 Honeycomb lattice with multiorbital structure: Topological and quantum anomalous Hall insulators with large gaps. GU-FENG ZHANG, Univ of California - San Diego, YI LI, Princeton University, CONJUIN WU, Univ of California - San Diego — We construct a minimal four-band model for the two-dimensional topological insulators and quantum anomalous Hall insulators based on the $p_z$- and $p_y$-orbital bands in the honeycomb lattice. The multiorbital structure allows the atomic spin-orbit coupling which lifts the degeneracy between two sets of on-site Kramers doublets $j_z = \pm \frac{3}{2}$ and $j_z = \pm \frac{1}{2}$. Because of the orbital angular momentum structure of Bloch-wave states at $\Gamma$ and $K(K')$ points, topological gaps are equal to the atomic spin-orbit coupling strengths, which are much larger than those based on the mechanism of the $s-\pi$ band inversion. The energy spectra and eigen wave functions are solved analytically based on Clifford algebra. The competition among spin-orbit coupling $\lambda$, sublattice asymmetry $m$, and the Néel exchange field $n$ results in band crossings at $\Gamma$ and $K(K')$ points, which leads to various topological band structure transitions. The quantum anomalous Hall state is reached under the condition that three gap parameters $\lambda$, $m$, and $n$ satisfy the triangle inequality. Flat bands also naturally arise which allow a local construction of eigenstates. The above mechanism is related to several classes of solid state semiconductor.

1:15PM M10.00011 Observation of topological surface state quantum Hall effect in an intrinsic three-dimensional topological insulator. YANG XU, IRENEUSZ MIOTKOWSKI, YONG CHEN, Department of Physics and Astronomy, Purdue University, West Lafayette, IN 47907, YONG P.CHEN'S GROUP IN PURDUE TEAM, CHIH-KANG SHIH'S GROUP IN UT-AUSTIN COLLABORATION, M. ZAHID HASAN'S GROUP IN PRINCETON COLLABORATION — A three-dimensional (3D) topological insulator (TI) is a novel quantum matter with a gapped insulating bulk yet a conducting surface hosting topologically-protected gapless surface states of Dirac fermions. One of the most distinct electronic transport signatures predicted for such topological surface states (TSS) is a half-integer quantum Hall effect (QHE) in a magnetic field. We have observed well-developed QHE arising from TSS in an intrinsic TI of Bi$_2$Se$_3$. Our samples can exhibit surface dominated conduction even close to room temperature, while the bulk conduction is negligible. At low temperatures and high perpendicular magnetic fields, the Hall conductance shows well quantized integer plateaux in exfoliated flake devices on SiO$_2$/Si substrates, where the top and bottom surface each contributing a half integer $e^2/h$ Hall conductance, accompanied by vanishing longitudinal resistance. We have also studied dual-gated devices where both the top and bottom surfaces can be independently gated. Such intrinsic 3D TI materials exhibiting no measurable bulk conduction and well-developed surface state QHE pave the way for further applications of topological quantum electronics.

[2] DARPA Meso program (Grant N66001-11-1-4107)

1:27PM M10.00012 Giant Band Gap Quantum Spin Hall Phase with Weak Spin-Orbit Coupling. ZHIGANG WU, MARC DVORAK, Colorado Sch of Mines — The typical quantum spin hall (QSH) insulator relies on spin-orbit (SO) coupling to open a band gap in the bulk material. However, the intrinsic SO coupling is often rather weak, especially in graphene, and most researchers have focused on enhancing the SO interaction, e.g., by adsorbing heavy adatoms, to increase the bulk band gap. We have demonstrated that if patterned properly, periodic defects on graphene are able to induce intervalley scattering between Dirac points and then open a large ($\sim 1$ eV) bulk band gap. Using both tight-binding method and density functional theory, we explore the possibility of creating a QSH insulator in a graphene nanomesh. We find that an arbitrarily weak SO coupling is able to induce the spin-filtered edge states to traverse the bulk band gap. Here the SO coupling is not responsible for band gap opening, but only serves to connect the K and K' points, leading to a QSH phase with a giant band gap without the existence of strong SO coupling.

[3] This work was supported by a U.S. DOE Early Career Award (Grant No. DE-SC0006433).

— Recently, this long-sought quantum anomalous Hall effect was realized in the magnetic topological insulator. However, the requirement of an extremely low temperature (~30 mK) hinders realistic applications. Based on honeycomb lattices comprised of Sn and Ge, which are found to be 2D topological insulators, we propose a quantum anomalous Hall platform with low energy gap of 0.34 and 0.06 eV, respectively. The ferromagnetic order forms in one sublattice of the honeycomb structure by controlling the surface functionalization rather than dilute magnetic doping, which is expected to be visualized by spin polarized STM in experiment. Strong coupling between the inherent quantum spin Hall state and ferromagnetism results in considerable energy splitting and consequently an ferromagnetic insulator with large energy gap. The estimated mean-field Curie temperature is 243 and 599 K for Sn and Ge lattices, respectively. The large energy gap and high Curie temperature indicate the feasibility of the quantum anomalous Hall effect in the near-room-temperature and even room-temperature regions. Ref: S.-C.Wu, G. Shan, B. Yan, arXiv:1405.4731 (2014).

1 We thank the helpful discussions with C. Felser, S. Kanugo, C.-X. Liu, Z. Wang, Y. Xu, K. Wu, and Y. Zhou.

1:51PM M10.00014 Electronic Structure of Quantum Spin Hall Parent Compound CdTe, GUANG BIAN, Department of Physics, Princeton University — Cadmium telluride, a compound widely used in devices, is a key base material for the experimental realization of the quantum spin Hall phase. The electronic structure of CdTe has been studied by various theoretical and experimental methods. However, high-resolution band mapping has been lacking to this date. The detailed low-energy electronic structure of CdTe is thus unavailable, but it is of fundamental importance for understanding the topological properties and trends of this type of materials. We report herein, for the first time, a systematic study of the electronic structure of CdTe by angle-resolved photoemission spectroscopy from well-ordered (110) surfaces. The results are compared with first-principles calculations to illustrate the topological distinction between CdTe and a closely related compound HgTe. In addition, topological phase transition from CdTe to HgTe upon alloying and the massless Dirac-Kane semimetal phase at the critical composition are illustrated by computations based on a mixed-pseudopotential simulation.

2:03PM M10.00015 Unexpected edge conduction in HgTe quantum wells under broken time reversal symmetry, ERIC YUE MA, M. REYES CALVO, JING WANG, BIAO LIAN, Stanford University, MATTHIAS MUEHLBAUER, CHRISTOPH BRUNE, Universität Würzburg, YONGTAO CUI, Stanford University, KEJI LAI, UT Austin, WORASOM KUNDHIKANJANA, YONGJIANG YANG, MATTHIAS BAENNINGER, MARKUS KONIG, Stanford University, CHRISTOPHER AMES, HARTMUT BUEHMANN, PHILIPP LEUBNER, LAURENS MOLENKAMP, Universität Würzburg, SHOU-CHENG ZHANG, DAVID GOLDBERGER-GORDON, MICHAEL KELLY, ZHI-XUN SHEN, Stanford University — A key prediction of quantum spin Hall (QSH) theory that remains to be experimentally verified is the breakdown of the edge conduction under broken TRS by a magnetic field. Here we use a unique cryogenic microwave impedance microscopy (MIM) on two HgTe QW devices, corresponding to a trivial (5.5 nm) and an inverted (7.5 nm) band structure, to find unexpectedly robust edge conduction under broken TRS. At zero field and low carrier densities, clear edge conduction is observed only in the local conductivity profile of the 7.5 nm device, consistent with QSH theory. Surprisingly, the edge conduction persists up to 9 T with little effect from the magnetic field, as confirmed by both transport and real space MIM images. This indicates physics beyond current simple QSH models, possibly associated with material-specific properties, other symmetry protection and/or electron-electron interactions.

Wednesday, March 4, 2015 11:15AM - 2:15PM – Session M11 DCMP: Superconductivity: Mostly Meso-Nano Scale 007B - Timir Datta, University of South Carolina

11:15AM M11.00001 Size dependent suppression of superconductivity in granular mesoscopic Nb islands. MALCOLM DURKIN, University of Illinois at Urbana-Champaign, SARANG GOPALAKRISHNAN, Harvard University, RITA GARRIDO MENACHO, NADYA MASON, University of Illinois at Urbana-Champaign — While the suppression of superconductivity has been studied in bulk, 2D, and 1D systems, it remains largely unstudied in systems of mesoscopic granular islands. We investigate critical temperature ($T_c$) suppression in mesoscopic granular Nb islands as a function of island diameter. By performing transport measurements, we find that superconductivity is suppressed at diameters considerably larger than the coherence length of Nb. This behavior cannot be explained by competition between charging and Josephson energies. Instead, variations in island $T_c$ for fixed diameters suggest that the onset—and suppression—of superconductivity may be determined by rare region effects.

11:27AM M11.00002 Origin of superconductivity and ferromagnetism in Bi/Ni/Bi sandwich trilayers1, WEIWEI ZHAO, Center for Nanoscale Science and Physics Department, PSU, CUI-ZU CHANG, Francis Bitter Magnet Lab, MIT, DUK-Y KIM, Physics Department, PSU, JAGADEESH MOODERA, Francis Bitter Magnet Lab and Physics Department, MIT, MOSES CHAN, Center for Nanoscale Science and Physics Department, PSU — Coexistence of superconductivity and ferromagnetism was experimentally observed in Bi/Ni bilayers [PRL 94, 037006 (2005)]. To reveal the origin of the superconductivity in this system, we here systematically studied the superconductivity and the ferromagnetism in Bi/Ni/Bi trilayers, Bi/Ni bilayers and Ni/bilayers. We found the superconducting transition temperature to be independent of the thickness of Ni layers from 1nm to 45nm in Bi/Ni/Bi trilayers. The superconducting critical magnetic fields of trilayers were higher than those of bilayers. In addition, we observed conventional ferromagnetism in both trilayers and bilayers. These observations can be explained by a model that the superconductivity originates from the Bi/Ni interfaces with spin triplet pairing.

1This research is supported by the NSF grants (DMR-0820404, Penn State MRSEC; DMR-1207469, MIT).

11:39AM M11.00003 Electron Pairing Without Superconductivity 1. JEREMY LEVY, G. CHENG, M. TOMCZYK, S. LU, University of Pittsburgh, J.P. VEAZEY, Grand Valley State University, M. HUANG, P. IRVIN, University of Pittsburgh, S. RYU, H. LEE, C.-B. EOM, University of Wisconsin-Madison, C.S. HELLBERG, Naval Research Laboratory — Strontium titanate (SrTiO$_3$) exhibits an extremely low carrier density threshold for superconductivity, and possesses a phases diagram similar to high-temperature superconductors. Two factors that suggest an unconventional pairing mechanism. We describe transport experiments with nanowire-based quantum dots localized at the interface between SrTiO$_3$ and LaAlO$_3$. Electrostatic gating of the quantum dot reveals a series of two-electron conductance resonances—paired electron states—that bifurcate above a critical magnetic field B$_c$, an order of magnitude larger than the superconducting critical magnetic field. For B$<$B$_c$, these resonances are insensitive to applied magnetic fields; for B$>$B$_c$, the resonances exhibit a linear Zeeman-like energy splitting. Electron pairing is stable at temperatures as high as an order of magnitude larger than the superconducting critical magnetic field. However, the requirement of an extremely low temperature (~30 mK) hinders realistic applications. Based on honeycomb lattices comprised of Sn and Ge, which are found to be 2D topological insulators, we propose a quantum anomalous Hall platform with low energy gap of 0.34 and 0.06 eV, respectively. The ferromagnetic order forms in one sublattice of the honeycomb structure by controlling the surface functionalization rather than dilute magnetic doping, which is expected to be visualized by spin polarized STM in experiment. Strong coupling between the inherent quantum spin Hall state and ferromagnetism results in considerable energy splitting and consequently an ferromagnetic insulator with large energy gap. The estimated mean-field Curie temperature is 243 and 599 K for Sn and Ge lattices, respectively. The large energy gap and high Curie temperature indicate the feasibility of the quantum anomalous Hall effect in the near-room-temperature and even room-temperature regions. Ref: S.-C.Wu, G. Shan, B. Yan, arXiv:1405.4731 (2014).

1This work was supported by ARO MURI W911NF-08-1-0317 (J.L.), AFOSR MURI FA9550-10-1-0524 (C.-B.E., J.L.) and FA9550-12-1-0342 (C.-B.E.), and grants from the National Science Foundation DMR-1104191 (J.L.), DMR.
11:51 AM M11.00004 Andreev Bound States in Confined Superconducting Semiconductor Nanowires1, GUANGLEI CHENG, MICHELLE TOMCZYK, SHICHEANG LIU, JOSH VEAZEY2, MENGCHEN HUANG, PATRICK IRVIN, JEREMY LEVY, University of Pittsburgh, HYUNGWOO LEE, SANWOON RYU, CHANG-BEOM EOM, University of Wisconsin-Madison — The hybridization of superconductors (SC) and semiconducting nanowires leads to a variety of interesting phenomena including nanoscale superconductivity and Majorana fermion physics. Andreev bound states (ABS), which are a discrete energy spectrum as a result of Andreev reflections of electrons and holes between two normal-SC interfaces, are predicted to support Majorana bound states under certain conditions. The LaAlO$_3$/SrTiO$_3$ interface possesses native superconductivity and strong spin-orbit coupling and is thus a promising platform for observing signatures of Majorana fermions. Here we investigate a superconducting nanowire quantum dot created by reversible “write” and “erase” processes using a conductive atomic force microscope tip. Transport studies show that electrons can travel in different regimes dominated by resonant pair tunneling and Andreev reflection in a single device.

1This work was supported by ARO (W911NF-08-1-0317), AFOSR (FA9550-10-1-0524 and FA9550-12-1-0342), and NSF (DMR-1104191, DMR-1124131, and DMR-1234096).

2Present Address: Grand Valley State University

12:03PM M11.00005 Detection of vortex trapping in mesoscopic single-crystal loops of NbSe$_2$ by magnetoresistance oscillations1, SHAUN MULLS, The Pennsylvania State University, CHENYI SHEN, ZHAUN XU, Zhejiang University, YING LIU, The Pennsylvania State University, Shanghai Jiao Tong University — Vortex crossing of a doubly-connected mesoscopic loop of a type II superconductor will lead to magnetoresistance oscillations because the free energy of the loop is modulated by the enclosed flux. The amplitude and temperature dependence of the oscillations in these mesoscopic loops of type II superconductors differ from the conventional Little-Parks effect. In addition to Abrikosov vortex crossing, vortex trapping within the arms of a mesoscopic loop should be possible. London calculations predict a phase shift in the free energy modulation when a single vortex is trapped within the arm of a superconducting loop. We present magnetoresistance measurements on mesoscopic, single-crystal NbSe$_2$ loops exhibiting the anticipated free energy modulation phase shift at a critical vortex trapping field that can be tuned by sample geometry, temperature, and external current in agreement with theoretical expectations.

1Work supported in part by the NSF under Grant DMR 0908700 with nanofabrication done at the Penn State MRI Nanofabrication Lab under NSF Cooperative Agreement 0335765, NNIN with Cornell University. Work in China supported by MOST of China and NSFC.

12:15PM M11.00006 Andreev states in the spin-symmetric solution of a quantum dot attached to superconducting leads, VAACLAV JANIS, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, VLADISLAV POKORYN, Institute of Physics, ASCR, Prague, Czech Republic — A quantum dot with Coulomb repulsion attached to left and right superconducting leads is studied via the perturbation expansion in the interaction strength. We use the Nambu formalism and the standard many-body diagrammatic representation of the impurity Green functions. We formulate the perturbation expansion in the spectral representation so that to be able to separate contributions from the isolated gap states (Andreev bound states) and from the continuous band states. We resolve exactly the spin-symmetric state in the asymptotic limit with Andreev states approaching the Fermi energy. We demonstrate that a spin-symmetric state reaches saturation at zero temperature at a critical interaction at which the Andreev states merge and freeze at the Fermi energy. There is no solution above this critical interaction with Andreev states split from the Fermi energy unless external magnetic field breaking the spin symmetry is applied and degeneracy of the ground state lifted.

12:27PM M11.00007 Splitting individual Cooper pairs and single photon detection in superconducting aluminium, MEGAN EDWARDS, NICHOLAS LAMBERT, ADAM ESMAIL, ANDREW FERGUSON, University of Cambridge, BRENDON LOVETT, University of St. Andrews, FELIX POLLOCK, University of Oxford, UNIVERSITY OF CAMBRIDGE TEAM, UNIVERSITY OF OXFORD/UNIVERSITY OF ST. ANDREWS TEAM1 — Using superconducting aluminium quantum dots, we demonstrate the splitting of individual Cooper pairs using microwave light [1]. Within our nanoscale devices, the competition at low temperatures between the charging energy, superconducting gap and Josephson energy enables single Cooper pairs to be split and reformed. The delivery of constituent quasi-particles to separate quantum dots has facilitated measurements of both splitting and recombination. The devices are probed by radio-frequency reflectometry, a technique sensitive to the ‘quantum capacitance’ of the device band structure [2]. We intentionally induce splitting via the application of a microwave field, indicating a system able to detect individual photons of microwave light [1]. To controllably separate a Cooper pair into two quasi-particles may have important implications for quantum information processing; future experiments will investigate the coupling of a double quantum dot to a microwave resonator for single photon detection [3], with applications to circuit quantum electrodynamics.


1Valuable contributions to this work have been made by a joint team from the Universities of Oxford and St. Andrews.

12:39PM M11.00008 Stripe-like nanoscale structural phase separation and optimal inhomogeneity in superconducting BaPb$_{1-x}$Bi$_x$O$_3$, PAULA GIRALDO-GALLO, Stanford University, YING ZHANG, Chinese Academy of Sciences, CAROLINA PARRA, Universidad Tecnica Federico Santa Maria, HARI MANOHARAN, MALCOLM BEASLEY, THEODORE GEBALLE, Stanford University, MATTHEW KRAMER, Ames Lab - Iowa State University, IAN FISHER, Stanford University — Structural phase separation in the form of partially disordered stripes, with characteristic length scales in the nanometer range, is observed for superconducting BaPb$_{1-x}$Bi$_x$O$_3$. The evolution of the superconducting coherence length with composition relative to the size of these stripes suggests an important role of the nanostructure in determining the shape of the superconducting dome. It is proposed that the maximum $T_c$ is determined by a kind of “optimal inhomogeneity,” characterized by a crossover from an inhomogeneous macroscopic superconductor to a granular superconductor for which phase fluctuations suppress $T_c$.

12:51PM M11.00009 ABSTRACT WITHDRAWN —
tunnel barrier strength at the critical angle as a criterion for establishing the topological nature of the observed signal. Majorana zero modes. We investigate the effect of tilting the magnetic field relative to the spin-orbit coupling direction in a simple continuum model and in the confined region on Cd$_3$3 measurements on the 3D Dirac semi-metal Cd$_3$3.

Therefore, in principle, it should be possible to drive them into exotic new phases by breaking certain symmetries. We will discuss point-contact spectroscopic circuits.

1Supported by EPSRC (UK)

1:15PM M11.00011 Strong effects of weak ac driving in short superconducting junctions

ROMAN-PASCAL RIFWAR, MANUEL HOUZET, JULIA S. MEYER, UNIV. GRENoble ALPES, INAC-SPSMS, F-38000 Grenoble, France; CEA, INAC-SPSMS, F-38000 Grenoble, France, YULI V. NAZAROV, Kavli Institute of NanoScience, TU Delft, Lorentzweg 1, NL-2628 CJ, Delft, The Netherlands — We study a short superconducting junction subject to a dc and ac phase bias. The ac modulation changes the occupation of the Andreev bound states formed at the constriction by transitions between bound states and the continuum. In a short junction, the non-equilibrium Andreev bound state population may relax through processes that conserve parity of the occupation number on the same bound state and processes that do not conserve it. We argue that the parity conserving processes occurs on a much faster time scale. In this case, even a weak driving may lead to a large deviation of the supercurrent from its equilibrium value. We show that this effect is accompanied by a quasiparticle current which may lead to a measurable charge imbalance in the vicinity of the junction. Furthermore, we study the time evolution of the supercurrent after switching off the ac drive. On a time scale where parity relaxation is negligible, the supercurrent relaxes to a stationary non-equilibrium state. Finally, we briefly outline the regime of ultraweak driving where the ac-induced processes occur on a time scale comparable to parity relaxation.

1This work has been supported by the Nanosciences Foundation in Grenoble, in the frame of its Chair of Excellence program.

1:27PM M11.00012 Weber blockade in superconducting nanowires

TYLER MORGAN-WALL, BENJAMIN LEITH, NIKOLAUS HARTMAN, ATIKUR RAHMAN, NINA MARKOVIC, Johns Hopkins University — Vortices in superconductors are topological excitations that carry quantized magnetic flux and can be viewed as basic degrees of freedom that describe the low-energy states of the system. Here we show that a short superconducting nanowire can behave as a quantum dot for vortices. In the range of magnetic fields in which vortices can enter the nanowire in a single row, we find regular oscillations of the critical current as a function of magnetic field, with each oscillation corresponding to the addition of a single vortex to the nanowire. A charge-vortex dual of the Coulomb-blockaded quantum dot for electrons, the nanowire shows diamond-shaped regions of zero resistance as a function of current and magnetic field, in which the number of vortices is fixed. Besides demonstrating that macroscopic objects such as vortices can behave as fundamental particles, the fine control over critical currents and vortex configurations may prove useful for quantum devices that employ superconducting circuits.

1This work was supported by NSF DMR-1106167.

1:39PM M11.00013 Generation of photon pairs at different frequencies: route toward quantum microwave source

DANIEL ESTEVE, OLIVIER PARLAVECCHIO, CARLES ALTIRMAS, PHILIPPE JOYEZ, DENIS VION, PATRICE ROCHE, FABIEN PORTIER, Service de Physique de l’Etat Condensé (CNRS URA 2464), IRAMIS, CEA Saclay, 91191 Gif-sur-Yvette, France, NANOELECTRONICS-QUANTRONICS GROUPS COLLABORATION — The dynamical Coulomb blockade (DCB) is a quantum phenomenon that隧tunneling of charge through a tunnel junction is modified by its electromagnetic environment. The sudden charge transfer generates photons in the electromagnetic modes. We coupled a Josephson junction to two resonators at frequencies $\nu_1 \neq \nu_2$ when voltage-biased at $2\nu_1 = h\nu_1 + h\nu_2$. Cooper pairs can tunnel only if two photons, one at each frequency, are simultaneously emitted. We measured the cross-correlations between the emission rates and showed that a Cauchy-Schwarz inequality is violated. This result, in agreement with theoretical prediction made by Leppakkangas and coworkers, reveals the amplitude two-mode squeezing. Our setup is a easy way to produce non-classical microwave radiation from a battery. We believe that this source is a good candidate for producing pairs of entangled photons with high rate (few hundreds of MHz).


1:51PM M11.00014 Point-contact spectroscopy on the 3-Dimensional Dirac Semi-metal Cd$_3$As$_2$

GOUTAM SHEET, ABHISHEK GAURAV, Indian Institute of Science Education and Research, Mohali, GOHIL SINGH THAKUR, ZEBA HAQUE, Department of Chemistry, Indian Institute of Technology, New Delhi, ASHOK KUMAR GANGULI, Institute of Nano Science & Technology, Mohali, LEENA AGGARWAL, Indian Institute of Science Education and Research, Mohali — The three dimensional (3D) Dirac semi-metals exist close to topological phase boundaries. Therefore, in principle, it should be possible to drive them into exotic new phases by breaking certain symmetries. We will discuss point-contact spectroscopic measurements on the 3D Dirac semi-metal Cd$_3$As$_2$ using several normal metallic tips. We have found that the mesoscopic point-contacts between elemental normal metals (like silver (Ag), platinum (Pt) and gold (Au)) and Cd$_3$As$_2$ exhibit signatures of certain exotic new phases. The possible origin of such phases in the confined region on Cd$_3$As$_2$ will also be discussed.

2:03PM M11.00015 Tilting of the magnetic field in Majorana nanowires

STEVEN REX, ASLE SUDBO, Department of Physics, Norwegian University of Science and Technology — Semiconductor nanowires with strong spin-orbit coupling and proximity-induced $s$-wave superconductivity in an external magnetic field have been the most promising settings for approaches towards experimental evidence of topological Majorana zero modes. We investigate the effect of tilting the magnetic field relative to the spin-orbit coupling direction in a simple continuum model and provide an analytical derivation of the critical angle, at which the topological states disappear. We also obtain the differential conductance characteristic of a junction with a normal wire for different tilting angles and propose a qualitative change of the dependence of the zero-energy differential conductance on the tunnel barrier strength at the critical angle as a criterion for establishing the topological nature of the observed signal.

1Supported by the Norwegian Research Council, Grant Nos. 205591/V20 and 216700/F20.

Wednesday, March 4, 2015 11:15AM - 2:15PM — Session M12 DCMP: Exotic Topological Superconductors II 007C - Dale Van Harlingen, University of Illinois
11:15AM M12.00001 Symbiosis of ferromagnetism and superconductivity in topological insulators1 Y. S. HOR, Y. QIU, K. N. SANDERS, J. E. MEDVEDEVA, T. VOJTA, Missouri University of Science and Technology, J. DAI, W. WU, Rutgers University, P. GHAEMI, City College of the City University New York — Three-dimensional topological insulators (TIs) have been found to depict topological distinct phases of matter and have attracted great interest due to helical spin texture on the surfaces. By Nb-doping in bismuth selenide, the TI turns into a type-II bulk superconductor while maintaining its helical metallic surface state in its normal state. However, at high magnetic field this doped TI behaves superparamagnetically. Niobium is usually considered a non-magnetic cation but it exhibits a unique magnetic behavior in this doped TI. Moreover, magnetic correlations appear in the system when the superconductivity emerges at below 3.2 K, presenting novel magnetic coupling of the Nb cations through modification of supercurrents mediated by Nb magnetic moments. As a consequence, ferromagnetism is induced in the superconducting regime below the upper critical field. Magnetic susceptibility of the TI shows paramagnetic behavior at high field due to destruction of the superconductivity which is the underlying bases for ferromagnetic coupling of Nb moments. The superconductivity and ferromagnetism, which are usually mutually destructive, can mutually benefit each other in the system giving rise to a zero-field magnetization which results in a symbiotic relationship between ferromagnetism and superconductivity.

1This work was supported primarily by the National Science Foundation under Award Number DMR-1255607

11:27AM M12.00002 High field magnetization of Half-Heusler compound LuPdBi BENJAMIN LAWSON, GANG LI, COLIN TINSMAN, FAN YU, TOMOYA ASABA, Univ of Michigan - Ann Arbor, XIAOFENG WANG, JOHNPIERRE PAGLIONE, University of Maryland, LU LI, Univ of Michigan - Ann Arbor — Topological insulators and topological superconductors are a novel phases of matter that have been an area of rich new physics in recent years. Half-Heusler compound LuPdBi has been suggested to have a topologically nontrivial phase by theoretical calculations and has been shown to have superconductivity and weak antilocalization in magneto-transport measurements. Given the promise of this compound, we performed and report here preliminary results of magnetization measurements in LuPdBi at high magnetic fields up to 45T.

11:39AM M12.00003 Superconductivity induced by In substitution into the topological crystalline insulator Pb0.5Sn0.5Te RUIDAN ZHONG, JOHN SCHNEELOCH, TIANSHENG LIU, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, NY 11973, USA, FERNANDO CAMINO, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973, USA, JOHN TRANQUADA, GENDA GU, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, NY 11973, USA — Indium substitution turns the topological crystalline insulator (TCI) Pb0.5Sn0.5Te into a possible topological superconductor. To investigate the effect of the indium concentration on the crystal structure and superconducting properties of (Pb0.5Sn0.5)xInxTe, we have grown high-quality single crystals using a modified floating-zone method and have performed systematic studies for indium content in the range 0 ≤ x ≤ 0.35. We find that the single crystals retain the rocksalt structure up to the solubility limit of indium (x ∼ 0.30). Experimental dependencies of the superconducting transition temperature (Tc) and the upper critical magnetic field (Hc2) on the indium content x have been measured. The maximum Tc is determined to be 4.7 K at x = 0.30, with μ0Hc2(T = 0) ≈ 5T.

11:51AM M12.00004 mk-STM study of Cu0.2Bi2Se3 with W and Nb Tips RAMI DANA, WAN-TING LIAO, University of Maryland, IRENEUSZ MIOTKOWSKI, YONG P. CHEN, Purdue University, MICHAEL DREYER, University of Maryland — The Cu intercalated Bi2Se3 is predicted to be a time-reversal invariant topological superconductor with Majorana bound state in the vortex core. The samples are characterized by intrinsic inhomogeneity and disorder. Using mk-STM, a variety of high resolution superconducting gaps and sub-gap structures were observed. Our data from SIN and SIS junctions, using W and Nb tips on Cu0.2Bi2Se3 and while applying of a magnetic field will be discussed in details.

12:03PM M12.00005 Quasiparticle Interference Patterns on the Surface of a Topological Insulator with Superconductivity AARON FARRELL, McGill University, MAXIME BEAUDRY, University of Montreal, TAMIR PEREG-BARNEA, McGill University, MARCEL FRANZ, University of British Columbia — When the electrons on the surface of a strong topological insulator are forced to undergo superconductive pairing (perhaps via proximity effect) a topological superconducting state is formed. Such a state is of interest as it plays host to Majorana modes on its boundaries and in vortex cores. For this reason it is currently of great interest to develop a theoretical understanding of any experimental probes of such systems. In this talk we will discuss the theory of one such probe. Namely, we present results for local density of states measurements in a Dirac system with superconductivity added. These results should be relevant to measurements in Scanning Tunnelling Spectroscopy (STS) on the surface of strong topological insulators with pairing either naturally arising or driven by proximity effect. By considering a variety of different impurity scatterers and tunings of the chemical potential in the system, we discuss different probes of the underlying Dirac physics present in these patterns.

12:15PM M12.00006 Topological superconductors with unconventional pairing symmetry characterized by monopole harmonics YI LI, Princeton University — We study the topological structure of Cooper pairing whose symmetry is characterized by the monopole harmonic functions instead of the usual spherical harmonic functions. This pairing symmetry can be either driven by the non-trivial topology of the Fermi surface or by interaction effects. The Bogoliubov quasi-particles are nodal which can either exhibit time-reversal invariant Dirac type spectrum or the time-reversal symmetry breaking Weyl spectra with the winding numbers determined the monopole harmonic functions. The non-trivial electromagnetic responses are also discussed. These exotic pairing symmetry can be realized in 3D Weyl metal and fermion systems with magnetic dipolar interactions.

12:27PM M12.00007 Low-energy phonons and superconductivity in Sn5In2Te3 GUANGYONG XU, Brookhaven National Laboratory, ZHIJUN XU, UC Berkeley, JOHN SCHNEELOCH, RUIDAN ZHONG, Brookhaven National Laboratory, J.A. RODRIGUEZ-RIVERA, L. HARRIGER, NIST Center for Neutron Research, ROBERT BIRGENEAU, UC Berkeley, GENDA GU, JOHN TRANQUADA, Brookhaven National Laboratory — We present neutron scattering measurements on low-energy phonons from a superconducting (Tc = 2.7 K) Sn5In2Te3 single crystal sample. The longitudinal acoustic phonon mode and one transverse acoustic branch have been mapped out around the (002) Bragg peak for temperatures of 1.7 K and 4.2 K. We observe a substantial energy width of the transverse phonons at energies comparable to twice the superconducting gap; however, there is no change in this width between the superconducting and normal states. We also confirm that the compound is well ordered, with no indications of structural instability.

1This work is supported by the Office of Basic Energy Sciences, DOE.
Discovery of superconductivity in Bi$_2$Te: evidence of universal behavior in an infinitely adaptive series under compression

We study a two-band model of fermions in a 1D chain with an antisymmetric hybridization that breaks inversion symmetry. We show that by imposing a reality constraint on the order parameter, the resulting zero energy junction bound state can be mapped onto a soliton solution of a Jackiw-Rebbi type Dirac equation similar to that in polyacetylene. Further, we consider $\pi$-junctions where the order parameter phase winds across the junction so that the aforementioned bound state generically acquires a gap. We relate these observations to the classification of the junctions according to their anti-unitary symmetries.

We wish to thank the Brazilian agencies, CAPES, FAPERJ, CNPq and FAPEMIG for financial support. We (DN and NT) would like to acknowledge funding from Grant No. NSF DMR-1309461.

12:39PM M12.00008 Superconductivity near a 3-Dimensional Dirac Semimetal: Topological Crystalline Insulator (Pb$_{1-x}$Sn$_x$)$_{1-y}$In$_y$Te near the Inversion Transition

12:51PM M12.00009 Superconductivity near 3D Dirac Semimetal: Topological Crystalline Insulator (Pb$_{1-x}$Sn$_x$)$_{1-y}$In$_y$Te near the Inversion Transition

1:03PM M12.00010 Entanglement Entropy and Entanglement Spectrum of Disordered Topological Superconductors

1:15PM M12.00011 One dimensional parafermionic phases and topological order

1:27PM M12.00012 Topological aspects of Josephson $\pi$-junctions in Kitaev wires

1:39PM M12.00013 Topological states in normal and superconducting p-wave chains

1Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under contract DE-AC52-07NA27344.

2Princeton University
explore the consequences of bulk quantum fluctuations of the order parameter in Hamiltonians by Bogoliubov-de Gennes Hamiltonians. Band insulators and superfluids are, however, fundamentally different. In particular, unlike the static energy gap of a band insulator, the gap in a superfluid is due to a dynamical order parameter that is subject to both thermal and quantum fluctuations. We explore the consequences of bulk quantum fluctuations of the order parameter in $^3\text{He}-B$ on the topologically protected Majorana surface states. We find that one of the three spin-orbit Goldstone modes couples to the surface Majorana fermions, which induces an effective short-range two-body interaction between the Majorana fermions with coupling constant inversely proportional to the strength of the nuclear dipole-dipole interaction. A mean-field theory estimate of the value of this coupling suggests that the surface Majorana fermions in $^3\text{He}-B$ are in the vicinity of a quantum phase transition to a gapped time-reversal symmetry breaking phase.

2:03PM M12.0015 Conditions for Non-Abelian Braiding in Time-Reversal Invariant Topological Superconductors, PIN GAO, VIC KAM TUEN LAW, Hong Kong Univ of Sci & Tech, XIONG-JUN LIU, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China — We study the validity of the non-Abelian braiding in 1D time-reversal invariant (DIII class) topological superconductors which host Majorana Kramer’s pairs in the ends. It has been shown that braiding two Majorana Kramer’s pairs can generically be reduced to two independent braiding processes of two different time-reversed copies, while the local noise or perturbations may lead to decoherence in the braiding operations. Here we examine in detail the braiding of Majorana Kramer’s pairs in the presence of disordered local couplings and noises, and show the generic conditions under which the decoherence effects are negligible and the non-Abelian braiding can be validated.

Wednesday, March 4, 2015 11:15AM - 2:15PM
Session M13 DMP: Focus Session: Complex Oxide Interfaces - LaAlO$_3$/SrTiO$_3$ I

11:15AM M12.0001 Emergent Phenomena in Oxide Superlattices from DFT+DMFT, CHRIS MARIANETTI, Columbia Univ — Density functional theory plus dynamical mean-field theory (DFT+DMFT) has proven to be an instrumental tool in describing transition metal-oxides, and DFT+DMFT is well poised to search the rich phase space of oxide superlattices for emergent phenomena. In this talk, we focus on double-perovskite heterostructures of the form $AA’BB’O_6$. Our two separate goals are to design new ferroelectric Mott insulators and high temperature ferromagnetic Mott insulators. In the context of ferroelectric Mott insulators, we demonstrate the ability to design in-plane ferroelectrics based upon transition metal charge transfer and $A/A’$ cation size mismatch, harnessing displacements of both the A-site and B-site. In the context of ferromagnetic Mott insulators, we detail the different mechanisms for obtaining high temperature ferromagnetic Mott states, and we present new candidates for high temperature ferromagnetic insulators. Finally, we discuss the prospect of coupling magnetic and ferroelectric states in addition to potential applications.

The authors acknowledge support from FAME, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA.

11:51AM M13.00002 Structural, chemical and electronic changes at LaAlO$_3$/SrTiO$_3$ interfaces near the critical thickness, ROHAN MISHRA, S.T. PANTELIDES, Vanderbilt University, Oak Ridge National Laboratory, JAUME GAZQUEZ, G. HERRANZ, M. STENGEL, M. SCIGAJ, N. DIX, F. SANCHEZ, J. FONTCUBERTA, Institut de Ciència de Materials de Barcelona, M. VARELA, Oak Ridge National Laboratory, Universidad Complutense de Madrid, A.Y. BORISEVICH, Oak Ridge National Laboratory — The formation of two-dimensional electron gas (2DEG) at the n-type LaAlO$_3$/SrTiO$_3$(LAO/STO) heterostructure is a paradigmatic example for emergent functionalities at oxide heterointerfaces. However, the origin of this 2DEG at the LAO/STO interface still remains unclear. In this work, we use scanning transmission electron microscopy and electron energy loss spectroscopy (STEM/EELS) to study a series of (LAO)$_n$(STO) films, both below (n=3) and above (n=5,7) the critical thickness for the formation of the 2DEG (n>$\approx$3). From STEM imaging, we observe dramatic changes in the polar distortion of the AIO$_3$ layers in response to the built-in electrostatic potential in the three films. We also observe changes in the octahedral tilts across the interface for different LAO thicknesses. We obtain information about cation intermixing across the heterointerface from EELS. We combine these results with density functional theory calculations to discuss the effect of each of these different structural and chemical changes on the electronic property of the interfaces. Overall, our results present a detailed understanding of the role of electronic and atomic reconsctructions and defects on the emergence of 2DEG at these interfaces.

12:03PM M13.00003 Surface charging in LaAlO$_3$/SrTiO$_3$ heterostructures, KARTHIK KRISHNASWAMY, CYRUS E. DREYER, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — The two-dimensional electron gas (2DEG) observed at the interface between LaAlO$_3$(LAO) and SrTiO$_3$(STO) is known to depend on its proximity to the LAO surface (thickness of LAO) and the conditions to which the surface is exposed. It has been proposed that electrons from the 2DEG can leak to surface states, resulting in a charged surface. Using first-principles calculations, we determine the electronic structure of the LAO surface and the coupling between the surface of LAO and the interface 2DEG. We develop a methodology for treating charged dielectric surfaces and apply it to LAO. This allows for the determination of the 2DEG density as well as the stable surface terminations and reconstructions of LAO on STO as a function of LAO thickness, under any given experimental conditions. Under oxygen-rich conditions, we find an increase in critical thickness required to form the 2DEG, and under hydrogen-rich environment the critical thickness decreases.

This work was supported by the LEAST Center (SRC/DARPA) and by ARO.

12:15PM M13.00004 Understanding enhanced UV photo-response of Pd nanoparticle-coated LaAlO$_3$/SrTiO$_3$ using ambient control Kelvin probe force microscopy, DONG-WOOK KIM, HAERI KIM, Department of Physics, Ewha Womans University, NGAI YUI CHAN, JIYAN DAI, Department of Applied Physics, The Hong Kong Polytechnic University — Significant enhancement in photoresponse of Pd nanoparticle-coated LaAlO$_3$/SrTiO$_3$(LAO/STO) heterostructure is observed under UV illumination compared with a bare LAO/STO sample. Clear ambient dependence suggests crucial roles of gas adsorption/desorption and resulting carrier transfer in the enhanced UV response. In this work, we have measured surface work function of the samples with and without UV light using Kelvin probe force microscopy (KPFM). We perform both transport and the surface potential measurements at the same time. Such simultaneous measurements can help us to improve our understanding regarding the light sensing and strong ambient dependence of the LAO/STO heterointerface.
12:27PM M13.00005 Increasing the capacitance beyond the classical limits in capacitors with free-electron like electrodes, JAVIER JUNQUERA, PABLO GARCIA-FERNANDEZ, PABLO DE CASTRO-MANZANO, CITIMAC, Universidad de Cantabria, Avda. de los Castros s/n, E-39005 Santander, Spain, MASSIMILIANO STENGEL, Institut de Ciència de Materials de Barcelona (ICMAB-CSIC) Campus UAB, E-08193 Bellaterra, Barcelona, Spain — Capacitors are ubiquitous in solid state devices like metal oxide semiconductors field effect transistors (MOSFET). For energy efficiency, the MOSFET should operate at small gate voltages. In this regime, to increase the channel conductivity and performance, the capacitance of the capacitor between the gate and the channel should be made as large as possible. Recently, an enhancement of the capacitance of up to 40 % with respect this classical limit has been reported in two-dimensional electron gases formed at the interface between two oxides, SrTiO$_3$ and LaAlO$_3$. A first theoretical analysis pointed to the quantum exchange-energy in the electron-electron interactions as the driving force to explain the anomalous behavior. The exchange-interaction would produce a lowering of the chemical potential of the electron system as the electronic density increases (the negative compressibility effect). Here we test the validity of the approach, carrying out self-consistent calculations on a capacitor where the metallic plates are simulated by a jellium. We study the effect of the thickness of the metallic electrode and the density of the free electron, on the spillage of the electronic clouds into the dielectric and the variation of the chemical potential.

12:39PM M13.00006 2D charge confinement in oxide heterostructures: fundamentals from First-Principles, ALESSIO FILIPPETTI, CNR-IOM UOS Cagliari, c/o Physics Dept. University of Cagliari, Italy — The accurate description of the fundamental properties of complex oxides by First-Principles (FP) is tantamount with the possibility of achieving reliable theoretical design. Here we use the variational pseudo-self-interaction corrected density functional theory (VPSIC) to investigate structural and electronic properties of several exceptionally interesting heterostructures (the STO/LAO interface, the Nb-doped STO superlattice, the SrTiO$_3$/SrZrO$_3$ superlattice, the SrTiO$_3$ surface). The key features which are at the fundament of the 2DEG formation (film polarity, band disalignment, doping, structural and electronic screening, chemistry of 3d orbitals) are described and discussed. Furthermore, we propose a combined VPSIC plus Bloch-Boltzmann approach as reliable and efficient method, applicable to generic doped oxides, to obtain thermolectric and transport properties in satisfying agreement with the available experimental data. Our theoretical analysis consents to relate the calculated transport properties to the specific features of the band structure at the interface, e.g. on-site and inter-site band splitting, which govern the confinement process. This is instrumental to achieve guidelines for the design of interfaces with enhanced transport and thermolectric functionalities.

12:51PM M13.00007 Role of Oxygen in the Resistance Upturn of LaAlO$_3$/SrTiO$_3$ Heterostructures1. H. ZHANG, University of Toronto, J.H. NGAI, University of Texas at Arlington, C. AHN, Yale University, C. MCMAHON, D.G. HAWTHORN, University of Waterloo, J.Y.T. WEI, University of Toronto and the Canadian Institute for Advanced Research — Among the phenomena exhibited by LaAlO$_3$/SrTiO$_3$ (LAO/STO) heterostructures, the appearance of a low-temperature resistance upturn has attracted much recent debate [1-4]. This phenomenon has been observed to co-occur with both nonlinear Hall effect and negative magnetoresistance, and attributed to either the Kondo effect, multiband conduction, or weak localization. More importantly, it is primarily seen in samples grown by pulsed laser deposition, and is sensitive to film layer thickness, growth condition and electrostatic gating, all of which could affect the oxygen content. In this work, we study the occurrence of resistance upturn in samples grown by molecular beam epitaxy, and how the sheet resistance and Hall conductance are affected by post-growth oxygenation. X-ray photoelectron spectroscopy is used to monitor the cation valences, and correlate them with the conduction and magnetic properties. Our results are analyzed in terms of oxygen vacancies in the presence of polar charge transfer, and the effect of these vacancies on the resistance upturn in LAO/STO heterostructures.

1Work supported by NSERC, CFI-OIT, the Canadian Institute for Advanced Research, and National Science Foundation Grant #1119826.

1:03PM M13.00008 The Role of Lattice Mismatch and Polar Fluctuation at the Conducting Oxide Interfaces, ZHEN HUANG, NUSNNI-NanoCore, National University of Singapore, KUN HAN, Department of Physics, National University of Singapore; NUSNNI-NanoCore, National University of Singapore, SHENGWEI ZENG, MALLIKARJUNA MOTAPOTHULA, WEIMING LÜ, YONGLIANG ZHAO, CHANGJIAN LI, NUSNNI-NanoCore, National University of Singapore, WENXIONG ZHOU, Department of Physics, National University of Singapore; NUSNNI-NanoCore, National University of Singapore, MICHAEL COEY, School of Physics and CRANN, Trinity College; NUSNNI-NanoCore, National University of Singapore, ARIANDO ARIANDO, Department of Physics, National University of Singapore; NUSNNI-NanoCore, National University of Singapore — Two key questions have been raised since the discovery of two-dimensional electron gas (2DEG) at the interface between insulating oxides LaAlO$_3$ and SrTiO$_3$. One is the origin for such 2DEG, and the other is how to improve carrier mobility. By replacing LaAlO$_3$ with the cubic polar perovskite insulator (La$_0.35$Sr$_0.7$)(Al$_0.65$Ta$_0.35$)O$_3$ (LSAT), carrier mobility can be increased by 30 times and reach 35,000 cm$^2$/V·s at 2 K, accompanied by reducing lattice mismatch from 2.98% to 0.96%. Moreover, two critical thicknesses for LSAT/SrTiO$_3$(001) interface are found: one is 5 unit cells for 2DEG appearance, and the other is around 12 unit cells for carrier mobility optimization. This phenomenon can be explained in terms of polar fluctuation in LSAT(001), while the conducting (110)- and (111)-orientated LSAT/STO interfaces without such polar fluctuation shows less thickness-dependent carrier mobility.

1:15PM M13.00009 Interface orientation dependent carrier distribution in LaAlO$_3$/SrTiO$_3$ heterostructures, TULA R. PAUDEL, EUGENY Y. TSYMBAL, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE 68588 — Carrier distribution in widely studied LaAlO$_3$/STO$_3$ heterostructures depends upon the directionality of the interface. From the first-principles calculations, we find that, for the (001) interface, most carriers are localized at the interface and have the $d_{xy}$ character, which decays away from the interface on the scale of 1 nm. The $d_{xy}$ and $d_{x^2-y^2}$ carrier concentration increases, peaks at about three unit cells (1.15 nm), and then decays very slowly away from the interface. For the (111) interface, we find that the total carrier distribution is similar to that of $d_{xy}$ and $d_{x^2-y^2}$ in the (001) heterostructure. It has a maximum that lies at about four-bilayers (0.89 nm) away from interface and then decays very slowly producing a long-ranged tail. This difference in the carrier distribution is controlled by the $d$-orbital splitting which depends on the interface orientation. For the (001) interface, the tetragonal distortion brings the in-plane $d_{xy}$ orbital to about 0.5 eV below the Fermi energy, creating a deep localized state, whereas the $d_{x^2-y^2}$ and $d_{z^2}$ orbitals are much shallower and hence less localized. For the (111) interface, the rhombohedral distortion splits the $d$-orbitals by about 0.1 eV so that they are all located in vicinity of the Fermi energy and therefore less localized at the interface.
1:27PM M13.00010 Scanning Tunneling Microscopy of 2DEG in Complex Oxide Interfaces and Heterostructures, IGOR ALTZFEDER, Air Force Research Laboratory, HYUNGWOO LEE, University of Wisconsin-Madison, ALP SEHIRLIOGLU, Case Western Reserve University, CHANG-BOOM EOM, University of Wisconsin-Madison, ANDREY VOEVODIN, Air Force Research Laboratory — New experimental data clarifying the origin of 2DEG at LaAlO3 (LAO) - SrTiO3 (STO) interfaces will be presented. The materials that have been studied include (a) 4 unit cells of LAO on STO and (b) symmetric n-type 2DEG bilayer heterostructures prepared by atomic layer engineering method [1]. All studied materials are grown by pulsed laser deposition (PLD). UHV STM results obtained on 4LAO/STO samples do not confirm the prediction of electronic reconstruction model [2]. On the other hand, UHV STM results obtained on symmetric n-type 2DEG bilayer heterostructures indicate that the formation of n-type 2DEG is caused by complex interplay of oxygen vacancy doping and interfacial band bending at LaO-TiO2 interfaces. The physical mechanisms of interface induced charge density multiplication effect will be discussed.

[1] H. W. Jang et al., Science 331, 886 (2011);

1:39PM M13.00011 The role of La displacement in Titanium $d_{xy}$ ferromagnetism at the LaAlO$_3$/SrTiO$_3$ — double-exchange like mediation$^1$, SUNG-HYON RHIM, Univ of Ulsan, DORJ ODKHUU, Inchen National University, DONGBIN SHIM, NOEJUNG PARK, Ulsan National Institute of Science and Technology — In this talk, we argue that La site polar distortion is the key for magnetism without oxygen vacancy, whereby coupling between La $d_{z^2}$ and O $2p_{x,y}$ offer a pathway for double-exchange like interaction to support Ti $d_{xy}$ ferromagnetism. While ferromagnetism found in the n-type LAO/STO has been mainly attributed to oxygen vacancy near the interface, the mechanism we propose a possibility of ferromagnetism without any defect. We show that there is a phase separation between charge-order and half-metallicity that can be characterized by La displacement - this can be tailored through adsorption on the outer AlO$_2$ surface or electrostatic bias.

$^1$Supported by NRF of Korean (NRF-2013R1A1A0207910) and NRF by the Ministry of Education(2009-0093818)

1:51PM M13.00012 Importance of the surface in interfacial conductivity in LaAlO$_3$ thin films on SrTiO$_3$. C. STEPHEN HELLBERG, Naval Research Lab — Careful growth of LaAlO$_3$ thin films on SrTiO$_3$ by molecular beam epitaxy has shown that the La/Al ratio of the film is key to the formation of a two-dimensional electron liquid at the interface—metallic conductivity is only observed in Al-rich films. The interfacial electron liquid forms due to the polar catastrophe, the diverging potential caused by the atomic layer arrangement at the interface when polar LaAlO$_3$ is grown on TiO$_2$-terminated non-polar SrTiO$_3$. The system eventually reconstructs, moving negative charges to the interface to screen the diverging potential. I will present density functional calculations showing the defects that form in the film depend on the stoichiometry, and these defects lead to electronic reconstruction in Al-rich films and ionic reconstruction in La-rich films. The stoichiometry of the surface differs from that of the bulk of the film, and I will show that the LaAlO$_3$ surface is unstable to phase separation. The interaction between surface and bulk leads to a scenario where the insulating La-rich films have an Al-rich surface.

2:03PM M13.00013 Effects of structural phase transitions on the interface of perovskite oxides$^1$, NICHOLAS J. GOBLE, Department of Physics, Case Western Reserve University, RICHARD AKROBETU, ALP SEHIRLIOGLU, Department of Materials Science and Engineering, Case Western Reserve University, THONG Q. NGO, JOHN G. EKERD'T, Department of Chemical Engineering, University of Texas at Austin, KRISTY J. KORMONDY, ALEXANDER A. DEMKOV, Department of Physics, University of Texas at Austin, XXUAN P.A. GAO, Department of Physics, Case Western Reserve University — Conductivity at the interface of perovskite oxides such as LaAlO$_3$/SrTiO$_3$ is a wildly growing area of research. These interfaces are rich in phenomena including superconductivity, large negative in-plane magnetoresistance, giant persistent photoconductivity, and ferromagnetism. Although this field has seen rapid growth in the recent decade, there is yet to be a systematic study on what effect structural phase transitions in strontium titanate play on the interface. It is well understood that strontium titanate transitions from a cubic to tetragonal phase most notably at 105K, but how this effects oxide interface conductivity has yet to be reported on. Through transport measurements, we observe evidence of structural phase transitions in LaAlO$_3$/SrTiO$_3$ and Al2O3/SrTiO3 interfaces at 80K and 200K. These effects are enhanced when the scale of the devices is reduced to a few microns.

$^1$The authors thank AFOSR for funding support (grant number FA9550-12-10494 and FA9550-12-1-0441).

Wednesday, March 4, 2015 11:15AM - 2:15PM —
Session M14 DMP: Focus Session: Mesoscopic Electronic Phenomena —
008A - Juan M. Merlo, Boston College

11:15AM M14.00001 Hydrodynamic Coulomb drag, magnetodrag and Hall drag of strongly correlated electron liquids$^1$, STANISLAV APOSTOLOV, ALEX LEVCHENKO, Michigan State University, ANTON ANDREEV, University of Washington — We develop a theory of Coulomb drag in ultraclean double layers with strongly correlated carriers. In the regime where the equilibration length of the electron liquid is shorter than the interlayer spacing the main contribution to the Coulomb drag arises from hydrodynamic density fluctuations. The latter consist of plasmons driven by fluctuating longitudinal stresses, and diffusive modes caused by temperature fluctuations and thermal expansion of the electron liquid. We express the drag resistivity in terms of the kinetic coefficients of the electron fluid. Our results are nonperturbative in interaction strength and do not assume Fermi-liquid behavior of the electron liquid.

$^1$This work was supported by NSF Grant No. DMR-1401908.

11:27AM M14.00002 Spin-charge scattering in generic Luttinger liquids$^1$, ALEX LEVCHENKO, Michigan State University — We discuss the violation of spin-charge separation in generic nonlinear Luttinger liquids and investigate its effect on the relaxation, electrical and thermal transport of genuine spin-1/2 electron liquids in ballistic quantum wires. We identify basic scattering processes compatible with the symmetry of the problem and conservation laws that lead to the decay of plasmons into the spin modes and Brownian backscattering of spin excitations. We derive a closed set of coupled kinetic equations for the spin-charge excitations and solve the problem of conductance of interacting electrons for an arbitrary relation between the quantum wire length and spin-charge relaxation length.

$^1$This work was supported by NSF Grant No. DMR-1401908.
11:39 AM M14.00003 Determination of time-reversal symmetry breaking lengths in an InGaAs Sagnac interferometer array. SHAOLA REN, J.J. HEREMANS, Virginia Tech, C.K. GASPE, S. VIJAYARAGUNATHAN, T.D. MISHIMA, M.B. SANTOS, University of Oklahoma — Time-reversed trajectories in Aharonov-Bohm ring Sagnac interferometers yield AAS oscillations if time-reversal symmetry is preserved. The quantum interference oscillations can be used to quantify time-reversal symmetry breaking, more particularly the mesoscopic dephasing length associated with time-reversal symmetry breaking under applied magnetic field, an effective magnetic length. We measured AAS oscillations with periodicity 13 G, corresponding to h/2e flux in the 650 nm radius rings of a 5 × 5 Sagnac interferometer array fabricated on a 2D electron system in an InGaAs/InAlAs heterostructure at 0.4 K. The oscillation amplitudes were investigated over magnetic field spanning 2.2 T, with the amplitude estimated by Fourier transform of the oscillation. For a magnetic field, the oscillation amplitudes depend on the magnetic field, the magnetic field increases, the amplitude decreases due to time-reversal symmetry breaking by the magnetic field in the interferometer arms. A dephasing model for coherent networks allows extraction of the effective magnetic length. In wide diffusive system this length corresponds theoretically and experimentally to the usual magnetic length, whereas the data show that corrections enter for ballistic quasi-1D systems (DOE DE-FG02-08ER46532, NSF DMR-0520550).

11:51 AM M14.00004 Quantum interference and correlations in single dopants and exchange-coupled dopants in silicon1 JOE SALFI, Centre for Quantum Computation and Communication Technology, University of New South Wales — Quantum electronics exploiting the highly coherent states of single dopants in silicon invariably requires interactions between states and interfaces, and inter-dopant coupling by exchange interactions. We have developed a low temperature STM scheme for spatially resolved single-electron transport in a device-like environment, providing the first wave-function measurements of single donors and exchange-coupled acceptors in silicon. For single donors, we directly observed valley quantum interference due to linear superpositions of the valleys [1], and found that valley degrees of freedom are highly robust to the symmetry-breaking perturbation of nearby (3 nm) surfaces. For exchange-coupled acceptors, we measured the singlet-triplet splitting, and from the spatial tunneling probability, extracted enough information about the 2-body wavefunction amplitudes to determine the entanglement entropy [2], a measure of the quantum inseparability (quantum correlations) generated by the interactions between indistinguishable particles. Entanglement entropy of the J=3/2 holes was found to increase with increasing dopant distance, as Coulomb interactions overcome tunneling, coherently localizing spin towards a Heitler-London singlet, mimicking 5=1/2 particles [3]. In the future these capabilities will be exploited to peer into the inner workings of few-dopant quantum devices and shed new light on multi-dopant correlated states, engineered atom-by-atom.


1Primary financial support from the ARC.

12:27PM M14.00005 Spin Technologies in Silicon Carbide1, PAUL KLIMOV2, University of California, Santa Barbara and University of Chicago — Over the past several decades SiC has evolved from being a simple abrasive to a versatile material platform for high-power electronics, optoelectronics, and nanomechanical devices. These technologies have been driven by advanced growth, doping, and processing capabilities, and the ready availability of large-area, single-crystal SiC wafers. Recent advances have also established SiC as a promising host for a novel class of technologies based on the spin of intrinsic color centers. In particular, the divacancies and related defects [1,2] have ground-state electronic-spin triplets with ms-long coherence times that can be optically addressed near telecom wavelengths [3] and manipulated with magnetic, electric [4], and strain fields [5]. Recently, divacancy addressability has been extended to the single defect level [6], laying foundation for single spin technologies in SiC. This rapidly developing field has prompted research into the SiC material host to understand how defect-bound electron spins interact with their surrounding nuclear spin bath. Although nuclear spins are typically a major source of decoherence in color-center spin systems, they are also an important resource since they interact with magnetic fields orders of magnitude more weakly than electronic spins. This fact has motivated their use for quantum memories and ultra-sensitive sensors. In this talk I will review advances in this rapidly developing field and discuss our efforts towards this latter goal.


1This work was supported by the AFOSR, DARPA, and the NSF.

3In collaboration with Abram L. Falk, Bob B. Buckley, and David D. Awschalom

1:03PM M14.00006 Al Nanowire Arrays For Plasmonic Devices1 NATHAN T. NESBITT, AARON H. ROSE, YITZI M. CALM, JUAN M. MERLO, STEVE SHEPARD, GREG MCMAHON, CHIA-KUANG TSUNG, MICHAEL J. BURNS, MICHAEL J. NAUGHTON, Boston College — Aluminum nanowires have been fabricated in ordered vertical arrays on bulk Al foil with controlled wire dimensions and spacing. Large aspect ratio wires were obtained, including sub-micron wire diameters and supra-10 µm height. The somewhat novel method of fabrication utilizes nanoimprint lithography and the economical electrochemical anodization process used to make anodized aluminum oxide (AAO) templates, suggesting potential facile production and scalability. To our knowledge, arrays of vertical metallic nanowires (i.e. differing from semiconductor nanowire or carbon nanofiber arrays) of the obtained dimensions have not been previously reported. These dimensions may be favorable for nanoscale photonic and plasmonic transmission, nanoax solar cells, and non-diffraction-limited optical microscopy.

1This material is based upon work supported by the National Science Foun- dation Graduate Research Fellowship under Grant No. (DGE-1258923).

1:15PM M14.00007 ABSTRACT WITHDRAWN

1:27PM M14.00008 Dielectric tuned surface plasmon resonances on metallic gratings1, ADAM HAUSER, BILL FLAHERTY, KA MING LAW, EVGENY MIKHEEV, ADAM KAUDOS, SUSANNE STEMMER, S. JAMES ALLEN, Univ of California - Santa Barbara — We explore the effect of substrate dielectric constant on the dispersion of infrared surface plasmons supported by micron scale metal gratings. Of particular interest are substrate dielectrics that can be tuned by electric fields and thereby make possible gated plasmonic devices. Angle resolved s and p polarized reflectivity is used to observe the plasmon dispersion for Pt gratings on various oxide dielectrics and heterostructures, LSAT, SrTiO3, Nb:SrTiO3 and LSAT/SrTiO3/GdTiO3. Most striking is the shift in the plasmon dispersion upon Nb doping of SrTiO3 caused by the free carrier contribution to the dielectric constant. We focus our attention on a metal-oxide-metal heterostructure, Pt/Ba0.3Sr0.7TiO3/Pt-grating that serves to confine the infrared field to the electric field modulated region enhancing the potential for a gated plasmonic structure.

1Supported by the ONR MURI “Extreme electron density electronics” N00014-12-0976.
V reasonable assumptions, the “localization product” $\kappa a V$. Low temperature resistance measurements show a characteristic dependence of $R$ on external parameters such as pH (T. Simon et al., Nature Mat. 13, 1013 (2014)).

2:03PM M14.00011 Interferometric Plasmonic Lensing with Nanohole Arrays, YU GONG, ALAN JOLY, PATRICK EL-KHOURY, WAYNE HESS, Pacific Northwest National Laboratory, CHEMICAL PHYSICS TEAM — Nonlinear photoemission electron microscopy (PEEM) is used to map propagating surface plasmons launched from lithographically patterned isolated nanoholes and nanohole arrays in gold films. A damped elongated ring-like photoemission beat pattern is observed from individual nanoholes. Strong near field photoemission patterns are observed in the PEEM images, recorded following low angle of incidence irradiation of the plasmonic nanohole arrays with sub-15 fs laser pulses centered at 780 nm. The recorded photoemission patterns are attributed to constructive and destructive interference between propagating surface plasmons launched from the individual nanoholes which comprise the array. By exploiting the wave nature of propagating surface plasmons, we demonstrate how varying the array geometry (hole diameter, pitch, and number of rows/columns) ultimately yields intense localized photoemission patterns. Through a combination of PEEM experiments and finite-difference time-domain simulations, we identify the optimal array geometry for efficient light coupling and interferometric plasmonic lensing. We also describe an exemplary practical application of the nanohole array-based plasmonic lenses, namely, enhanced photoemission from a vertex of a strategically positioned gold triangle.


11:15AM M15.00001 Photocatalytic Solar Fuel Generation on Semiconductor Nanocrystals1, JOCHEN FELDMANN, Photonics and Optoelectronics Group, Ludwig-Maximilians-Universitaet (LMU), Munich, Germany — I will review our scientific work on photocatalytic solar fuel generation utilizing colloidal semiconductor nanocrystals decorated with catalytic metal clusters. In particular, nanocrystals made of CdS, TiO$_2$ and organo-metal halide perovskites will be discussed. Key issues are the role of hole scavengers (M. Berr et al., Appl. Phys. Lett. 100, 223903 (2012)), the size and density of catalytic clusters (M. Berr et al.: Appl. Phys. Lett. 97, 093108 (2010) and Nano Letters 12, 5903 (2012) , and dependencies on external parameters such as pH (T. Simon et al., Nature Mat. 13, 1013 (2014)).

Financially supported by the Bavarian Research Cluster "Solar Technologies Go Hybrid: SolTech"

1All aspects of this work supported by the U.S. Department of Energy Office of Basic Energy Sciences, Division of Materials Science and Engineering, under Award No. DE-SC0002158.

11:51AM M15.00002 Gate-Induced Carrier Delocalization in Quantum Dot Field Effect Transistors1, M.E. TURK, J.-H. CHOI, S.J. OH, A.T. FAFARMAN, B.T. DIROLL, C.B. MURRAY, C.R. KAGAN, J.M. KIKKAWA, University of Pennsylvania — We study the low temperature resistance and transport properties of high-mobility indium-doped CdSe quantum dot (QD) field effect transistors [1]. Low temperature resistance measurements show a characteristic dependence of $R(T) = R_0 \exp (T_0/T)^p$ with $p = 2/3$, consistent with a recent model based on Coulomb gap variable range hopping plus thermal broadening. We show that using the gate bias $V_G$ to accumulate electrons in the QD channel increases the “localization product” $a a$ (localization length $a$, dielectric constant $\kappa$), as expected for Fermi level changes near an Anderson mobility edge. Under any reasonable assumptions, $a$ increases significantly beyond the QD diameter as gate bias is applied. Magnetoresistance (MR) measurements display both positive and negative MR contributions that vary with $V_G$ and $T$. For each $V_G$, we observe a universal negative MR line shape for higher temperatures ($T > 20K$) that scales as $T^{-4/3}$, consistent with Zeeman MR for $p = 2/3$ with a gate bias-modulated mobility gap ($\Delta \varepsilon$).

1All works of this aspect by the U.S. Department of Energy Office of Basic Energy Sciences, Division of Materials Science and Engineering, under Award No. DE-SC0002158.

12:03PM M15.00003 Charge trapping and de-trapping in isolated CdSe/ZnS nanocrystals under an external electric field: indirect evidence of a permanent dipole moment, HUIDONG ZANG, MINGZHAI LIU, FERNANDO CAMINO, MIRCEA COTLET, Brookhaven National Laboratory, CENTER FOR FUNCTIONAL NANOMATERIALS TEAM — The charge trapping and de-trapping processes in single CdSe/ZnS nanocrystals under external electric field were systematically studied. The results clearly demonstrated that the external electric field can reversibly modulate the exciton dynamics and photoluminescence blinking, which provide further evidence for the existence of a permanent ground state dipole moment in isolated nanocrystals. A model which assumes energetically deep charge traps is proposed to explain on/off blinking in isolated CdSe/ZnS nanocrystals with the presence of a permanent dipole moment.
12:15PM M15.00004 Probing Energy Levels of Large Array Quantum Dot Superlattice by Electronic Transport Measurement, S.Z. BISRI, RIKEN-CEMS, Japan, E. DEGOLI UNIMORE, Italy, N. SPALLANZANI, Univ.Rome II, Italy, G. KRISHNAN, B. KOOI, Univ.Groningen, Netherlands, C. GHICA, NIMB-Bucharest, Romania, M. YAREMA, Univ.Linz, Austria, L. PROTESCIU, ETHZurich, Switzerland, W. HEISS, Univ.Linz, Austria, M. KOVALENKO, ETHZurich, Switzerland, O. PULCI, Univ.Rome II, Italy, S. OSSICINI, UNIMORE, Italy, Y. IWASA, RIKEN-CEMS, Japan, M. LOI, Univ.Groningen, Netherlands — Colloidal quantum dot superlattice (CQDS) emerges as new type of hybrid solids allowing easy fabrication of devices that exploits the quantum confinement properties of individual QD. This materials displays peculiar characters, making investigation of their transport properties nontrivial. Besides the bandgap variations, 0D nature of QD lead to the formation of discrete energy subbands. These subbands are crucial for multiple exciton generation (for efficient solar cell), thermoelectric material and multistate transistor. Full understanding of the CQDS energy level structure is vital to use them in complex devices. Here we show a powerful method to determine the CQDS electronic energy levels from their intrinsic charge transport characteristics. Via the use of ambipolar transistors with CQDS as active materials and gated using highly capacitive ionic liquid gating, Fermi energy can be largely tuned. It can access energy levels beyond QD’s HOMO & LUMO. Ability to probe not only the bandgap, but also the discrete energy level from large assembly of QD at room temperature suggests the formation of energy minibands in this system.

12:27PM M15.00005 Singlet and Triplet Exciton Harvesting in the Thin Films of Colloidal Quantum Dots Interfacing Phosphorescent Small Organic Molecules, BURAK GUZELTURK, PEDRO LUDWIG HERNANDEZ-MARTINEZ, Nanyang Technological University, Bilkent University, DEWEI ZHAO, XIAO WEI SUN, Nanyang Technological University, HILMI VOLKAN DEMIR, Nanyang Technological University, Bilkent University — Efficient nonradiative energy transfer is reported in an inorganic/organic thin film consists of a CdSe/ZnS colloidal quantum dot (QD) layer interfaced with a phosphorescent small organic molecule (Frlpic) coated fluorphore host (TCTA). The nonradiative energy transfer in this films has a cascaded energy transfer behaviour: first from the fluorescent host TCTA to phosphorescent Frlpic and then to QDs. The nonradiative energy transfer in these films enables very efficient singlet and triplet state harvesting by the QDs with a fluorescence enhancement factor of 2.5-fold, while overall nonradiative energy transfer efficiency is over 90%. The experimental results are nicely supported by the theoretical model which includes exciton diffusion assisted Förster-type near-field dipole–dipole coupling within the films.

12:39PM M15.00006 Electron-Exciton and Electron-Phonon interactions effects on the tunnel electronic spectrum of PbS quantum dots, HONGYUE WANG, EMMANUEL LHUILLIER, QIAN YU, ALIREZA MOTTAGHAZI, Laboratoire de Physique et d’Etude des Matériaux, UMR 8213, ESPCI-ParisTech-CNRS-UPMC, 10 rue Vauquelin, 75231 Paris, France — We present a tunnel spectroscopy study of the electronic spectrum of single PbS Quantum Dots (QDs) trapped between nanometer-spaced electrodes, measured at low temperature T=5 K. The carrier filling of the QD can be controlled either by the drain voltage in the shell filling regime or by a gate voltage. In the empty QD, the tunnel spectrum presents the expected signature of the 8x degenerated excited levels. In the shell filled regime, the levels degeneracies are lifted by the global electrostatic Coulomb energy of the QD; in the gate controlled shell filling regime, the levels degeneracies are lifted by the intra-Coulomb interactions. In the charged quantum dot, electron-phonons interactions lead to the apparition of Franck-Condon side bands on the single excited levels and possibly Franck-Condon blockade at low energy. The sharpening of excited levels at higher gate voltage suggests that the magnitude of electron-phonon interactions is decreased upon increasing the electron filling in the quantum dot.

12:51PM M15.00007 Impact of particle interactions on the photoluminescent stability of silicon nanocrystal clusters, JOSEPH B. MILLER, Rice University, NAVEEN DANDU, NDSU, REBECCA J. ANTHONY, UWE R. KORTSHAGEN, UMN, DANIEL M. KROLL, SVETLANA KILINA, ERIK K. HOBBIE, NDSU — We combine experiments, Monte Carlo simulations and ab initio calculations to explore the influence of inter-particle interactions on the photoluminescent stability of silicon nanocrystal (SiNC) clusters. The time-dependent photoluminescence (PL) emitted by structures ranging in size from a single nanocrystal to collections of several thousand SiNCs is compared with Monte Carlo simulations of non-interacting nanocrystal ensembles. The discrepancy is modeled using calculations of the energy transfer rate between neighboring SiNCs as a function of material composition and shape, bringing the possibility to control the photoluminescent stability of silicon nanocrystal clusters.

1:03PM M15.00008 Plasmonic Cavity Transparency Induced by a Single Quantum Dot, THOMAS HARTSFIELD, Department of Physics, The University of Texas at Austin, WEI-SHUN CHANG, Department of Physics, Rice University, SUNG-CHEOL YANG, TZUHSUAN MA, Department of Physics, The University of Texas at Austin, JINWEI SHI, Department of Physics, Beijing Normal University, LIUYANG SUN, GENNADY SHVETS, Department of Physics, The University of Texas at Austin, STEPHAN LINK, Department of Physics, Rice University, XIAOQIN LI, Department of Physics, The University of Texas at Austin — There are a large number of studies devoted to designing and characterizing plasmonic cavities. However, few experiments investigate interaction of individual quantum absorbers and emitters with a plasmonic cavity, which is essential for exploring cavity quantum electrodynamic (QED) effects. The main experimental challenge lies in the difficulty of placing an absorber and emitter at the desired positions. The very virtue of the small mode volume of plasmonic cavities demands precise spatial placement of emitters. Here, we study the simplest plasmonic cavity: a spherical metallic nanoparticle (MNP). By placing a semiconductor quantum dot (QD) controllably in the close proximity of the MNP cavity, its scattering spectrum is modified drastically. A Fano resonance is observed due to interference between the plasmonic resonance of the MNP and the exciton resonance in the QD. The experiment demonstrates that transparency of the MNP cavity can be effectively induced by a single quantum dot, achieving an important step toward realizing plasmonic quantum devices.

1:15PM M15.00009 Ultrafast Excitonic and Plasmonic Processes at the Nanoscale: Understanding Energy Flow in Hybrid Nanostructures, GARY WIEDERRECHT, Center for Nanoscale Materials, Argonne National Laboratory — Nanoscale plasmonic and excitonic structures frequently possess ultrafast processes that can be initiated and monitored by light. Nanoscale structures lend themselves to strong light-matter interactions for a variety of reasons, including a tendency towards large optical extinction and polarizability. Many times these nanostructures have strong resonances due to collective excitations with coherence, a property that lends itself very well to optical control opportunities. These types of collective excitations can also couple strongly to excitations of other nanostructures with different composition and with disparate properties in order to realize hybrid excitations. Hybridization presents unique opportunities for inducing directional energy and charge flow initiated by light. Thus, using ultrafast pulses of appropriate photon energy, combined with considerations of material composition and shape, brings the possibility to control energy flow in excitonic and plasmonic hybrid nanostructures. In this talk, I discuss our recent efforts to create and characterize electronically coupled nanostuctures and the impact this has on ultrafast photoreponse. These processes have strong impact on applications such as light harvesting and nonlinear optical responses in nanoscale structures. Use of the Center for Nanoscale Materials was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357.
1:27PM M15.00010 Directed synthesis of Mn\textsubscript{1-x}Ti\textsubscript{x}O\textsubscript{2} tunnel structured materials for energy applications, TIM DROUBAY, ANNE CHAKA, SEBASTIEN KERISIT, EUGENE MILTON, Pacific Northwest National Laboratory — Mn oxides with tunnel structures are crucial in technological applications such as Li batteries, catalysis, fuel cells, electrochemical capacitors, sensors, and groundwater remediation. However, the complexity and poor quality of natural Mn oxide has hindered efforts to understand their fundamental structure-property relationships. To address this issue, we used PLD to make high-quality Mn\textsubscript{1-x}Ti\textsubscript{x}O\textsubscript{2} single-crystal films. Attempts to synthesize pure $\beta$-MnO\textsubscript{2} thin films on TiO\textsubscript{2} substrates resulted in Mn\textsubscript{2}O\textsubscript{3} dominant films. Results of ab initio thermodynamics to explain film stability as a function of growth conditions and Mn/Ti composition suggest that “protecting” the Mn in a TiO\textsubscript{2} matrix by co-deposition would be beneficial. This approach has met with initial success even though the resultant films have oxygen vacancies. XPS indicates that (110) oriented films are Mn-rich near the surface while (001)-oriented films are Mn-rich near the interface. XRD shows that the films are coherently strained to the substrate which may influence the oxygen non-stoichiometry. Aberration corrected TEM results corroborate the XPS and XRD results and indicate a potential Mn-dependent defect. These films will be discussed along with multilayered (MnO\textsubscript{2})\textsubscript{m}–(TiO\textsubscript{2})\textsubscript{n} films. Atomic modeling shows that alternating cation rows that only contained Ti or Mn (m,n = 1) greatly lower the activation energy for Li diffusion relative to films where Mn and Ti were homogeneously mixed.

1:39PM M15.00011 Energy filtering in nanowires, MAARTEN THEWISSEN, BART SORÈE, WIM MAGNUS, Univ of Antwerp, IMEC COLLABORATION — Nanowires present a viable geometry to allow for future semiconductor device scaling. When the dimensions of these nanowires become comparable to the wavelength of the carriers, quantum effects may have a profound impact on the transport properties of the wire. An example of such effect, theoretically investigated here, is the introduction of a periodic potential profile along the transport direction. This could be achieved by repeatedly varying the diameter of the wire, by including a superlattice perpendicular to the wire, by applying a periodic electric field etc. The consequent resonances will effectively block electrons at some energies, while allowing others to pass, and hence function as an energy filter. Such property might be beneficial for its use in a transistor. The transmission of electrons through the wire is examined here, by solving Schrödinger’s equation in the effective mass approximation and Poisson’s equation self-consistently. As for the contacts, quantum transmitting boundary conditions are used as suggested by Lent. The result shows that energy filtering as described can indeed occur in realistic device structures.

1:51PM M15.00012 Influence of non-gaussian statistics and dynamic non-locality in temporal evolution of open quantum systems, CARLOS FLOREZ, LEONARDO PACHÓN, Univ de Antioquia — The study of quantum dissipation and non-local dynamics in phase space demands an extension of the Ullersma-Caldeira-Leggett framework to include non-linearities either in the system or the bath or even in the couplings between them. In this work, the special case of a linear open system interacting with a harmonic thermal bath by means of non-linear couplings is considered. This framework is constructed by extending the path integral formulation into phase space and applying the Feynman-Vernon influence functional theory to study the perturbative regime at different orders in the couplings. In doing so, the formal correspondence between the perturbative contributions and the Feynman diagrams that arise from the $n$-point correlation functions in the canonical variables are used. The effect of the non-local behavior induced by the non-linear contributions on the dissipative and decohering mechanisms are analyzed. The main features are the presence of non-Gaussian statistics and multiplicative, instead of additive, noises.

2:03PM M15.00013 First-Principles Approach to Transient Heat Flow in Quantum Systems\textsuperscript{1}, KAMIL WALCZAK, Department of Chemistry and Physical Sciences, Pace University, One Pace Plaza, New York City, NY 10038, KIRK YERKES, Aerospace Systems Directorate, Air Force Research Laboratory, Wright-Patterson AFB, OH 45433, NANOSCALE PHYSICS DIVISION TEAM, THERMAL MANAGEMENT CENTER COLLABORATION — We examine heat transfer via quantum advection modes (coherently correlated quantum states) between two thermal baths of different temperatures mediated by quantum system with discrete spectrum of accessible energy levels. Nanoscale transport is treated within the first-principles method by including the superposed wave functions into the quantum expression for heat flux. Our results show the specific modifications of heat transport characteristics due to the dynamics of quantum systems under consideration. Such dynamics is captured by non-steady-state solutions to time-dependent Schrödinger wave equation or by specific solutions of interrelated Pauli rate equations. Since the applicability of Fourier’s law is questionable at nanoscale and in the case of transient heat conduction, we pay particular attention to the new physics of post-Fourier heat transport and its further consequences. For instance, the non-equilibrium conditions may establish and maintain certain degree of coherence between correlated quantum states which are involved into the energy conduction process. Understanding and gaining control of coherent manipulations of qubits (two-level quantum systems) is crucial for further development of quantum informatics.

\textsuperscript{1}This work was supported by Pace University Start-up Grant and the Air Force Office of Scientific Research (AFOSR).

Wednesday, March 4, 2015 11:15AM - 1:51PM —
Session M16 DMP: Focus Session: Designed Function in Reduced Dimensional Materials and Clusters 101AB - Raghunathan Ramakrishnan, University of Basel, Switzerland

11:15AM M16.00001 Topologically nontrivial electronic bands and tunable Dirac cones in graphynes with spin-orbit coupling\textsuperscript{1}, VLADIMIR JURICIC, GUIDO VAN MIERT, CRISTIANE MORAIS SMITH, Univ of Utrecht — Graphynes represent an emerging family of carbon allotropes that differ from graphene by the presence of the triple bonds (-C≡C-) in their band structure. They have recently attracted much interest due to the tunability of the Dirac cones in the band structure. I will show that the spin-orbit coupling in $\beta$-graphyne could produce various effects related to the topological properties of its electronic bands. Intrinsic spin-orbit coupling yields high- and tunable Chern-number bands, which may host both topological and Chern insulators, in the presence and absence of time-reversal symmetry, respectively. Furthermore, Rashba spin-orbit coupling can be used to control the position and the number of Dirac cones in the Brillouin zone\textsuperscript{1}. Finally, I will also discuss the electronic properties of $\alpha$- and $\gamma$-graphyne in the presence of the spin-orbit coupling within recently developed general theory of spin-orbit couplings in graphynes\textsuperscript{2}.

\textsuperscript{1}G. van Miert, C. Morais Smith, and V. Juricic, Phys. Rev. B 90, 081406(R) (2014).


\textsuperscript{1}Work supported by the Netherlands Organization for Scientific Research (NWO).
11:27AM M16.00002 Chemical Trends for Transition Metal Compound Bonding to Graphene, JOERN LANGE, VOLKER BLUM, Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC, USA — Transition metal compounds are of interest as catalysts for the hydrogen evolution reaction (HER). However, a perfect candidate to replace expensive platinum has not yet been identified. To tailor a specific compound, several properties come into play. One is the bonding to the underlying substrate, for which π-bonded carbon nanostructures are promising candidates. Here we analyze the bonding of small transition metal compound nano-clusters to a graphene layer for a range of chemical compositions: M₆A₈ (M = Mo, Ti; A = S, O, B, N, C). The clusters are generated by an unbiased random search algorithm. We perform total energy calculations based on density functional theory to identify lowest energy clusters. We calculate binding energies using the PBE and HSE functionals with explicit van der Waals treatment[1] and benchmark those against RPA cluster calculations. Our results indicate that molybdenum-carbides and -nitrides tend to bond tightly to graphene. Mo-oxides and -sulfides show small binding energies, indicating van der Waals bonding.


11:39AM M16.00003 Density-Functional Theory Study of Nucleation and Growth of Metallic Nanoparticles on MoS₂(001), WISSAM A. SAIDI, Mechanical Engineering and Materials Science, Univ of Pittsburgh — The dispersion of metallic Pt nanoparticles (NPs) on MoS₂ monolayers is systematically analysed using first-principles density functional theory calculations. The nucleation of the NPs is followed step-by-step where we find that n = 5 is the cluster size where the growth of the NPs transforms from 2-dimensional (2D) to 3D. Owing to the topography of MoS₂(001), the 2D NPs mostly attach to the support via a direct bonding with Mo atoms that sit in the troughs of the surface, while the 3D NPs are bonded to the sulfur atoms that are more extended in the vacuum region. Furthermore, we find that Pt is sufficiently mobile on the surface where the number of hopping events per second is ≈ 10⁹ s⁻¹. Moving from smaller width to a larger width, nanoribbons were showing more of a sheet like character. Other properties of these nanoribbons will also be discussed.

11:50AM M16.00004 Li Storage Properties of Disordered Single- and Bi-Layer Graphene, H. YILDIRIM, Purdue University School of Chemical Engineering, ALPER KINACI, Argonne National Laboratory, ZHI-JIAN ZHAO, Purdue University School of Chemical Engineering, MARIA CHAN, Argonne National Laboratory, JEFFREY P. GREELEY, Purdue University School of Chemical Engineering — Due to the limited capacity of the traditional intercalation-type graphite materials (373 mAh/g, LiC₆), much effort has been made to explore new anode materials to meet the increasing demand for batteries of high energy density. Among them, graphene has much attracted attention as an ideal platform for higher Li storage capacity, and for obtaining fundamental understanding of Li-C interaction. In this respect, we performed extensive first-principles calculations to model Li adsorption and intercalation in single- and bi-layer graphene, which are activated by defects for Li adsorption. For a wide range of Li coverages, the calculations predict that defect-free single layer graphene is not thermodynamically favorable compared to bulk metallic Li. However, graphene activated by defects are generally found to bind Li more strongly, and the interaction strength is sensitive to both the nature of defects and their densities. A rigorous thermodynamic analysis establishes the theoretical Li storage capacities of the defected graphene, and in some cases, these capacities are found to approach, although not exceed, those of bulk graphite. We will provide a performance comparison between defected single- and bi-layer graphene and bulk-graphite for Li storage capacities. A detailed analysis of the effect of the van der Walls (vdW) interactions will also be presented.

12:03PM M16.00005 Structure and electronic properties of alkali and alkaline-earth metals on graphene, JIAN ZHOU, Virginia Commonwealth University, SHUNHONG ZHANG, QIAN WANG, QIANG SUN, Peking University, PURUSOTTAM JENA, Virginia Commonwealth University — A thorough search of the monolayer structure of Li, Na, K, and Ca atoms on graphene, based on a synergistic combination of density functional theory and particle swarm optimization algorithm, yielded unusual deposition patterns. For Li atoms, we show that they prefer to cluster on graphene, irrespective of their concentration. We further show that an external electric field applied vertically to the graphene surface or doping with boron can prevent this clustering, leading to the homogeneous growth of Li. For larger atoms Na, K, and Ca, they distribute uniformly when their coverage ratio M:C is 1:6, but the Na and Ca atoms self-assemble to form parallel quasi-one-dimensional chains when their coverage is reduced to 1:8. Electron-phonon coupling calculations further show that the NaC₆ is a superconductor with critical temperature of 5.8 K. At low concentration (M:C = 1:8) and depending on metal species, well-aligned atomic metal chains interact with graphene with varying intensity, making it possible to achieve either rigid or non-rigid band doping in graphene.

1This work is partially supported by grants from the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award #DE-FG02-96ER45579 and the National Grand Fundamental Research 973 Program of China

12:15PM M16.00006 The effect of depolarization fields on the electronic properties of two-dimensional materials, YOUNG-HAN SHIN, HYE JUNG KIM, MOHAMMAD NOOR-A-ALAM, Department of Physics, University of Ulsan, Ulsan 680-749, Republic of Korea — Graphene is a two-dimensional semimetal with a zero band gap. By weakening the sp² covalent bonding of graphene with additional elements such as hydrogen or fluorine, however, it is possible to make it insulating. We can expect that the band gap converges to that of a three-dimensional analogue by repeating such two-dimensional layers along the normal to the layer. If we control the position of additional elements to make a dipole monolayer, the system will have an intrinsic internal field decreases as the number of layers increases. But, for two-dimensional bilayers, depolarization field is so strong that its electronic properties can be much different from its monolayer analogue. In this presentation, we show that the internal fields induced by dipole moments can change electronic properties of two-dimensional materials such as graphene-like structures and complex metal oxides.

1This work was supported by the National Research Foundation of Korea Grant by the Ministry of Education, Science, and Technology (2009-0093818, 2012-014007, 2014M3A7B4049367)

12:27PM M16.00007 First-principles studies of hematite nanoribbons, PRABATH WANAGURU, JIAO AN, QIMING ZHANG, The University of Texas at Arlington — We study two types of hematite nanoribbons, based on density functional theory has been performed. Geometry and magnetic order of these nanoribbons were optimized using DFT+U method implemented in VASP suite of software. It is found that the band gaps decreases from the value of ~ 2.0eV to ~ 1.7eV as the widths increase from 6Å to more than 40Å. Despite the bulk hematite is indirect in band gap nature, one type of nanoribbons show direct band gap nature in several widths. Cleaving energies are positive with respect to the hematite sheet and as width increases it is decreasing. Moving from smaller width to a larger width, nanoribbons were showing more of a sheet like character. Other properties of these nanoribbons will also be discussed.

1This research is supported by NSF SusChEM Program (Award DMR-1306291).
12:39PM M16.00008 Getting the Most from 2-D Materials: the Role of Device Dimensionality
HUAISHAN LI, DAVID STRUBBE, JEFFREY GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology — While the control of material dimensionality has been widely used as an important design means, the device dimensionality, which relates to the regularity of the material ensemble rather than the material itself, has received far less attention. Recently, both vertical [1,2] and lateral [2] heterojunctions based on 2-D materials have been successfully synthesized, which provides an unprecedented opportunity to renew our understanding of the concept of “dimensionality.” In this study, we propose a design strategy of controlling device dimensionality by computationally investigating a “1.5-dimensional” solar cell device made of a 2-dimensional graphene based material. According to the predicted optical properties and charge dynamics, this prototype system has the potential to achieve desirable characteristics of robustness against defects, efficient polaron pair dissociation, broad tunability with surface functionalization and the possibility to form tandem cells. In addition, the optimization of correlated light harvesting procedures simultaneously becomes attainable in such 1.5-d solar cell due to the extra degree of freedom to manage the flux of mass and energy.

12:51PM M16.00009 Structure Matters More than Size: Tuning the Electronic Properties of (TiO$_2$)$_n$ Clusters, NOA MAROM, Tulane University, New Orleans, LA, USA, SASWATA BHATTACHARYA, LUCA GHIRINGHELLI, Fritz-Haber-Institut der MPG, Berlin, Germany — To design (TiO$_2$)$_n$ clusters with desired properties we implemented a suite of three genetic algorithms (GA) tailored to optimize for low total energy (EGA), high vertical electron affinity (VEA-GA), and low vertical ionization potential (VIP-GA). The property-based GAs are an extension of the cascade GA reported in [1]. Analysis of the structures found by the VEA-GA and the VIP-GA vs. the EGA reveals structure-property relations. A high VEA is correlated with the presence of several dangling-O atoms (typically 3-4), rather than the previously suggested tri-coordinated Ti atom [2]. A low VIP is correlated with low bond connectivity (typically 2) between two dangling-O atoms. We show that the electronic properties of (TiO$_2$)$_n$ clusters with n up to 20 correlate more strongly with the presence of these structural features than with size. We further propose that the presence of these structural features causes the observed large magnitude of the dipole moment of TiO$_2$ clusters.


1:03PM M16.00010 Electronic and optical properties of ultrathin silicon nanomembranes: A first-principles investigation, WOOSUN JANG, SU-HYUN YOO, ALOYSIUS SOON, Global E3 Institute and Department of Materials Science and Engineering, Yonsei University, Seoul 120-749, Korea — Owing to its unique and exotic physical and chemical properties, there has been a lot of effort undertaken to explore and study ultrathin low-dimensional nanomaterials (e.g. graphene and MoS$_2$). Of late, two-dimensional (2D) nanomembranes of silicon — a well-known prototypical bulk semiconductor - have attracted much attention, and has found its potential in niche nanodevice applications e.g. field effect transistors (FET) and secondary battery anodes. In this work, after considering various nanomembranes of Si with varying thicknesses, we study geometric and electronic structures using first-principles density-functional theory calculations (and beyond). Here, we consider both bulk-terminated pristine Si nanomembranes as well as surface-reconstructed ones, as motivated by available experimental and theoretical reports. To understand the influence of growth conditions on these Si nanomembranes, we have also studied the role of surface-passage (e.g. with O, H, and OH) on their electronic and optical properties. Namely, we carefully investigate their thickness-dependent electronic band structure (i.e. both their fundamental and optical band gap energies), so as to elucidate their intrinsic structure-property relations for designing future technologically important nanodevices.

1:15PM M16.00011 What is the work function of a small nanocrystal?, LINGYUAN GAO, JAIME SOUTO, ALEX DEMIKOV, JAMES CHELIKOWSKY, Univ of Texas, Austin — The work function is defined as the difference between the electrostatic potential energy (\(\phi\)) of an electron in the vacuum near the metal surface and the metal’s Fermi energy. For a single crystal metal, the measured work function typically depends on the orientation of the metal surface. This seems counterintuitive, as the Fermi energy is the same across the metal sample, and the vacuum energy is also expected not to depend on the direction. The problem becomes even more interesting for a metallic nanocrystal, where facets of different orientation meet. We undertake to explore and study ultrathin low-dimensional nanomaterials (e.g. graphene and MoS$_2$). Of late, two-dimensional (2D) nanomembranes of silicon — a well-known prototypical bulk semiconductor - have attracted much attention, and has found its potential in niche nanodevice applications e.g. field effect transistors (FET) and secondary battery anodes. In this work, after considering various nanomembranes of Si with varying thicknesses, we study geometric and electronic structures using first-principles density-functional theory calculations (and beyond). Here, we consider both bulk-terminated pristine Si nanomembranes as well as surface-reconstructed ones, as motivated by available experimental and theoretical reports. To understand the influence of growth conditions on these Si nanomembranes, we have also studied the role of surface-passage (e.g. with O, H, and OH) on their electronic and optical properties. Namely, we carefully investigate their thickness-dependent electronic band structure (i.e. both their fundamental and optical band gap energies), so as to elucidate their intrinsic structure-property relations for designing future technologically important nanodevices.

1:27PM M16.00012 Effects of Interaction Range and Strength on the Phase Behavior of Small Clusters of Colloidal Particles, RAY SEHAGL, DIMITRIOS MAROUDAS, Univ of Mass - Amherst — We report the findings of a computational study of the phase behavior of thermodynamically small assemblies (clusters) of colloidal particles interacting via a potential that includes electrostatic repulsion and depletion-based attractive interactions. We applied the data mining technique of diffusion mapping to determine the dimensionality of an appropriate coarse-grained description of the phase behavior and to assess the suitability of chosen order parameters. The results of this technique indicate that two coarse variables, which represent metrics of assembly density and crystallinity, are required to describe the phase behavior of these colloidal assemblies. We generate free-energy landscapes (FELs) in this well-justified coarse-variable space using Monte Carlo umbrella sampling. We constructed these FELs over a range of interaction strength changes and obtained a comprehensive picture regarding the possible stable configurations of such colloidal assemblies at equilibrium and the phase changes observed between them. In particular, we observe an order-to-disorder transition between crystalline and liquid-like phases as well as a polymorphic transition between relaxed face-centered cubic and hexagonal close-packed structures.


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1 Funded by Recruitment Program of Global Experts of China and China Postdoctoral Science Foundation.
Wednesday, March 4, 2015 11:15AM - 2:15PM  
Session M17 DCMP: Graphene: Terahertz Physics and Plasmons 102AB - Junichiro Kono, Rice University

11:15AM M17.00001 Optimizing Broadband Terahertz Modulation with Hybrid Graphene/Metasurface Structures , SUFEI SHI, BO ZENG, HUI-LING HAN, XIAOPING HONG, HSIN-ZON TSAI, HAE SAE, ALEX ZETTL, MIKE CROMMIE, FENG WANG, UC Berkeley, UC BERKELEY TEAM — We demonstrate efficient terahertz (THz) modulation by coupling graphene strongly with a broadband THz metasurface device. This THz metasurface, made of periodic gold slit arrays, shows near unity bandwidth transmission that arises from coherent radiation of the enhanced local field in the slits. Utilizing graphene as an active load with tunable conductivity, we can significantly modify the local-field enhancement and strongly modulate the THz wave transmission. This hybrid device also provides a new platform for possible nonlinear THz spectroscopy study of graphene.

11:27AM M17.00002 Full-range Gate-controlled Terahertz Phase Modulation with Graphene Metasurfaces , QIONG WU, ZIQI MIAO, XIN LI, DING KUN, QIONG HE, ZHENHUA AN, YUANBO ZHANG, LEI ZHOU, Fudan Univ, LEI ZHOU’S GROUP COLLABORATION, YUANBO ZHANG’S GROUP, ZHENHUA AN’S GROUP TEAM — Local phase control of electromagnetic wave is the basis of a diverse set of applications such as hologram imaging, polarization manipulations and wave-front controls. Here, we demonstrate full-range THz phase modulation realized on a metasurface featuring magnetic resonators that are coupled with graphene as a tunable loss. A gate bias applied through liquid ion tunes graphene’s optical conductivity, turns the coupled system from an under-damped resonator to an over-damped one, and induces dramatic modulation in the phase of the reflected wave. Our one-port resonator (i.e. resonator with only reflection channel) model reveals the underlying mechanism of our extreme phase modulation, and points to general guidelines for achieving large, tunable phase modulation in THz regime. A gate-tunable polarizer will be presented as an early demonstration of the capability of our graphene metasurfaces.

11:39AM M17.00003 Coupling of strongly localized graphene plasmons to molecular vibrations , DAMON FARMER, IBM T. J. Watson Research Center, YILEI LI, Columbia Univ, HUGEN YAN, IBM T. J. Watson Research Center, XIANG MENG, Columbia Univ, WENJUN ZHU, IBM T. J. Watson Research Center, RICHARD OSGOOD, TONY HEINZ, Columbia Univ, PHAEDON AVOURIS, IBM T. J. Watson Research Center — In this work, we present a new mechanism to couple graphene plasmons to vibrations in the PMMA molecules. The enhanced interaction is manifested through induced transparency in the graphene plasmon optical response when the plasmon and the vibrational frequencies are matched. We also show that this coupling is of an electromagnetic nature by comparing the evolution of the line shape as a function of the detuning of the two frequencies to simulations using the finite-difference time-domain method.

11:51AM M17.00004 Effects of screening on the propagation of graphene surface plasmons , KEN-ICHI SASAKI, NORIO KUMADA, NTT Basic Research Laboratories — We investigated surface plasmons in epitaxial graphene, while paying particular attention to the effect of interface states and resistivity on the transport properties[1,2]. The propagation velocity of the surface plasmons is much slower than the electron Fermi velocity when the screening effect induced by interface states is taken into account. Furthermore, slow-moving surface plasmons undergo a strong diffusion when the Fermi energy is near the Dirac point. This is shown by a numerical simulation of an RLC circuit model and its continuum approximation known as the telegrapher’s equation. We could explain recent experimental results for the surface plasmons satisfactorily. [1] Kumada et al., New J. Phys. 16, 063055 (2014). [2] Sasaki and Kumada, Phys. Rev. B 90, 035449 (2014).

12:03PM M17.00005 Retardation effect in graphene plasmonics , HUGEN YAN, IBM T. J. Watson Research Center — Localized plasmons in graphene micro- and nano-structures have attracted lots of attention recently. Typically the size of the graphene structure is much smaller than the on-resistance light wavelength and the quasi-electrostatic treatment of the light-matter interaction is sufficient. However, with increasing graphene structure size and stacked layer thickness, the quasi-electrostatic treatment fails. Retardation effect and dynamic depolarization have to be taken into account. In the paper, we’ll focus on two major topics related to the retardation effect. First, ultralow damping of graphene plasmons can be achieved in ultra-large graphene disk and ribbon arrays. Second, the coupling of graphene structures in the same array is radiative in nature and the resonance associated with the periodic lattice of the graphene disk or ribbon arrays play an role in the plasmonic response.

12:15PM M17.00006 Plasmon-enhanced terahertz photodetection in graphene1 , XINGHAI CAI, ANDREI SUSHKOV, CNAM, University of Maryland, College Park, MOHAMMAD JADIDI, IREAP, University of Maryland, College Park, R.L. MYERS-WARD, A.K. BOYD, R.M. DANIELS, D. KURT GASKILL, U.S. Naval Research Laboratory, Washington, DC, THOMAS MURPHY, IREAP, University of Maryland, College Park, H. DENNIS DREW, CNAM, University of Maryland, College Park, MICHAEL FUHRER, School of Physics, Monash University, Victoria, Australia — Graphene is a promising material for high speed room-temperature terahertz photodetection. However, the limited absorption in monolayer graphene remains a key challenge. We present here a large area terahertz detector that utilizes a plasmonic resonance in sub-wavelength graphene micro-rubbons to increase the absorption efficiency, and exploits the hot-electron photothermoelectric effect for detection. Through Fourier transform infrared spectroscopy we show that by tailoring the orientation of the graphene ribbons with respect to an array of sub-wavelength bimetallic electrodes, the plasmonic resonance can be efficiently excited, with a gate-tunable resonance frequency across the terahertz range. Polarization-dependent photoresponse measurements show an enhanced photothermal voltage between the outermost electrodes due to the plasmonically enhanced absorption.

1This work was sponsored by the US ONR (N000140911064, N000141310712 and N000141310865), the US NSF (ECCS 1309750), IARPA, and the Australian Research Council.

12:27PM M17.00007 Controlling Terahertz Waves using Graphene Supercapacitors , NURBEK KAKENOV, Osman Balcı, EMRE O. POLAT, Bilkent University, HAKAN ALTAN, Middle East Technical University, COSKUN KOÇABAS, Bilkent University — Ability to control density of high mobility charge carriers on graphene provides a unique platform to control electromagnetic waves in a broad spectrum. In this work, we demonstrate a terahertz intensity modulator using a graphene supercapacitor which consists of two large area graphene electrodes and electrolyte medium. This simple device structure enables us to modulate THz waves in a broad spectrum without any metallic gate electrodes. The mutual electrostatic gating between the graphene electrodes provides a very efficient electrostatic doping with Fermi energies of 1 eV. We show that, the graphene supercapacitor yield more than 50% modulation between 0.1 to 1.4 THz with operation voltages less than 3V. The low insertion losses, the simplicity of the device structure and polarization independent device performance are the key attributes of graphene supercapacitors for THz applications.
12:39PM M17.00008 THz pump-THz probe study of electrostatically gated graphene1, JINGDI ZHANG, MENGKUN LIU, MARTIN WAGNER, D. N. BÁSOV, RICHARD D. AVERITT, Univ of California - San Diego — We investigate ultrafast carrier dynamics in graphene using THz-pump THz-probe spectroscopy. In contrast to recent studies using optical excitation [1] [2], THz excitation exclusively initiates intra-band transitions, resulting in an increase in the carrier scattering rate. The corresponding transient peak of the transmitted probe signal scales linearly with the E-field of the incident THz pump pulse. Further, the decay time of the excited carriers is independent of the gating voltage. As the Fermi level is tuned toward the charge neutral point (CNP) by varying the electrostatic gate voltage, the induced increase in transmission is strongly suppressed. We believe that the low density of states near the CNP is responsible for this suppression. [1] Shi, S. F., Tang, et. al. Nano Lett., 14(3), 1978-1982 (2014). [2] A. J. Frenzel, et. al. Phys. Rev. Lett. 113, 056602 (2014).

1Work supported by DOE-BES. RDA and JZ also with Boston University. ML also with Stony Brook University.

12:51PM M17.00009 Top Gated Graphene PN junctions for THz detection1, ANTHONY BOYD, US Naval Research Laboratory, ANINDYA NATH, George Mason University, MEHDI JADIDI, RYAN SUESS, ANDREI SUSHKOV, GREGORY JENKINS, H. DENNIS DREW, THOMAS MURPHY, University of Maryland, RACHEL MYERS-WARD, KEVIN DANIELS, D. KURT GASKILL, US Naval Research Laboratory — The search for terahertz (THz) detectors based on graphene is encouraged by the fact that the ballistic regime in graphene occurs at room temperature over a distance of few dozens of nanometers. The naturally occurring 2-D carriers have extremely high intrinsic mobility at room temperature. Despite being only one atomic layer thick, graphene still absorbs several percent of incoming THz radiation well. THz detectors are fabricated on epitaxial graphene using an improved lithography process using lift off resist to achieve low contact resistance [1]. The devices are field effect transistors constructed with a thin asymmetric nichrome (NiCr) top gate that facilitates tuning the photovoltaic effect. The thin NiCr gate possesses a sheet resistance of 390 ohms which enables better matching of free space and does not block the incoming THz radiation.


1:03PM M17.00010 Strong exciton-plasmon coupling in graphene-semiconductor structures , TIGRAN V. SHAHBAZYAN, Jackson State Univ, KIRILL A. VELIZHANIN, Los Alamos National Lab — We study strong coupling between plasmons in monolayer doped graphene and excitons in narrow gap semiconductor quantum well separated from graphene by a potential barrier. We show that Coulomb interactions between excitons and plasmons result in mixed states described by Hamiltonian similar to one describing exciton-polaritons and derive the exciton-plasmon coupling parameter that depends on system geometry and material properties. We calculate numerically the Rabi splitting of exciton-plasmariton states and discuss the manifestation of these states in optical and electrical measurements. We also study how the contacts affect the coupling to and from free-space radiation. This provides insight to design and optimize plasmonic devices in the terahertz spectral range that can be tuned by application of a gate voltage. These features make graphene an attractive candidate for a variety of electrically tunable and broad bandwidth photodetectors of the THz regime.

1:15PM M17.00011 Plasmons in metal contacted graphene1, M.M. JADIDI, Institute for Research in Electronics and Applied Physics(IREEAP), Univ of Maryland, College Park, A.B. SUCHKOV, Center for Nanophysics and Advanced Materials(CNAM), Univ of Maryland, College Park, R.L. MYERS-WARD, A.K. BOYD, K.M. DANIELS, D.K. GASKILL, US Naval Research Laboratory, H.D. DREW, CNAM, Univ of Maryland, College Park, T.E. MURPHY, IREEAP, Univ of Maryland, College Park — Subwavelength graphene structures exhibit standing-wave plasmon resonances throughout the terahertz spectral range that can be tuned by application of a gate voltage. These features make graphene an attractive candidate for a variety of electrically tunable terahertz devices, including filters, sensors, sources, and modulators. Plasmonic modes have been observed and analyzed in finite-size graphene elements such as ribbons and disks. However, nearly all optoelectronic applications require electrical connection to the graphene element, which drastically alters the plasmonic boundary conditions and mode structure. We present a study of the effects of conductive electrical contacts on the plasmonic modes of a graphene channel, and examine how the contacts affect the coupling to and from free-space radiation. We show that radiation effects are essential in defining and understanding the properties and linewidths of these modes. We also study how the graphene plasmon mode interacts with the antenna modes of the contacts. These results provide valuable insight for designing antenna-coupled graphene plasmonic devices, including detectors and emitters.

1This work was sponsored by the US ONR (N000141310865) and the US NSF (ECCS 1309750)

1:27PM M17.00012 Electro-optic and Many-body Effects on Optical Absorption of Twisted Bilayer Graphene , KAN-HENG LEE, LUJIE HUANG, CHEOL-JOO KIM, JIWOOONG PARK, Cornell University — In twisted bilayer graphene (tBLG), the interlayer rotation angle between the two graphene layers induces additional angle-dependent van Hove singularities (vHSs) in its band structure where the two Dirac cones from each layer intersect. These vHSs introduce extra angle-dependent absorption peaks in the optical absorption spectra of tBLG. Here, we experimentally investigate the overall doping and the interlayer potential on these interlayer absorption features at various angles. We independently tune the doping concentration of each layer with a newly-developed, optically transparent, dual-gate transistor geometry to perform simultaneous optical and electrical measurements. Our data show strong electro-optic phenomena in the optical absorption of tBLG, the peak energy and width of the interlayer resonance feature sensitively depends on the overall doping and interlayer potential. We explain our observation using a simple band picture as well as many-body effects. Our study provides a powerful experimental platform for studying more complicated structures such as rotated tri- and multi-layer graphene systems in the future. Moreover, the understanding of electro-optic and many-body effects in these materials opens up a way for novel electrochromic devices.

1:39PM M17.00013 Doping and Field Dependent Electrical Conductivity of Angle-Resolved Twisted Bilayer Graphene , LUJIE HUANG, CHEOL-JOO KIM, Cornell, ADAM WEI TSEN, Columbia, LOLA BROWN, JIWOOONG PARK, Cornell — In twisted bilayer graphene (tBLG), the interlayer interaction induces additional van Hove singularities (VHS) and mini-gaps near the intersections between the Dirac cones of the two layers; this results in several electrical and optical phenomena at an energy level that monotonically increases with the twist angle θ. While there exist previous studies on the electrical properties of tBLG, the electrical conductivity of tBLG and its dependence on the overall doping and interlayer potential (field) have not been measured using tBLG samples with known θ. Here, we report the electrical conductivity of θ-resolved tBLG in a dual-gate field effect transistor geometry which allows an independent control of the doping and interlayer potential. In large θ tBLG, the total conductivity is approximately proportional to the total carrier density (the sum of the carrier number densities from the top and the bottom layers), indicating that large θ tBLG acts as two independent single layers carrying the electrical current in parallel. Among tBLG samples with a small θ, however, we observe an extra resistance peak besides the Dirac point, which may correspond to the minigap near the VHS. In order to perform further experiments for this small-θ tBLG samples, we use a doubletransfer of CVD grown graphene films with a uniform lattice orientation over a large scale. This allows a direct optical characterization in the relevant IR wavelengths, a critical capability for determining and the twist angle θ.

1This work was sponsored by the US ONR (N000141310865) and the US NSF (ECCS 1309750)
1:51PM M17.00014 Resonant Tunneling and Intrinsic Bistability in Twisted Graphene Structures, JOAQUIN RODRIGUEZ-NIEVA, MILDRED DRESSELHAUS, LEONID LEVITOV, MIT — Bistable systems exhibit several distinct macroscopic states and can switch between them upon variation of some control parameter. Nonvolatile electronic systems that exhibit intrinsic bistability and fast switching times are desirable for low-power memory and logic. Experimental realizations of such systems, however, are scarce. We propose a novel mechanism for intrinsic bistability in van der Waals heterostructures formed by twisted graphene monolayers. Bistability in these systems originates from resonant tunneling and charge coupling between different graphene layers. These characteristics, governed by Dirac-like spectrum and Moiré periodicity of the tunneling Hamiltonian, allow multiple stable states in the sequential tunneling regime. In the bistability region, an intermediate electrically decoupled graphene layer can, for the same external bias, be either in a resonant or non-resonant state with respect to the top/bottom layer. Features of interest, such as resonant tunneling, negative differential resistance and bistability, are controlled by parameters easily accessible in experiments, namely the twist angle and interlayer conductances. We estimate the power required to retain this state, switching times, and assess volatility of such intrinsically bistable systems.

2:03PM M17.00015 Discovery of bound excitons in twisted bilayer graphene, HIRAL PATEL, Department of Physics, Oregon State University, JIWOOG PARK, Department of Chemistry, Cornell University, MATT GRAHAM, Department of Physics, Oregon State University — Recent first principle Bethe-Salpeter simulations of twisted bilayer graphene (tBLG), predict that the unique geometry of tBLG’s overlapping interlayer 2p orbitals produce a strong destructive coherence effect that results in stable, strongly bound exciton states. We directly probe the electronic dynamics of twisted bilayer graphene for the first time by developing a unique ultrafast confocal microscopy approach that combines transient absorption, and transmission electron microscopy. We find resonantly excited twisted bilayer regions display distinct, long-lived dynamics that are not present in 0° stacked bilayers. We further map out the electronic structure using one and two-photon transient absorption microscopy to observe signatures of both unbound and strongly bound excitonic states predicted by the theory. The probable existence of the stable excitons opens up the possibility of efficient carrier extraction by exploiting the unusual hybrid metallic-excitonic nature in twisted bilayer graphene systems.

Wednesday, March 4, 2015 11:15AM - 2:15PM

11:15AM M18.00001 From ground-state densities to entangled wave functions: an exploration for the Hubbard model, KLAUS CAPELLE, Universidade Federal do ABC (UFABC), Sao Paulo — The fundamental Hohenberg-Kohn theorem of density-functional theory (DFT) guarantees that, in principle, all information about a many-body system is contained in its ground-state density. Most effort in DFT is thus directed at finding ways to reliably calculate this density and to extract useful information from it. Quantum-information theory (QIT), on the other hand, is little concerned with ground-state densities, focusing instead on wave functions and density matrices, with a view on exploiting entangled states in information processing. In spite of these different philosophies, many connections exist between both approaches. In this talk, I review how some of these connections have been discovered and quantified in the context of the Hubbard model: (i) DFT calculations for a model Hamiltonian serve to relate the entanglement entropy to phase transitions; (ii) a local-density-type approximation can be used to calculate the entanglement entropy of spatially inhomogeneous systems, such as cold atoms in optical traps and large superlattices, where traditional numerical methods encounter difficulties; (iii) a combination of DFT with a Bethe-ansatz ansatz allows one to calculate the values of system-specific parameters in expressions for the block-block entanglement that remain undetermined in scaling approaches; (iv) the construction of suitable metrics shines light on how the Hohenberg-Kohn theorem relates densities and wave functions for different systems.

11:51AM M18.00002 Time-Dependent Density Functional Theory for Universal Quantum Computation, DAVID TEMPEL, Harvard University — In this talk, I will discuss how the theorems of TDDFT can be applied to a class of qubit Hamiltonians that are universal for quantum computation. The theorems of TDDFT applied to universal Hamiltonians imply that single-qubit expectation values can be used as the basic variables in quantum computation and information theory, rather than wavefunctions. From a practical standpoint this opens the possibility of approximating observables of interest in quantum computations directly in terms of single-qubit quantities (i.e. as density functionals). Additionally, I will discuss how TDDFT provides an exact prescription for simulating universal Hamiltonians with other universal Hamiltonians that have different, and possibly easier-to-realize two-qubit interactions.

12:27PM M18.00003 The computational complexity of many-electron problems and Density Functional Theory, NORBERT SCHUCH, RWTH Aachen University — Quantum computation and complexity has helped us to sharpen our understanding of the common origin for the difficulty of a wide range of problems in quantum many-body physics. In my talk, I will discuss the implications of quantum complexity theory to understanding systems of interacting electrons, and show how it allows us to determine the fundamental limitations to any numerical method for the simulation of those systems, including our ability to approximate the universal functional in Density Functional Theory.

1:03PM M18.00004 What Density Functional Theory could do for Quantum Information, ANN MATTSSON, Sandia National Laboratories, Albuquerque NM — The Hohenberg-Kohn theorem of Density Functional Theory (DFT), and extensions thereof, tells us that all properties of a system of electrons can be determined through their density, which uniquely determines the many-body wave-function. Given access to the appropriate, universal, functionals of the density we would, in theory, be able to determine all observables of any electronic system, without explicit reference to the wave-function. On the other hand, the wave-function is at the core of Quantum Information (QI), with the wave-function of a set of qubits being the central computational resource in a quantum computer. While there is seemingly little overlap between DFT and QI, reliance upon observables form a key connection. Though the time-evolution of the wave-function and associated phase information is fundamental to quantum computation, the initial and final states of a quantum computer are characterized by observables of the system. While observables can be extracted directly from a system’s wave-function, DFT tells us that we may be able to intuit a method for extracting them from its density. In this talk, I will review the fundamentals of DFT and how these principles connect to the world of QI. This will range from DFT’s utility in the engineering of physical qubits, to the possibility of using it to efficiently (but approximately) simulate Hamiltonians at the logical level. The apparent paradox of describing algorithms based on the quantum mechanical many-body wave-function with a DFT-like theory based on observables will remain a focus throughout. The ultimate goal of this talk is to initiate a dialog about what DFT could do for QI, in theory and in practice. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

1:39PM M18.00005 Density Functional Theory and Quantum Computation, FRANK GAITAN, University of Maryland — No abstract available.
Wednesday, March 4, 2015 11:15AM - 1:39PM

11:15AM M19.00001 Advances in Additive Manufacturing, VLASTIMIL KUNC, ORNL — No abstract available.

11:51AM M19.00002 3D Printing of Human Tissue Mimics via Layer-by-Layer Assembly of Polymer/Hydrogel Biopapers, BRADLEY RINGEISEN, Naval Research Laboratory — The foundations of tissue engineering were built on two fundamental areas of research: cells and scaffolds. Multipotent cells and their derivatives are traditionally randomly seeded into sophisticated polymer or hydrogel scaffolds, ultimately with the goal of forming a tissue-like material through cell differentiation and cell-material interactions. One problem with this approach is that no matter how complex or biomimetic the scaffold is, the cells are still homogeneously distributed throughout this three dimensional (3D) material. Natural tissue is inherently heterogeneous on both a microscopic and macroscopic level. It also contains different types of cells in close proximity, extracellular matrix, and a complex vascularized network. Recently deposited 3D cell and organ printers may be able to enhance traditional tissue engineering experiments by building scaffolds layer-by-layer that are crafted to mimic the microscopic and macroscopic structure of natural tissue or organs. Over the past decade, my laboratory has developed a capillary-free, live cell printer termed biological laser printing, or BioLP. We find that printed cells do not express heat shock protein and retain >99% viability. Printed cells also incur no DNA strand fracture and preserve their ability to differentiate. Recent work has used a layer-by-layer approach, stacking sheets of hybrid polymer/hydrogel biopapers in conjunction with live cell printing to create 3D tissue structures. Our specific work is now focused on the blood-brain-barrier and air-liquid interface and will be described during the presentation.

12:27PM M19.00003 3-D Constructs—Molded vs. Printed: The differences from a cell based perspective, MARCIA SIMON, Professor and Director of Graduate Studies, School of Dental Medicine, Stony Brook — Additive manufacturing technologies are increasingly being used to replace standard subtractive molding methods in engineering polymeric biomedical implants and devices. The principal advantage of this new technology is the ability to print directly from a scan and hence produce parts which are an ideal fit for an individual, which eliminates much of the sizing and fitting associated with standard manufacturing methods. The question though arises whether devices which may be macroscopically similar, serve identical functions, and be produced from the same polymeric material, in fact interact in the same manner with living tissue. Here we will discuss the differences in the surface structures produced by these manufacturing methods and the interactions of dental pulp stem cells with structures of multiple length scales as they impact cell differentiation and tissue mineralization.

In collaboration with Kuan Che Feng, Mariah Geritano, Michael Cuiffo, and Gary Halada, Materials Science and Engineering, Stony Brook University; Adriana Pinkas-Sarafova, Oral Biology and Pathology and Materials Science and Engineering, Stony Brook University; Sihana Rugova, Oral Biology and Pathology, Stony Brook University; and Miriam Rafailovich, Materials Science and Engineering, Stony Brook University.

1:03PM M19.00004 Novel Patterning Approaches for Continued Device Scaling, FLORIAN Gstrein, Intel Corporation — Top-down patterning techniques based on optical lithography have made semiconductor products ever more powerful, ubiquitous and affordable. This is largely due to the ability of conventional lithographic techniques to transfer trillions of mask features to wafers at defect densities approaching virtually zero throughout high-volume manufacturing. As features continue to shrink, the ability to print and to correctly place tight-pitch patterns have quickly emerged as two of the greatest challenges to scaling. Given the fundamental physical limitations of conventional optical lithography, complimentary patterning techniques and bottom-up patterning approaches are needed to overcome shortcomings in resolution and pattern placement accuracy. This presentation will focus on the enabling role novel materials can play in achieving both critical dimension scaling and reduced pattern placement errors. The talk will first outline how extreme UV lithography (EUV) and directed self-assembly (DSA) can simplify patterning and improve multilayer pattern placement by reducing the number of masks and associated overlay steps required to achieve the desired resolution. Novel EUV resist materials require amplification mechanisms that overcome acid blur and new strategies to improve shot noise limitations and mechanical stability. For DSA, novel block co-polymers are needed with a higher chi parameter to yield tighter pitch and improved roughness. The second part of the talk will highlight opportunities for self-aligned patterning with a special emphasis on the emerging field of selective deposition. Atomic layer deposition (ALD) is derived from the chemical nature of precursors and co-reactants. The ability of these molecules to recognize chemical functionalities and surfaces, results in the deposition of thin films only where they are desired. Selective deposition is a powerful and so far unexploited patterning tool capable of further reducing or even eliminating pattern placement errors.

Wednesday, March 4, 2015 11:15AM - 1:45PM
Session M20 FEb: Invited Session: Reichert Award Session: Re-imagining the Advanced Lab Ballroom B - Randall Knight, California Polytechnic State University

11:15AM M20.00001 Reichert Award Talk: Preparing Physics Students in an Era of Virtual Reality, CARL Akerlof, RAMON TORRES-ISEA, University of Michigan — Like many other institutions with a large and active faculty, the University of Michigan Physics Department has a rich curriculum of undergraduate courses that focus on the use of 19th Century mathematics to understand the behavior of matter and energy. Most people who have pursued a career in this field appreciate that success usually depends on a much wider variety of skills. Addressing those needs has been the major emphasis of our undergraduate advanced lab program. This covers a broad range of topics. First of all, physics will continue to enlarge its encroachment into new areas. Thus, we have added experiments in radio astrophysics and non-linear dynamics. Computational and statistical methods are integrated into the experiments as appropriate and development of effective communication skills is heavily stressed. While there are efforts elsewhere to replace traditional hands-on experimentation with simulations, interactive video-based laboratory modules, and remotely controlled laboratory experiments, we consider these tools to be appropriate only for pre-lab and post-lab activities. None of these tools can provide the long-lasting experimental skills and knowledge-packed memories that a well-designed teaching experiment can. Hence, we choose to focus on providing a comprehensive list of experiments in a safe, well-equipped, teaching environment. The overall guiding principle is to provide a multi-faceted introduction to a rewarding career in science.

11:45AM M20.00002 A hands-on introduction to quantum mechanics, DAVID JACKSON, Dickinson College — At Dickinson College, we have designed a series of experiments that are designed to expose students to the strange and fascinating world of quantum mechanics. These experiments are employed in our sophomore-level course titled Introduction to Relativistic and Quantum Physics, our version of the traditional Modern Physics course. The experiments make use of a correlated light source produced via the process of Spontaneous Parametric Down Conversion (SPDC). Using such a light source, students can experimentally verify that when a single photon is incident on a beam splitter, the photon is either transmitted or reflected — it never goes both ways. If instead the photons are directed into a Mach-Zehnder interferometer, students then observe an interference pattern, suggesting that each photon must somehow take both paths in the interferometer (in apparent contradiction of the first experiment). Finally, the interference pattern is observed to disappear if the photons are “tagged” to distinguish which path they take, only to mysteriously reappear if that path information is “erased” after emerging from the interferometer. In this talk, I will provide an overview of these experiments and the accompanying theory that students learn in this course.

This work was supported, in part, by NSF grant 0737230.
12:15PM M20.00003 Preparing students for experimental research through instructional labs, HEATHER LEWANDOWSKI, University of Colorado — Preparing undergraduate physics majors for future careers in experimental science is one of the main goals of our current physics education system. At the University of Colorado, we have been working to transform our upper-division laboratory courses to better prepare students for future undergraduate, industrial, or graduate experimental work. Through this process, we have developed learning goals, curricular materials, and assessments for two upper-division lab courses. The transformation process and measured outcomes will be presented.

12:45PM M20.00004 Autonomy, D.A. VAN BAALK, TeachSpin, Inc. — Advanced-laboratory experiences have long been a formative part of the undergraduate curriculum, and this presentation reviews some of the purposes that they serve. One under-acknowledged purpose for these laboratories is the role they serve in cultivating students’ capacity for exercising autonomy as scientists. Overt recognition of this implicit purpose of laboratory courses has implications for the organization and execution of such courses.

1:15PM M20.00005 Investigating student learning in upper-division laboratory courses on analog electronics1, MACKENZIE STETZER, University of Maine — There are many important learning goals associated with upper-division laboratory instruction; however, until recently, relatively little work has focused on assessing the impact of these laboratory-based courses on students. As part of an ongoing, in-depth investigation of student learning in upper-division laboratory courses on analog electronics, we have been examining the extent to which students enrolled in these courses develop a robust and functional understanding of both canonical electronics topics (e.g., diode, transistor, and op-amp circuits) and foundational circuits concepts (e.g., Kirchhoff’s laws and voltage division). This focus on conceptual understanding is motivated in part by a large body of research revealing significant student difficulties with simple dc circuits at the introductory level and by expectations that students finish electronics courses with a level of understanding suitable for building common, practical circuits in a real-world environment. Recently, we have extended the scope of our investigation to include more laboratory-focused learning goals such as the development of (1) troubleshooting proficiency and (2) circuit chunking and design abilities. In this talk, I will highlight findings from written questions and interview tasks that have been designed to probe student understanding in sufficient depth to identify conceptual and reasoning difficulties. I will also use specific examples to illustrate the ways in which this research may inform instruction in upper-division laboratory courses on analog electronics.

1This work has been supported in part by the National Science Foundation under Grant Nos. DUE-1323426, DUE-1022449, DUE-0962805, and DUE-0618185.


11:15AM M21.00001 Measurement and Instrumentation Challenges at X-ray Free Electron Lasers1, YIPING FENG, SLAC National Accelerator Laboratory — X-ray Free Electron Laser sources based on the Self Amplified Spontaneous Emission process are intrinsically chaotic, giving rise to pulse-to-pulse fluctuations in all physical properties, including intensity, position and pointing, spatial and temporal profiles, spectral content, timing, and coherence. These fluctuations represents special challenges to users whose experiments are designed to reveal small changes in the underlying physical quantities, which would otherwise be completely washed out without using the proper diagnostics tools. Due to the X-ray FEL’s unique characteristics such as the unprecedented peak power and nearly full spatial coherence, there are many technical challenges in conceiving and implementing these devices that are highly transmissive, provide sufficient signal-to-noise ratio, and most importantly work in the single-shot mode.

1Portions of this research were carried out at the Linac Coherent Light Source (LCLS) at the SLAC National Accelerator Laboratory. LCLS is an Office of Science User Facility operated for the U.S. Department of Energy Office of Science by Stanford Univ.


12:27PM M21.00003 LCLS-II: Upgrade Plans for the Linac Coherent Light Source–Including New Scientific Opportunities1, WILLIAM SCHLOTTER, LCLS, SLAC National Accelerator Laboratory, LCLS-II TEAM — The Linac Coherent Light Source (LCLS) is planning a major upgrade that will provide revolutionary new scientific capabilities for exploring materials on the atomic and nano-scale with element specificity and ultrafast temporal resolution. The LCLS is an x-ray free electron laser with six experimental instruments accessible via a peer-reviewed proposal process. The upgraded LCLS-II facility will continuously deliver ultrafast x-ray pulses at repetition rates greater than 100kHz with photon energies tunable between 250 eV and 5 keV. The upgrade will also produce pulses with photon energies as high as 25 keV at a repetition rate of 120 Hz. These capabilities will enable new scientific methods that will revolutionize the study of highly correlated electron systems, magnitization dynamics and nanoscale fluctuations in soft matter to name a few. Expected capabilities and prospective experimental examples will be presented.

1The Linac Coherent Light Source (LCLS) at the SLAC National Accelerator Laboratory. LCLS is an Office of Science User Facility operated for the U.S. Department of Energy Office of Science by Stanford University.

12:39PM M21.00004 Fourier transform inelastic x-ray scattering from phonons using Free Electron Laser pulses, MARIANO TRIGO, SLAC/Stanford University, THOMAS HENIGHAN, Stanford University, DAVID REIS, SLAC/Stanford University — We demonstrate that ultrafast x-ray scattering at Free Electron Lasers (FELs) provides a new approach for measuring phonon dispersion relations spanning the entire Brillouin zone, without the need for complex monochromators and spectrometers. Our method uses an ultrafast optical laser as pump and the dynamics are probed using femtosecond x-ray pulses from an FEL. We obtain the entire transverse acoustic phonon dispersion in germanium with ~ 0.5 meV energy resolution by a simple Fourier transform of the oscillatory dynamics of the scattered x-ray intensity. Using coherent control with a pair of pump pulses, we show that the femtosecond laser couples to pairs of phonons, analogous to a second order Raman scattering mechanism, which also explains the excitation of large-wavevector phonons by the long wavelength (optical) pump pulse. This shows that the generation mechanism is quite general and thus this ultrafast approach could be applicable as a general spectroscopic tool of phonons near to and far from equilibrium.

12:51PM M21.00005 ABSTRACT WITHDRAWN –
The frequency of the AIDT excitation. Diffraction measurements of a Pt thin film grown on the LiNbO
the strain is identical to that measured using light reflectivity. From x-ray diffraction measurements, we obtained a quantitative measure of the strain amplitude,
the ring frequency of the Advanced Photon Source, where x-ray diffraction measurements were carried out with a focus of 7
µ3
follow the constant velocity curve of the piezoelectric surface to focus the strain wave over a small focal area. A detailed analysis of the strain around the focal
waves can be used to determine the charge and vibrational asymmetry in the bulk crystal. These effects are demonstrated with in situ synchrotron x-ray scattering measurements on S(111)7x7 surfaces with and without Ag films.

Support is gratefully acknowledged from NSF DMR-0706278 and DGE-1069091. The Advanced Photon Source at Argonne National Laboratory is supported by the US-DOE W-31-109-Eng-38.

A MEMS-based device used for alignment and manipulation of MLL x-ray focusing optics, WEIHE XU, KENNETH LAUER, HUI YAN, Brookhaven Natl Lab, VELIKO MILLANOVIĆ, Mirrorce Technologies, Inc, EVGENY NAZARETSKI, Brookhaven Natl Lab, BROOKHAVEN NATL LAB TEAM, MIRRORCLE TECHNOLOGIES, INC. TEAM — Multilayer Laue lenses (MLLs) X-ray microscopy is a powerful tool used for materials research. To push the spatial resolution of x-ray microscopy studies below 10 nm the system needs to be compact and rigid. Applications of MEMS based tip-tilt stages used for alignment and manipulation of nanofocusing optics is a promising route to achieve high stability. In this work, we report characterization and stability testing of a MEMS device suitable for manipulation of nanofocusing optics. We developed two closed-loop circuits implemented in a MEMS tip-tilt device utilizing capacitive and laser interferometry techniques. Test results demonstrate better than 10 mille-degree resolution when using capacitive sensors and better than 0.8 mille-degree resolution when using interferometry sensing respectively.

Forbidden Reflections in X-ray Crystal Truncation Rods: Using Surface Reference Waves to Distinguish Charge and Vibrational Asymmetry in Bulk Silicon1, JESSE KREMEN-NAK, YIYAO CHEN, SHAWN HAYDEN, MICHAEL GRAMLICH, PAUL MICELI, University of Missouri — X-ray reflections from diamond crystal structures with Miller indices that satisfy h+k+l = 4n+2, where n is an integer, are considered to be forbidden by crystal symmetry. However, asymmetry from valence charge distribution as well as anharmonic vibrations break the symmetry and result in non-zero intensity “forbidden reflections.” Due to the absence of phase information, considerable effort, involving combined temperature-dependent x-ray and neutron scattering studies, was previously required to determine the contributions of charge and vibrations to these reflections. In the present work, we demonstrate that useful phase information can be gained in x-ray reflectivity and crystal truncation rod measurements where there is interference between waves scattered from the bulk and the surface. In this manner, surface reference waves can be used to determine the charge and vibrational asymmetry in the bulk crystal. The DOD-AFOSR Award FA9550-14-1-0363 and the LANSCE-ROSEN Professorship supported work at NMSU/LANL. Research at UCSD was supported by the NSF & NIH/NIGMS via NSF award DMR-1332208.

Phonon Mapping in Flowing Equilibrium1, J.P.C. RUFF, CHESS, Cornell University — When a material conducts heat, a modification of the phonon population occurs. The equilibrium Bose-Einstein distribution is perturbed towards flowing-equilibrium, for which the distribution function is not analytically known. Here I argue that the altered phonon population can be efficiently mapped over broad regions of reciprocal space, via diffuse x-ray scattering or time-of-flight neutron scattering, while a thermal gradient is applied across a single crystal sample. When compared to traditional transport measurements, this technique offers a superior, information-rich new perspective on lattice thermal conductivity, wherein the band and momentum dependences of the phonon thermal current are directly resolved. The proposed method is benchmarked using x-ray thermal diffuse scattering measurements of single crystal diamond under transport conditions.

CHESS is supported by the NSF & NIH/NIGMS via NSF award DMR-1332208.

Mapping of Strain Inhomogeneity within a Single Ni-NiO Core-Shell Nanoparticle using Bragg Coherent Diffraction Imaging1, ERANDI WIJERATHNA, NMSU, R. HARDER, APS, Argonne National Laboratory, J. CLARK, SLAC National Accelerator Laboratory, B. KIEFER, NMSU, E. FULLERTON, O. SHPYRKO, UCSD, E. FOHTUNG, NMSU — We report on recent progress in mapping strain inhomogeneity within a single core/shell ferromagnetic/antiferromagnetic Ni-NiO nanoparticle (NP) using Bragg Coherent X-ray Diffraction Imaging (CXDI). By collecting CXD maps from the NP in the vicinity of two different reciprocal lattice points we observe variations in the sign and magnitude displacement gradients within the core and shell regions indicative of anisotropy and inhomogeneity. We utilize computations with atomic resolution to model a guess of the deformations within the core structure. This serves as guide for apriori support. Finite difference analysis is used alongside CXDI to reconstruct the core-shell regions. This approach opens new avenues in studying buried structures and multifunctional properties using CXDI.

Work at UNL is supported by NSF Grant No. 1409622 and MRSEC DMR-0820521, and at Argonne by DE-AC02-06CH11357.

Measurement of fast dynamic strain generated by focusing of surface acoustic waves1, UDAY SINGH, Univ of Nebraska - Lincoln, Y. LI, D.A. WALKO, Argonne National Lab, S. ADENWALLA, Univ of Nebraska - Lincoln — We have measured the spatial and temporal dependence of high frequency (88 MHz) strain waves in a focused surface acoustic wave (FSAW). Increasing the strain generated by a SAW to levels that are comparable with epitaxial strains in thin films (~ 1%) necessitate annular inter-digital transducers (AIDT) that follow the constant velocity curve of the piezoelectric surface to focus the strain wave over a small focal area. A detailed analysis of the strain around the focal center of an AIDT patterned on 128 Y-cut LiNbO3 shows shifts in the (104) x-ray diffraction peak. The AIDT spacing was chosen to produce a resonance at the ring frequency of the Advanced Photon Source, where x-ray diffraction measurements were carried out with a focus of 7 µm. The spatial dependence of the strain is identical to that obtained measuring light reflectivity. From x-ray diffraction measurements, we obtained a quantitative measure of the strain amplitude, 0.5% at an AIDT excitation power of 24 dBm. The temporal dependence showed a sinusoidally varying strain that cycles between compressive and tensile at the frequency of the AIDT excitation. Diffraction measurements of a Pt thin film grown on the LiNbO3 show significant strain transfer. These data lay the groundwork for future experiments that involve tuning the physical properties of strain sensitive thin film materials at high frequencies.

Work at UNL is supported by NSF Grant No. 1409622 and MBSEC DMR-0820521, and at Argonne by DE-AC02-06CH11357.

Wednesday, March 4, 2015 11:15 AM - 2:03 PM –
Session M22 DCMP: Heavy Fermions: Ce-115 and Yb-based Compounds: Experiment 202A -
Steven Dissler, NIST
11:15AM M22.00001 An Angle Resolved Photoemission Survey of the Band Structure of the Heavy Fermion Superconductor, CeCoIn$_5$.

THEODORE REBER, JONATHON RAMEAU, RONGWEI HU, CEDOMIR PETROVIC. peter johnson, Brookhaven National Lab — With the highest $T_c$ of the non-radioactive heavy fermion materials, CeCoIn$_5$ has been extensively studied by a host of techniques. However direct measurements of the band structure via angle resolved photo-emission spectroscopy has been limited to just a few experiments. We will present our studies of the momentum, temperature, photon energy and polarization dependence of the band structure of CeCoIn$_5$. We will compare our results with theory and other experimental results.

1Present address: Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University

11:27AM M22.00002 Landau Renormalizations of Superfluid Density in the Heavy-Fermion Superconductor CeCoIn$_5$.

LEI SHU, Fudan University, D.E. MACLAUGHLIN, C.M. VARMA, UC Riverside, O.O. BERNAL, California State U. LA, P.-C. HO, R.H. FUKUDA, California State U. Fresno, X.P. SHEN, Fudan University, M.B. MAPLE, UC San Diego — The formation of heavy fermion (HF) bands can occur by means of the conversion of a periodic array of local moments into itinerant electrons via the Kondo effect and the huge consequent Fermi-liquid(FL) renormalizations. Leggett predicted for liquid $^3$He that FL renormalizations change in the superconducting state, leading to a temperature($T$) dependence of the London penetration depth $\lambda$ quite different from that in the BCS theory. Using Leggett’s theory, as modified for HF, it is possible to extract from the measured $T$ dependence of $\lambda$ in high quality samples both Landau parameters $F_0$ and $F_1$; this has never been accomplished before. A modification of the $T$ dependence of the specific heat $C_\lambda$, related to that of $\lambda$, is also expected. We have carefully determined the magnitude and $T$ dependence of $\lambda$ in CeCoIn$_5$ by muon spin relaxation rate measurements to obtain $F_0=36\pm1$ and $F_1=1.2\pm0.3$, and find a consistent change in the $T$ dependence of electronic specific heat $C_\lambda$. This, the first determination of $F_1$ with a value $< F_0$ in a HF compound, tests the basic assumption of the theory of HF, that the frequency dependence of the self-energy is much more important than its momentum dependence.

1This research is supported by the NSF of China (11204041), NSF of Shanghai (12ZR1401200), USDoE (DE-FG02-04ER46105), and U.S. NSF(DMR 0802478, 0801407, 1206298, 1104544, 1105380).


ELI LEVENSON-FALK, JOSHUA STRAUQUADINE, ELIZABETH SCHEMM, AHARON KAPITULNIK, Stanford University, PRISCILLA ROSA, ZACHARY FISK, Department of Physics, UC Irvine — The heavy-fermion superconductor CeCoIn$_5$ is of great interest, as it shares many features with high-$T_C$ d-wave superconductors, with unconventional pairing and competition between superconducting and magnetic phases. Understanding the mechanisms of superconductivity in this material can elucidate the physics of high-$T_C$ and of unconventional superconductivity in general. We present measurements of the polar Kerr effect in CeCoIn$_5$ using a zero-area Sagnac interferometer. We observe an onset of Kerr rotation near the superconducting transition temperature, indicating an order parameter which breaks time reversal symmetry. We discuss the relation of this symmetry breaking to the superconducting state, and place our measurement in context with other experiments on this material.

11:51AM M22.00004 Ultrafast dynamics in CeCoIn$_5$.

INNA VISHIK, FAHAD MAHMOOD, ZHANYBEK ALPICHSHEV, Massachusetts Institute of Technology, SHANTA SAHA, JOHNPIERRE PAGLIONE, University of Maryland, College Park, NUH GEDIK, Massachusetts Institute of Technology — We present ultrafast pump-probe and transient grating spectroscopy studies of the heavy Fermion superconductor CeCoIn$_5$. In pump-probe experiments, a 100-femtosecond 800nm-wavelength pulse creates transient electronic excitations whose decay is probed by studying transient changes in reflectivity as a function of time. We observe changes in pump-probe decay dynamics across the Kondo coherence temperature. In transient grating spectroscopy, two pump-pulses are interfered to produce a spatially periodic excitation, and the system’s response to this periodic perturbation is studied through a diffracted probe beam. The temporal evolution of this signal indicates a non-trivial motion of the excitation grating in the heavy electron regime.

12:03PM M22.00005 Field induced density wave in the heavy fermion compound CeRhIn$_5$.

PHILIP MOLL, Department of Physics, University of California, Berkeley, California 94720, USA, BIN ZENG, LUIIS BALICAS, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, USA., STANISLAW GALESKI, Solid State Physics Laboratory, ETH Zurich, Switzerland, FEDOR BALAKIREV, National High Magnetic Field Laboratory, LANL, E536, Los Alamos, NM 87545, USA, ERIC BAUER, FILIP RONNING, Los Alamos National Laboratory, Los Alamos, NM 87545, USA.187 — We will present evidence for a magnetic field induced phase-transition to a state akin to a density-wave (DW) in the heavy fermion superconductor CeRhIn$_5$. The DW state is signaled by a hysteretic anomaly in the in-plane resistivity accompanied by the appearance of non-linear electrical transport at high magnetic fields ($>27T$), which are distinctive characteristics of density-wave states. The differential resistance $dV/dI$ is strongly suppressed by currents in excess of an critical electric field $E_c$, 15mV/cm, which would be a typical value for depinning thresholds in incommensurate density waves such as NbSe$_2$ or TaS$_2$. Intriguingly, the out-of-plane resistivity as well as the magnetic torque remain unaffected by the transition.

12:15PM M22.00006 Observation of field-induced Fermi surface reconstruction in CeRhIn$_5$.

HUIQIU YUAN, LIN JIAO, ZONGFA WENG, YE CHEN, Zhejiang Univ, FRANK STEGLICH, Zhejiang Univ/Max-Planck Institute for Chemical Physics of Solids, DAVID GRAF, Florida State University, JOHN SINGLETON, MARCELO JAIME, ERIC BAUER, JOE THOMPSON, Los Alamos National Lab — CeRhIn$_5$ provides a prototype compound for studying quantum criticality and its interplay with superconductivity. Application of pressure suppresses the antiferromagnetic (AF) order and gives rise to superconductivity [1]. A sharp change of Fermi surface was observed just at the pressure-tuning AF quantum critical point (QCP) [2], which was argued to support the scenario of local quantum criticality [3]. By measuring the dHvA oscillations and specific heat in a pulsed magnetic field, we have demonstrated the existence of a field-induced AF QCP around $B_c$=50T in this compound [4]. In this presentation, we will report the measurements of dHvA effect and Hall resistivity of CeRhIn$_5$ performed by using the 45T hybrid magnet and the pulsed field magnet at NHMFL. Field-induced changes of the dHvA frequencies and Hall coefficient are observed around $B^*=31T$. Detailed analyses suggest that the Fermi surface reconstruction at $B^*$ corresponds to a localized-itinerant transition of Ce 4f-electrons attributed to the Kondo effect. Our results indicate that multiple quantum phase transitions may exist in CeRhIn$_5$ which can be classified by the measurements of Fermi surface topology. [1] T. Park et. al., Nature 440, 65 (2006). [2] H. Shishido et. al., J Phys Soc Jpn 74, 1103 (2005). [3] Q. Si, F. Steglich, Science 329,1161 (2010). [4] L. Jiao et al., arXiv:1308.0294.
12:27PM M22.00007 The magnitude of the magnetic exchange interaction in the heavy fermion antiferromagnet CeRhIn$_5$; P. DAS, Ames Laboratory, IA, USA; Los Alamos National Laboratory, NM, USA, S.-Z. LIN, N.I. GHIMIRE, F. RONNING, E.D. BAUER, J.D. THOMPSON, C.D. BATISTA, M. JANOSCHEK, Los Alamos National Laboratory, NM, USA, K. HUANG, University of California, San Diego, CA, USA, G. EHLERS, Oak Ridge National Laboratory, TN, USA — The family of heavy fermion compounds CeTIn$_5$ ($T=Co$, Rh, Ir) has been a fertile ground to explore and understand the interplay between magnetism, unconventional superconductivity, and quantum criticality due to their tunability by pressure, substitution and magnetic field. CeRhIn$_5$ is a heavy fermion antiferromagnet which can be tuned to quantum criticality under pressure. The strength of the magnetic exchange interaction, which is a key parameter to understand its complex properties, however remained unknown. We have used high-resolution neutron spectroscopy to determine the complete spin wave spectrum in CeRhIn$_5$. The spin wave dispersion can be quantitatively reproduced with a simple frustrated $J_1-J_2$ model that also naturally explains the magnetic spin-spiral ground state of CeRhIn$_5$ and yields a dominant in-plane nearest-neighbor magnetic exchange constant $J_0 = 0.74(3)$ meV. Our results pave the way to a quantitative understanding of the rich low-temperature phase diagram of the prominent CeTIn$_5$ class of heavy fermion materials.

1Work at LANL was performed under the auspices of the US DOE, OBES, MSE division and partly funded by LDRD.

12:39PM M22.00008 Fine tuning of the quantum criticality in the heavy fermion superlattices CeRhIn$_5$/YbRhIn$_5$; RYOTA ENDO, RINTARO TODA, YOUSUKE HANAOA, MASAaki SHIMOZAWA, TAKUYA YAMASHITA, YUSUKE SHIMOYAMA, SHIGERU KASAHARA, YOSHI TOWKI, YUITI KASAHARA, Kyoto University, TAKASADA SHIBAUCHI, The university of Tokyo, TAKAHITO TERASHIMA, YUJI MATSUDA, Kyoto University — Bulk CeRhIn$_5$ shows an antiferromagnetic order at $T_N=3.8$ K. Using molecular beam epitaxy, we fabricate artificial superlattices CeRhIn$_5$(m)/YbRhIn$_5$($n$) containing $m$ layers of CeRhIn$_5$, alternating with seven layers of the nonmagnetic metal YbRhIn$_5$. With decreasing $m$, $T_N$ is seriously reduced and nearly vanishes at the $m=3$, indicating the dimensional tuning of the quantum critical point. When the magnetic field is applied to $m=3$ superlattice perpendicular to the plane, $T$-linear resistivity, a hallmark of non-Fermi liquid, persists down to 50 mK, demonstrating the fine tuning of the quantum critical point.

12:51PM M22.00009 Pressure studies of the quantum critical alloy Ce$_{0.93}$Yb$_{0.07}$CoIn$_{13}$; Y.P. SINGH, D.J. HANEY, X.Y. HUANG, Kent State University, B.D. WHITE, M.B. MAPLE, University of California, San Diego, M. DZERO, C.C. ALMASAN, Kent State University — We performed experimental and theoretical studies of the effect of pressure on the heavy fermion quantum critical alloy Ce$_{0.93}$Yb$_{0.07}$CoIn$_{13}$. As observed in resistivity measurements, the Ce$_{1-x}$Yb$_x$CoIn$_{13}$ system exhibits non-Fermi liquid behavior with two distinct contributions to resistivity (linear-in-$T$ and square-root-in-$T$). Our measurements suggest that linear in $T$ resistivity is governed by heavy/large Fermi surface and is suppressed with pressure, together with the suppression of the quantum fluctuations with pressure in Ce$_{0.93}$Yb$_{0.07}$CoIn$_{13}$. The square-root-in-$T$ dependence originates from two different physics: (i) the $\sqrt{T}$ dependence just above $T_c$ is suppressed with the application of pressure, and is a result of superconducting fluctuations; (ii) the higher temperature $\sqrt{T}$ contribution to resistivity remains insensitive to pressure, indicating that the scattering processes in this $T$ range are governed by the scattering of light electrons from the small Fermi surface. We demonstrate that the growth of the coherence temperature with pressure, as well as the decrease of the residual resistivity, can be accurately described by employing the coherent potential approximation for a disordered Kondo lattice.

1This work was supported by the National Science Foundation (grant NSF DMR-1006606) and Ohio Board of Regents (grant OBR-RIP-220573) at KSU, and by the U.S. Department of Energy (grant DE-FG02-04ER46105) at UCSD.

1:03PM M22.00010 Chemical substitution study on magnetism and superconductivity in Ce$_{1-x}$Sm$_x$CoIn$_{13}$; SOOYOUNG JANG, B.D. WHITE, D. YAZICI, A.S. WONG, M.B. MAPLE, Department of Physics, University of California, San Diego, La Jolla, CA 92039, USA — We have investigated the system Ce$_{1-x}$Sm$_x$CoIn$_{13}$ ($0 < x < 1$) by means of x-ray diffraction, electrical resistivity, specific heat, and magnetization measurements. We observe a crossover from a coherent Kondo lattice exhibiting superconductivity to a single-ion impurity Kondo effect coexisting with magnetic order on the Sm-rich side of the phase diagram. The superconducting transition temperature, $T_c$, and Kondo lattice coherence temperature, $T_K$, are suppressed near $x \sim 0.2$ and $x \sim 0.5$, respectively, which is consistent with the effect of substitution with other rare-earth (RE) ions on CeCoIn$_{13}$. After $T_{coh}$ is suppressed to 0 K, a single-ion impurity Kondo effect is observed for 0.5 $< x \leq 0.85$. The compound SmCoIn$_{13}$ exhibits three distinct magnetic phase transitions at roughly 8, 10, and 12 K, which are presumably associated with magnetic order; similar features are observed in the related compound SmIn$_3$. These transition temperatures are gradually suppressed by Ce substitution and completely vanish near $x \sim 0.2$. We establish the phase diagram of the system Ce$_{1-x}$Sm$_x$CoIn$_{13}$ and compare our results with those obtained from chemical substitution studies of CeCoIn$_{13}$ involving other RE ions.

1Research at UCSD was supported by the U. S. Department of Energy, Office of Basic Energy Science, Division of Material Science and Engineering under Grant DE-FG02-04ER46105.

1:15PM M22.00011 Tuning the Kondo effect in YbFe$_{1-x}$Co$_x$Zn$_{20}$; TAI KONG, VALENTIN TAUFOUR, SERGEY BUD’KO, PAUL CANFIELD, Ames Laboratory / Iowa State University — YbCo$_{20}$Zn$_{30}$ is a heavy fermion compound with a Sommerfeld coefficient, $\gamma$, value, of about 8000 mJ/mol-K$^2$ with an estimated single ion Kondo temperature, $T_K$, of about 1.5 K. One the other hand, YbFe$_2$Zn$_{20}$ is less heavy with an $\sim 500$ mJ/mol-K$^2$ and $T_K \sim 30$ K. From a generalized Kadowaki-Woods picture, degeneracies that relate to their Kondo phenomena are large while different: 8 for YbFe$_2$Zn$_{20}$ and 4 for YbCo$_{20}$Zn$_{30}$. In order to understand the effects of Fe-Co substitution on the Kondo effect, a family of YbFe$_{1-x}$Co$_x$Zn$_{20}$ were studied. We performed zero-field resistivity and specific heat measurements on single crystals of YbFe$_{1-x}$Co$_x$Zn$_{20}$ that were synthesized using a high-temperature solution growth technique [2]. The Kondo characteristic temperatures do not change monotonically in between pure YbFe$_2$Zn$_{20}$ and YbCo$_{20}$Zn$_{30}$. Data and a summarize phase diagram of characteristic temperatures as a function of Co doping will be presented and discussed.


1This work is supported by the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

1:27PM M22.00012 Thermal expansion and quantum criticality of the heavy fermion antiferromagnet YbBiP; RISHI BHANDIA, Occidental College, E.D. MUNN, Simon Fraser University, S.L. BUD’KO, P.C. CANFIELD, Ames Laboratory/Iowa State University, G.M. SCHMIEDESOff, Occidental College — YbBiP is a stoichiometric heavy fermion compound with an enormous Sommerfeld coefficient and an antiferromagnetic ground state that is suppressed by magnetic fields of about 0.4 T. Non-Fermi liquid behavior, and other signatures of field-induced quantum criticality have been observed. In this talk we will present measurements of the thermal expansion of YbBiP along the [111] axis from 30K to below 400 mK and in magnetic fields as high as 9 T. We will discuss the implications of our measurements on the quantum criticality of YbBiP and we will discuss an unusual feature in the data near 5K. Work at Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358. Work at Occidental College was supported by the National Science Foundation under DMR-1408598.
1:39PM M22.00013 Hybridization and coherence in the intermediate valence compound YbAl$_3$ via quasiparticle scattering spectroscopy (QPS). L.H. GREENE, S.M. NARASIWODEYAR, M. DWYER, W.K. PARK, University of Illinois at Urbana-Champaign, P.C. CANFIELD, Iowa State University — Band renormalization and hybridization in Anderson lattices has been a subject of continued interest [1]. The intermediate valence compound YbAl$_3$, which does not order magnetically nor superconducts, is a good model system for the study of the hybridization process. A microscopic understanding is still lacking although some characteristic temperature and energy scales have been identified. As shown by our previous works [1,2], QPS is a powerful tool to investigate the hybridization process via measurement of the hybridization gap. Here we report our recent QPS results on YbAl$_3$ [3]. Conductance spectra over a wide temperature range indicate that the hybridization process begins around 110 K, a new temperature scale found in this study, well before the full coherence is achieved (∼34 K). Our observations agree with the slow crossover scenario discussed recently in the literature [4]. The hybridization gap opens concomitantly with the emergence of a coherent Fermi liquid, suggesting that its measurement can be a more rigorous way to define the coherence temperature. *The work at UIUC is supported by the NSF DMR 12-06760 and the work done at Ames Lab. was supported under Contract No. DE-AC02-07CH11358.


1:51PM M22.00014 Visualizing Heavy Fermions in Thin Films by in situ ARPES. SHOUVIK CHATTERJEE, DARRELL SCHLOM, KYLE SHEN, Cornell University — Heavy Fermions are an important class of materials, which has attracted a lot of interest as they seemingly host a number of exotic ground states viz. unconventional superconductivity, Quantum Critical Fermi Liquid, FFLO states etc. Stabilizing these materials in a thin film form and extracting their spectral function via ARPES opens up new possibilities of dimensional and strain tunability and in understanding and designing materials with exotic emergent properties. I will present our recent efforts in stabilizing thin films of Yb based heavy fermion compound YbAl$_3$ and the conventional metal analog LuAl$_3$ on MgO substrates. With the aid of an Al buffer layer crystalline, phase pure and fully-oriented epitaxial thin films can be grown with sub-nm surface roughness. Using in situ angle resolved photoemission we, for the first time have been able to directly map out their electronic bandstructure and Fermi Surface. Measurements on LuAl$_3$ were found to be in good agreement with ab-initio calculations that provided us with an excellent reference to identify the signatures of heavy fermion formation in YbAl$_3$.

Wednesday, March 4, 2015 11:15AM - 1:51PM –
Session M23 DCOMP: Focus Session: Petascale Science and Beyond: Applications and Opportunities in Materials Science and Chemistry II
202B - Barry Schneider, National Institute for Standards and Technology

11:15AM M23.00001 DAG Software Architectures for Multi-Scale Multi-Physics Problems at Petascale and Beyond. MARTIN BERZINS, SCI INSTITUTE, UNIVERSITY OF UTAH — The challenge of computations at Petascale and beyond is to ensure how to make possible efficient calculations on possibly hundreds of thousands for cores or on large numbers of GPUs or Intel Xeon Phis. An important methodology for achieving this is present thought to be that of asynchronous task-based parallelism. The success of this approach will be demonstrated using the Uintah software framework for the solution of coupled fluid-structure interaction problems with chemical reactions. The layered approach of this software makes it possible for the user to specify the physical problems without parallel code, for that specification to be translated into a parallel set of tasks. These tasks are executed using a runtime system that executes tasks asynchronously and sometimes out-of-order. The scalability and portability of this approach will be demonstrated using examples from large scale combustion problems, industrial detonations and multi-scale, multi-physics models. The challenges of scaling such calculations to the next generations of leadership class computers (with more than a hundred petalapps) will be discussed.

*3Thanks to NSF, XSEDE, DOE NNSA, DOE NETL, DOE ALCC and DOE INCITE

11:51AM M23.00002 High performance electronic structure engineering. MARCO GOVONI, GIULIA GALLI, Institute for Molecular Engineering, The University of Chicago, Materials Science Division, Argonne National Laboratory — We discuss the efficiency of a recently proposed method for the calculation of energy levels in condensed and finite systems with density functional theory and many-body perturbation theory at the GW level. We present applications of this technique to the calculation of electronic properties of systems with thousands of electrons, including semiconductor nanoparticles, solid/liquid interfaces and defective materials. In addition we discuss the parallel performance and scalability on high performance architectures of a newly developed code [1], implementing the method.


12:03PM M23.00003 Excited calculations of large scale multiwalled nanotubes using real-space pseudopotential methods. CHARLES LENA, JAMES CHELIKOWSKY, University of Texas at Austin, JACK DESLIPPE, National Energy Research Scientific Computing Center, YOUSEF SAAD, University of Minnesota, CHAO YANG, Lawrence Berkeley National Laboratory, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory — One method for calculating excited states is the GW method. The GW method has many computational requirements. One of the bottlenecks is the calculation of numerous empty states. Within density functional theory, we use a real-space pseudopotential method (PARSEC) to calculate these empty states for multiwalled nanotubes. We illustrate the use of these empty states for calculating excited states using the GW method (BerkeleyGW). We demonstrate why using real-space density functional theory is advantageous for calculating empty states.

*3Support provided by the SciDAC program, Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences. Grant Numbers DE-SC0008877 (Austin) and DE-FG02-12ER4 (Berkeley)
12:15PM M23.00004 Scalable real space pseudopotential-density functional codes for materials applications

JAMES R. CHELIKOWSKY, CHARLES LENA, GRADY SCHOFIELD, University of Texas at Austin, YOUSEF SAAD, University of Minnesota, JACK DESLIPPE, National Energy Research Scientific Computing Center, CHAO YANG, Lawrence Berkeley National Laboratory — Real-space pseudopotential density functional theory has proven to be an efficient method for computing the properties of matter in many different states and geometries, including liquids, wires, slabs and clusters with and without spin polarization. Fully self-consistent solutions have been routinely obtained for systems with thousands of atoms. However, there are still systems where quantum mechanical accuracy is desired, but scalability proves to be a hindrance, such as large biological molecules or complex interfaces. We will present an overview of our work on new algorithms, which offer improved scalability by implementing another layer of parallelism, and by optimizing communication and memory management.

1Support provided by the SciDAC program, Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences. Grant Numbers DE-SC0008877 (Austin) and DE-FG02-12ER4 (Berkeley)

12:27PM M23.00005 Numerical solutions of the time-dependent Schroedinger equation for atoms and molecules in intense laser fields

XIAOXU GUAN, Louisiana State University — Recent progress in ab initio computational methods allows us to treat the laser-atom, laser-molecule interaction, and other collision processes with improved accuracy. Full-dimensional quantum calculations for even a few particles are extremely demanding because of the unfavorable scaling of the full quantum wave function, but they are of significant importance for understanding the entangled response of electrons and nuclei in a system strongly influenced by intense lasers and particle beams. In this talk I will concentrate on the applications of grid-based approaches to the time-dependent problems of atoms and molecules driven by intense ultrafast laser pulses. The spatial coordinates are discretized via the finite-element discrete-variable representation. Examples include ionization dynamics in complete breakup processes through few-phonon absorption in helium atoms and hydrogen molecules, and also time-delayed attosecond transient absorption spectra in helium.

1This work was supported by DOE DE-FG02-13ER16403, NSF PHY-0757755, NSF PHY-1068140, and XSEDE PHY-090031.

1:03PM M23.00006 Solving the Time Dependent Schroedinger Equation using the FEDVR/SIL Method

BARRY SCHNEIDER, NIST — In this talk we will explore how the finite element discrete variational representation coupled to the short iterative Lanczos method has enabled our group to make substantial progress in understanding the single and double ionization of atoms and simple diatomic molecules in short, intense electromagnetic fields. Particular attention will be paid to new time-dependent propagation techniques to shorten the computational times.

1:15PM M23.00007 Hybrid MPI/OpenMP First Principles Materials Science Codes for Intel Xeon Phi (MIC) based HPC: The Petascale and Beyond

ANDREW CANNING, Lawrence Berkeley National Laboratory and University of California, Davis, JACK DESLIPPE, Lawrence Berkeley National Laboratory, JAMES CHELIKOWSKY, University of Texas at Austin, STEVEN G. LOUIE, University of California, Berkeley and Lawrence Berkeley National Laboratory — Exploiting the full potential of present petascale and future exascale supercomputers based on many core chips requires a high level of threading on the node as well as reduced communications between the nodes to scale to large node counts. We will present results for a variety of first principles materials science codes (Berkeley-GW, PARATEC, PARSEC) on Intel Xeon Phi (MIC) based supercomputers for algorithms using hybrid OpenMP/MPI parallelism to obtain both efficiently threaded single chip performance and parallel scaling to large node counts.

1Support provided through the SciDAC program funded by U.S. Department of Energy, Office of Science, ASCR and BES under Contract No. DE-AC02-05CH11231 at LBNL and Award No. DESC0008877 at UT, Austin

1:27PM M23.00008 Time-Dependent Superfluids on Heterogeneous Computing Platforms

KENNETH ROCHE, Pacific Northwest National laboratory and University of Washington — The superfluid local density approximation (SLDA) and its time-dependent extension (TDSLDA) can be used to study strongly interacting fermion systems. SLDA and TDSLDA have been verified, and validated theoretically and experimentally for both homogeneous and inhomogeneous systems. Our numerical implementation enabled the first time-dependent simulations of fermionic superfluid systems within the DFT approach. Recently, we have developed novel algorithms for the efficient evaluation of the theory using hybrid CPU-GPU computer architectures. In this talk, I will focus on the challenges and implementation details of the hybrid CPU-GPU time-dependent code.

1:39PM M23.00009 Identification of metastable ultrasmall titanium oxide clusters using a hybrid optimization algorithm

ERIC INCLAN, Florida International University, Miami, FL 33174, DAVID GEOHEGAN, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — Nanostructured TiO₂ materials have interesting properties that are highly relevant to energy and device applications. However, precise control of their morphologies and characterization are still a grand challenge in the field. Using a hybrid optimization algorithm we theoretically explored configuration spaces of energetically metastable TiO₂ nanostructures. Our approach is to minimize the total energy of TiO₂ clusters in order to identify the structural characteristics and energy landscape of plausible (TiO₂)n (n = 1-100). The hybrid algorithm includes a modified differential evolution algorithm, a permutation operator to perform global optimization on a set of randomly generated structures, and then structure refinement using a BFGS Quasi-Newton algorithm. The results were compared against known physical structures and numerical results in the literature as well as our experimentally synthesized structures. Although the global minimum became more computationally expensive to locate with increasing number of TiO₂ units, the optimizer successfully identified numerous plausible structures along a range of energies close to the global minimum energy structure for all clusters in the given range.

1This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
The vacuum size. In contrast, the HGH and PAW PPs show fast and stable convergence with the same settings. The origin of these oscillations will be discussed.

for both TM and USPP PPs, the phonon energies at the Brillouin zone center exhibit oscillations and even large negative phonon modes with the increase of

Troullier-Martin (TM), Hartwigsen-Goedeker-Hutter (HGH), Projector Augmented-Wave (PAW), and ultrasoft pseudopotential (USPP), with the same PBE

atomic crystals. Using the 2D honeycomb lattice of lead (Pb) as a model system, we studied the convergence of the phonon energies on several important

model dramatically improves atomization energies for the AE6 test set, but remains an order of magnitude worse than a conventional Kohn-Sham GGA. We are

significant flaws in an earlier meta-GGA proposed by Perdew and Constantin. We find that these can be substantially fixed by revising an implicit constraint

set of molecules. Visualization of the KED, particularly in the region of localized electron pairs, such as atomic lone pairs and covalent bonds, pointed out

local Laplacian and gradient of the density, and based on insights gained in the visualization of the kinetic energy density (KED) for atoms and the AE6 test

set of molecules. Visualization of the KED, particularly in the region of localized electron pairs, such as atomic lone pairs and covalent bonds, pointed out

strong magnetic fields for Helium to Neon, Molecular Hydrogen, Water, Carbon dioxide and Benzene.

3Welch Fellowship (Grant J-1675), the ARO (Grant W911NF-13-1-0162), the Texas Southern University High Performance Computing Center (http://hpcc.tsu.edu/; Grant PHY-1126251) and NSF-CREST CRCN project (Grant HRD-1137732)

3Supported by the Towson University Faculty Development and Research Committee (grant OSPR # 140269), and the Fisher College of Science and Mathematics Fisher General Endowment.

11:15AM M24.00001 A Novel Gaussian-Sinc mixed Basis Set for Electronic Structure calculations1, JONATHAN JERKE, YOUNG LEE, C.J. TYMCZAK, Texas Southern University — A Gaussian-Sinc mixed basis set for the computation of the electronic structure of atoms and molecules is presented. Excellent bases functions are known for “core” and “valence” separately, such as Gaussians for the “core” wave functions and Plane-waves for “valence” wave functions, but as yet no method is known that can accurately deal with both regimes in a single basis. A Gaussian-Sinc mixed basis can do both. This method resolves several issues such as: i) the sincs basis spans the same space as the plane-waves basis, yet are semi-local enough to define all interaction elements including Exchange; ii) the Gaussians span the spherically symmetric core states and can be mixed with the sinc functions in a computationally efficient methodology; iii) together, this mixed basis set is a flexible, computationally efficient and a highly accurate method for solving atomic and molecular problems. This methodology has been implemented within the Hartree-Fock level of theory within ultra-strong magnetic fields. To demonstrate the utility of this new method, we calculated the ground state Hartree-Fock energies to five digits accuracy in ultra strong magnetic fields for Helium to Neon, Molecular Hydrogen, Water, Carbon dioxide and Benzene.

11:27AM M24.00002 Modeling the kinetic energy density of molecules – towards an orbital-free meta-GGA, ANTONIO CANCIO, DANE STEWART, JEREMY REDD, Ball State University — Driven by applications at high temperature and large system size, interest has recently turned to the construction of orbital-free density functionals, modeling the Kohn-Sham kinetic energy solely as a functional of the electron density and its derivatives. We report work on a metaGGA level orbital-free kinetic energy functional parametrized in terms of the local Laplacian and gradient of the density, and based on insights gained in the visualization of the kinetic energy density (KED) for atoms and the AE6 test set of molecules. Visualization of the KED, particularly in the region of localized electron pairs, such as atomic lone pairs and covalent bonds, pointed out significant flaws in an earlier metaGGA proposed by Perdew and Constantin. We find that these can be substantially fixed by revising an implicit constraint built into the prior model in the limit of strong electron localization – when the Kohn-Sham KED approaches the bosonic limit. A first attempt at an improved model dramatically improves atomization energies for the AE6 test set, but remains an order of magnitude worse than a conventional Kohn-Sham GGA. We are currently working to fix a notable over-correction of the PC meta-GGA for the electron localization limit that may lead to further improvement.

11:39AM M24.00003 Convergence of the phonon energy in two-dimensional atomic crystal of lead1, JIA-AN YAN, Department of Physics, Astronomy and Geosciences — Accurate phonon energies are important for the study of two-dimensional (2D) atomic crystals. Using the 2D honeycomb lattice of lead (Pb) as a model system, we studied the convergence of the phonon energies on several important parameters in supercell calculations based on the density-functional perturbation theory as implemented in Quantum Espresso code. These parameters include the planewave cut-off energy, the vacuum space size, the charge density cut-off, and FFT grid. The tested pseudopotentials (PPs) include the widely used Troullier-Martin (TM), Hartwigsen-Goedeker-Hutter (HGH), Projector Augmented-Wave (PAW), and ultrasoft pseudopotential (USPP), with the same PBE exchange-correlation functional. Surprisingly, the phonon energies calculated using these PPs exhibit quite distinct dependence on those parameters. Specifically, for both TM and USPP PPs, the phonon energies at the Brillouin zone center exhibit oscillations and even large negative phonon modes with the increase of the vacuum size. In contrast, the HGH and PAW PPs show fast and stable convergence with the same settings. The origin of these oscillations will be discussed.

11:51AM M24.00004 Implicit solvent models in VASP, KIRAN MATHEW, Cornell university, RICHARD HENNIG, University of Florida — Solid-liquid interfaces are at the heart of many modern-day technologies and presents challenges for materials simulation methods. A realistic first-principles computational study of such systems entails the inclusion of solvent effects. In our previous work, employing a linear implicit solvent model, we have demonstrated the importance of the inclusion of solvent effects on the calculation of reaction energy barriers and surface energies of semiconductor nanocrystals. In this work we propose to extend the implicit solvent model to incorporate the effects of the ions in the solvent and also to include the effects of dielectric saturation phenomenon. A solvation model that includes the effects of ionic solution at a first principle level, takes us one step closer to a more realistic simulation of an electrochemical interface. Incorporating the dielectric saturation effects further advance the capabilities of the state of the art DFT tools to study the Solid Electrolyte Interface(SEI) films formed on highly ionic surfaces such as Lithium halides.

12:03PM M24.00005 Compact wavefunctions from compressed imaginary time evolution, JAR- ROD MCCLEAN, ALAN ASPURU-GUZIK, Harvard University — Simulation of quantum systems promises to deliver physical and chemical predictions for the frontiers of technology. The success of approximation methods for quantum systems has hinged on the relative simplicity of physical systems with respect to the exponentially complex worst case. Exploiting this relative simplicity has required detailed knowledge of the physical system under study. In this talk, we will introduce a general and efficient black box method for many-body quantum systems that utilizes technology from compressed sensing to find the most compact wavefunction form possible without detailed knowledge of the system. It is a Multicomponent Adaptive Greedy Iterative Compression (MAGIC) scheme. No knowledge is assumed in the structure of the problem other than correct particle statistics. This method can be applied to many quantum systems such as spins, qubits, oscillators, or electronic systems. I will show the relation of this approach to matrix product states and discuss the implications. As a practical application, I use this technique to compute the ground state electronic wavefunction of hydrogen fluoride and recover 98

12:15PM M24.00006 First-Principles Studies of the Excited States of Chromophore Monomers and Dimers, SAMIA HAMED, University of California at Berkeley, SAHAR SHARIFZADEH, Boston University, JEFFREY NEATON, University of California at Berkeley — Elucidation of the energy transfer mechanism in natural photosynthetic systems remains an exciting challenge. Through the careful analysis of excited states on individual chromophores and dimers – and the predictive first-principles methods used to compute them – we are building towards an understanding of the nature of excitation transfer among arrays of chromophores embedded in protein environments. Excitation energies, transition dipoles, and natural transition orbitals for the important low-lying singlet and triplet states of experimentally-relevant chromophores are obtained from first-principles time-dependent density functional theory (TDDFT) and many body perturbation theory. The effects of the Tamm-Dancoff approximation and the performance of several exchange-correlation functionals, including an optimally-tuned range-separated hybrid, are evaluated with TDDFT, and compared to MBPT calculations and experiments. This work has been supported by the DOE; computational resources have been provided by NERSC.
12:27PM M24.00007 “Phantom” Modes in *Ab Initio* Tunneling Calculations: Implications for Theoretical Materials Optimization, Tunneling, and Transport. SERGEY V. BARABASH, DIPANKAR PRAMANIK, Intermolecular Inc. — Development of low-leakage dielectrics for semiconductor industry, together with many other areas of academic and industrial research, increasingly rely upon *ab initio* tunneling and transport calculations. Complex band structure (CBS) is a powerful formalism to establish the nature of tunneling modes, providing both a deeper understanding and a guided optimization of materials, with practical applications ranging from screening candidate dielectrics for lowest “ultimate leakage” to identifying charge-neutrality levels and Fermi level pinning. We demonstrate that CBS is prone to a particular type of spurious “phantom” solution, previously deemed true but irrelevant because of a very fast decay. We demonstrate that (i) in complex materials, phantom modes may exhibit very slow decay (appearing as leading tunneling terms implying qualitative and huge quantitative errors), (ii) the phantom modes are spurious, (iii) unlike the pseudopotential “ghost” states, phantoms are an apparently unavoidable artifact of large numerical basis sets, (iv) a presumed increase in computational accuracy increases the number of phantoms, effectively corrupting the CBS results despite the higher accuracy achieved in resolving the true CBS modes and the real band structure, and (v) the phantom modes cannot be easily separated from the true CBS modes. We discuss implications for direct transport calculations. The strategy for dealing with the phantom states is discussed in the context of optimizing high-quality high-κ dielectric materials for decreased tunneling leakage.

12:39PM M24.00008 Three- to two-dimensional crossover in time-dependent density-functional theory1, SHAHRZAD KARIMI, CARSTEN ULLRICH, University of Missouri — Quasi-2D systems, such as an electron gas confined in a quantum well, are important model systems for many-body theories. Earlier studies of the crossover from 3D to 2D in ground-state DFT showed that local and semilocal exchange-correlation functionals which are based on the 3D electron gas are appropriate for wide quantum wells, but eventually break down as the 2D limit is approached. We now consider the dynamical case and study the performance of various linear-response exchange kernels in TDDFT. We compare approximate local, semilocal and orbital-dependent exchange kernels, and analyze their performance for inter- and intrasubband plasmons as the quantum wells approach the 2D limit. 3D (semi)local exchange functionals are found to fail for quantum well widths comparable to the 2D Wigner-Seitz radius, which implies in practice that 3D local exchange remains valid in the quasi-2D dynamical regime for typical quantum well parameters, except for very low densities.

1Work supported by DOE Grant DE-FG02-05ER46213

12:51PM M24.00009 ABSTRACT WITHDRAWN

1:03PM M24.00010 Ultrafast coupled plasmon-phonon mode dynamics in GaAs, a combined experimental and theoretical study. EVAN THATCHER, CHRISTOPHER STANTON, Univ of Florida - Gainesville, KUNIE ISHIOKA, National Institute for Materials Science, Tsukuba, Japan, AMLAN BASAK, HRVOJE PETEK, Univ of Pittsburgh — We present results from a joint experimental and theoretical study exploring the excitation of coupled plasmon-phonon modes in GaAs. In contrast to previous coherent phonon studies in GaAs where electrons were generated primarily in the Γ valley, we use a pump-probe technique with a 10 fs pulse width and a shorter 400 nm laser wavelength to photoexcite electrons predominantly in the L valley. As a result: i) damping of the electron-hole plasma is faster and ii) diffusion of the carriers from the surface becomes important compared to the shorter absorption length. The probe pulses measure the time-dependent changes to the reflectivity due to the coupled plasmon-phonon modes created by the ultrafast photoexcitation and the subsequent depletion field screening. To model this, we solve for the time and density dependent coupled-mode frequencies allowing for ambiplar diffusion. Simulation of the coupled plasmon-phonon dynamics allows for comparison with, and a better understanding of experiments.

1Supported by the NSF through grants CHE-0650756, DMR-1311845, and DMR-1311849.

1:15PM M24.00011 Surface Dangling Bonds Are a Cause of Type-II Blinking in Si Nanoparticles1, NICHOLAS BRAWAND, MARTON VOROS, GIULIA GALLI, Univ of Chicago — Exponential blinking statistics was reported in oxidized Si nanoparticles and the switching mechanism was attributed to the activation and deactivation of unidentified nonradiative recombination centers. Using *ab initio* calculations, we predicted that Si dangling bonds at the surface of oxidized nanoparticles introduce defect states which, depending on their charge and local stress conditions, may give rise to ON and OFF states responsible for exponential blinking statistics. Our results are based on first principles calculations of charge transition levels, single particle energies, and radiative and nonradiative lifetimes of dangling bond defects at the surface of oxidized silicon nanoparticles under stress.

1Supported by the Department of Energy/Basic Energy Sciences grant No. DE-FG02-06ER46262.

1:27PM M24.00012 Auxiliary density functionals: a new class of methods for efficient, stable density functional theory calculations1, PHIL HASNIP, MATT PROBERT, University of York — *Ab initio* materials modelling methods have become an essential tool for physical scientists in a wide variety of fields. The advent of more and more powerful computers has allowed larger, more complex systems to be simulated and the dramatic improvements in both experimental growth and characterisation methods have allowed the length scale of theoretical simulations and experimental studies to coincide at the nanoscale. Whilst there has been undisputed success in the modelling of nanomaterials, the approach is not without its problems. As the size of the simulation system is increased, the conventional algorithms used to find the electronic ground state often show poor convergence, and for large or complex systems they may fail to converge at all. We present a new class of methods for solving the Kohn-Sham equations based on constructing a mapping dynamically between the Kohn-Sham system and an auxiliary system. This auxiliary system is not required to be fermionic, and an exemplar bosonic scheme is presented which captures the key features of the Kohn-Sham behaviour. This auxiliary scheme is shown to provide good performance for a variety of bulk materials, and a substantial improvement in the scaling of calculations with system size for a range of materials.

1Supported by the United Kingdom Car-Parrinello Consortium (UKCP) and EPSRC (grant ref. EP/K013564/1).

1:39PM M24.00013 Speeding up DFT: A new approach to k-point integration. JEREMY J. JORGENSEN, Brigham Young University, DEREK C. THOMAS, University of Texas at Austin, MATTHEW M. BURIDGE, Brigham Young University, IAN H. SLOAN, The University of New South Wales, CONRAD W. ROSENBROCK, RODNEY W. FORCADE, BRET C. HESS, GUS L.W. HART, Brigham Young University — The bottleneck for high throughput material property calculation is computational speed. Increasing the convergence rate of the band energy integration will decrease computation time. Band energy, despite its small contribution to the total energy, plays a large role in the calculation of formation enthalpies, where energy differences and not magnitudes are of greater importance. Current DFT codes generally choose k-points using the Monkhorst-Pack scheme, and then integrate the energy bands using the rectangle method. Instead, we interpolate the energy bands with splines, create a spline representation of the Fermi surface, and analytically integrate the energy bands beneath the Fermi surface to find the band energy. Our conservative estimate is a tenfold increase in computational efficiency for the band energy calculation.


2:03PM M24.00015 Ab-initio atomic level stress and role of d-orbitals in CuZr, CuZn and CuY, MADHUSUDAN OJHA, Univ of Tennessee, Knoxville, DON M. NICHOLSON, University of North Carolina Asheville, TAKESHI EGAMI, Univ of Tennessee, Knoxville — Atomic level stress offers a new tool to characterize materials within the local approximation to density functional theory (DFT). Ab-initio atomic level stresses in B2 structures of CuZr, CuZn and CuY are calculated and results are explained on the basis of d-orbital contributions to Density of States (DOS). The overlap of d-orbital DOS plays an important role in the relative magnitude of atomic level stresses in these structures. The trends in atomic level stresses that we observed in these simple B2 structures are also seen in complex structures such as liquids, glasses and solid solutions. The stresses are however modified by the different coordination and relaxed separation distances in these complex structures. We used the Locally Self-Consistent Multiple Scattering (LSMS) code and Vienna Ab-initio Simulation Package (VASP) for ab-initio calculations.


11:15AM M25.00001 Ab initio molecular dynamics simulations of electron doped ZrNCl, ANTHIAS R. A. BOTANA, FRANCOIS GYGI, WARREN E. PICKETT, University of California Davis — When electron doped, the layered transition metal nitride ZrNCl becomes superconducting with an impressive critical temperature $T_c = 15K$. Its isovalent sisters become superconducting at 17K (TaNCl) and 26K (HNCl). This class has very strong 2D character, as cuprates, iron pnictides, and MgB$_2$, but the pairing interaction is not magnetic nor conventional electron-phonon in origin. To explore the dynamical behavior of electrons doped into a highly ionic insulator, ab initio molecular dynamics calculations have been carried out on doped ZrNCl. The simulations allow us to analyze the electronic response in real space, and to study the differences in behavior of the two experimental mechanisms of doping electronic carriers: alkali metal intercalation and Cl vacancies, both of which give nearly the same high critical temperature.

11:27AM M25.00002 Density Functional Theory for Superconductors: new functionals and applications, ANTONIO SANNA, E.K.U. GROSS, Max Planck Institute of Microstructure Physics — Density functional theory for superconductors (SCDFT) is a fully parameter-free approach that allows for accurate predictions of the critical temperature and other properties of superconductors. We report on the most recent extensions of this theoretical framework, in particular the development of new functionals to:
- incorporate in a correct fashion Migdal's theorem;
- compute the excitation spectrum;
- include spin-fluctuation mediated pairing

Applications and predictions are shown for a set of materials including conventional and unconventional superconductors.

11:39AM M25.00003 Unconventional superconductivity and charge fluctuations in Li$_{x}$Mo$_6$O$_{17}$, NATALIA LERA, JOSE ALVAREZ, Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid — We study superconductivity in Li$_{x}$Mo$_6$O$_{17}$ considering charge and spin fluctuations as the pairing mechanism. We model the low-energy electronic properties of the material with a multiorbital extended Hubbard model and compute the superconducting vertex within the RPA. We found that charge collective modes induced by Coulomb repulsion favor the superconductivity both the singlet and triplet channels. Superconductivity is favored as the charge ordering transition of the model is approached by tuning the interaction. We compare with another quasi-one-dimensional approach where the superconductivity is an instability of a generalized Luttinger Liquid (LL) to higher dimensions, known as Quantum Smectic Metal or Sliding LL. We also discuss these results on the context of the dimensional crossover issue in the unconventional metallic phase of the material.

11:51AM M25.00004 Superconducting phase diagram of itinerant antiferromagnets, ASTRID ROEMER, Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark, ILYA EREMIN, Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany, PETER J. HIRSCHFELD, Department of Physics, University of Florida, Gainesville, USA, BRIAN M. ANDERSEN, Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark — We investigate the formation of Cooper pairs in systems with itinerant antiferromagnetic (AF) order. Our theory is a generalization of earlier studies of spin fluctuation mediated pairing on top of AF [1,2]. The AF order is manifested by gapless transverse spin waves as well as gaped longitudinal spin fluctuations. Both changes contribute to the Cooper pairing. We map out the superconducting gap as a function of electron doping and find a robust d-wave gap on the electron pockets in the anti-nodal regions with no nodes at the Fermi surface. Close to the critical doping of onset of AF order we observe a highly non-monotonic form of the superconducting gap due to enhancements at the "hot spots." In this doping regime we explore the presence of p- and f-wave triplet gaps competing with the d-wave solution [3].


12:03PM M25.00005 Dynamical Jahn-Teller instability in metallic fullerides, NAOYA IWAHARA, LIVIU CHIBOTARU, Theory of Nanomaterials Group, Katholieke Universiteit Leuven — Dynamical Jahn-Teller effect has escaped so far direct observation in metallic systems. It is particularly believed to be quenched also in correlated conductors with orbitally degenerate sites such as cubic fullerides. Here the Gutzwiller approach is extended to treat electron correlation over metals with Jahn-Teller active sites and applied to the investigation of the ground state of K$_3$C$_{60}$. It is shown that dynamical Jahn-Teller instability fully develops in this material when the interelectron repulsion $U'$ on C$_{60}$ sites exceeds some critical value. The latter is found to be lower than the current estimates of $U'$, meaning that dynamical Jahn-Teller effect takes place in all cubic fullerides. This leads to strong splitting of LUMO orbitals on C$_{60}$ sites and calls for reconsideration of the role of orbital degeneracy in the Mott-Hubbard transition in fullerides.

displays a characteristic Fano effect as an incipient charge density wave state forms. SLAC National Lab and Stanford University — I this talk I will present a theory for resonant photoexcitation of phonons using x-ray inelastic spectroscopy. I behavior as the dilution tends to the percolation threshold. The worm algorithm [PRL 87, 160601 (2001)]. We present results for the scalar susceptibility and O(N) conductivity in the critical region and follow the system's scaling in the vicinity of the quantum critical point [PRL 110, 140401 (2013)]. We report on the O(N) model with random site dilution, which we study using the worm algorithm [PRL 87, 160601 (2001)]. We present results for the scalar susceptibility and O(N) conductivity in the critical region and follow the system's behavior as the dilution tends to the percolation threshold.

12:39PM M25.00008 Amplitude mode in diluted O(N) models , YURY KISELEV, DANIEL AROVAS, Univ of California - San Diego — The relativistic O(N) model has recently been shown to exhibit a robust amplitude mode peak in its scalar susceptibility which exhibits scaling in the vicinity of the quantum critical point [PRL 110, 140401 (2013)]. We report on the O(N) model with random site dilution, which we study using the worm algorithm [PRL 87, 160601 (2001)]. We present results for the scalar susceptibility and O(N) conductivity in the critical region and follow the system's behavior as the dilution tends to the percolation threshold.

12:51PM M25.00009 Phonon Fano effect in RIXS across a CDW instability , THOMAS DEVEREAUX, SLAC National Lab and Stanford University — I this talk I will present a theory for resonant photoexcitation of phonons using x-ray inelastic spectroscopy. I will show how the strength of electron-phonon can be characterized in a momentum dependent way, and demonstrate how the phonon-continuum linehape displays a characteristic Fano effect as an incipient charge density wave state forms.

1:03PM M25.00010 Thermodynamics of superconducting quantum metamaterials , PIERRE-LUC DALLAIRE-DEMERS, FRANK WILHELM-MAUCH, Universite des Saarlandes — Left-hand matematerials are capacitively coupled layers of inductive pieces of conductors. These systems are well studied in the context of microwave metamaterials but their full quantum description or their embedding in highly correlated materials like superconductors are still an open problem. Notably, they are known to have a Van Hove singularity in the density of states at low energy and high pseudo-momentum that could effectively couple and condense Cooper pairs. The goal of this research is to analyze the thermodynamical properties of the order parameter of stacked layers of superconductors with a small repulsive Coulomb interaction. A 3D toy model of such a material is mapped to a Fermi-Hubbard lattice. The temperature independent anomalous correlation functions are computed variationally from a self-energy functional of a small cluster where inter-cluster tunneling is treated perturbatively. The effect of the repulsive interaction on the Cooper pairs binding can then be seen from the momentum distribution of the condensation amplitude. Such a material could potentially be realized with optical lattices or nanoscaled superconductors.

1:15PM M25.00011 Transport in thin insulating films close to the Boson-Fermion Crossover , J.C. JOY, X. ZHANG, S.M. HOLLEN, Department of Physics, Brown University, G. FERNANDES, J.M. XU, Division of Engineering, Brown University, J.M. VALLES, JR., Department of Physics, Brown University — In two-dimensional systems, sufficient levels of disorder are known to localize Cooper Pairs into a phase incoherent insulating state. While many theoretical and experimental works have shown this state's existence, its ubiquity close to the disorder tuned Superconductor to Insulator transition is still an open problem. Recent experiments on nanopatterned Pb0.5Sr1.5 films have suggested a crossover from Bosonic to Fermionic transport deep in the insulating phase, indicating that the Cooper Pair Insulator (CPI) only persists to a finite level of microscopic disorder. The normal state resistance at which this crossover occurs is governed by the extent coupling constant inhomogeneities on the scale of the coherence length, which allow the formation of locally phase coherent superconducting islands in the insulating state. By tuning the scale of these inhomogeneities and examining the extent of the CPI state, we argue that the disorder tuned Superconductor to Insulator transition proceeds via pair breaking and Anderson localization of fermions when the level spacing in the islands approaches the size of the mean field gap. This work was supported by the NSF through grants No. DMR-1307290 and DMR-0907357 and by the AFRL, the ONR, and the AFSOR.


1:39PM M25.00013 Probing the charge-vortex duality near the superfluid-to-insulator transition , SNIR GAZIT, DANIEL PODOLSKY, ASSA AUERBACH, Technion - Israel Institute of Technology — We study the charge vortex duality near the superfluid-to-insulator quantum phase transition in d=2–1 dimensions. We use a generalized reciprocity relation between charge and vortex conductivities at complex frequencies to identify the capacitance in the insulating phase as a measure of vortex condensate stiffness. We then compute the ratio of boson superfluid stiffness to vortex condensate stiffness at mirror points to be 0.21(1). This corroborates and provides a quantitative measure to the non self-dual nature of the charge-vortex duality. We further study deviations from self-duality at finite frequency by computing the product of Matsubara frequency conductivities at mirror points across the phase transition. Finally, we propose experimental realizations that test our predictions in THz spectroscopy of disordered superconductors and cold atomic systems trapped in an optical lattice. [1] S. Gazit, D. Podolsky, A. Auerbach, arXiv:1407.1055 (2014)
1:51PM M25.00014 Theory of phase-slip-center effects on superconducting kinetic inductance

MASAHIKO MACHIDA, YUKIHIRO OTA, Japan Atomic Energy Agency — Fluctuations significantly alter the conventional picture on transport phenomena in 1D superconductors. We study the current-dependence of the kinetic inductance in superconducting wires using the Ginzburg-Landau approach with fluctuations. We obtain a non-monotonic current-dependence of the kinetic inductance when the thermal fluctuations predominate the behaviors of the superconducting phase. This result is ascribed to the occurrence of phase-slip centers from thermally-activated processes. We also find that our approach qualitatively reproduces the experiment by Anzunziata et al. [Nanotechnology 21, 445202 (2010)]. Moreover, we discuss the effects of thermal fluctuations on the characteristics of superconducting detectors. We will also discuss the effects of quantum phase slips on superconducting detectors.

2:03PM M25.00015 Pairing in doped Hubbard model on a honeycomb lattice: A quantum Monte Carlo study

TIANXING MA, Department of Physics, Beijing Normal University — Inspired by the recent discovered graphene, we performed a systematic QMC study of the magnetic and pairing correlation in the t-U-V Hubbard model on a honeycomb lattice. Close to half filling, we find that pairing with d+id symmetry dominates over pairing with extended-s symmetry. As the doping increases, the next-nearest-neighbor t' tends to be important and when $t'/t < -0.65$, the single-particle spectrum is featured by the continuously distributed Van-Hove saddle points at the band bottom, where the density of states diverges in power-law. We investigate possible unconventional superconductivity in such system with Fermi level close to the band bottom, and our studies reveal a possible triplet p+ip superconductivity with appropriate interactions. By including the spin-orbit coupling, it is shown that the d+id pairing is enhanced while the p+ip pairing is decreased by increasing spin-orbit coupling. Our results might provide a possible route to look for triplet superconductivity with relatively-high transition temperature in a doped graphene and other similar systems.

Wednesday, March 4, 2015 11:15AM - 2:15PM –
Session M26 DCMP: Nanowires: Mechanical, Electronic, Optical, and Transport Properties

204A - Luis Balicas, Florida State University

11:15AM M26.00001 Synthesis and Photoresponse of Hydrothermally Grown ZnO Nanowires

AHMED AL-ASADI, LUKE HENLEY, SUJOY GHOSH, ABDIEL QUETZ, IGOR DUBENKO, Department of Physics, Southern Illinois University Carbondale, Carbondale-IL 62901, United States, NIHAR PRADHAN, LUIS BALICAS, National High Magnetic Field Laboratory, Florida State University, Tallahassee-FL 32310, United States, SAIKAT TALAPATRA, NAUSHAD ALI, Department of Physics, Southern Illinois University Carbondale, Carbondale-IL 62901, United States — We will present our results of hydrothermally grown ZnO nanowires (NWs) using ZnO nanoparticles as seeds. The seed layer was prepared simply by spraying commercially obtained ZnO nanoparticles with a diameter ~20 nm mixed with Isopropanol (IPA) onto Si/SiO2. A detailed structural characterization of the ZnO nanowires indicate that highly crystalline nanowires with an average diameter 45-55 nm and length 1 ~ 1.3 µm with an optical band gap of ~3.7 eV can be obtained using this method. We also show that a significant amount of photocurrent is generated in these nanowires when illuminated with UV radiation. The variation of photo response with light intensity as well as the nature of rise and decay of photocurrent will be presented and discussed in the light of available theoretical models.

11:27AM M26.00002 Controlling the electrical impedance of nanomechanical oscillators by electromigration

FENGPEI SUN, JIE ZOU, HO BUN CHAN, The Hong Kong University of Science and Technology — Detection of nanomechanical motion is of fundamental and practical interests. For doubly clamped nanobeams, a common method is the magnetomotive reflection technique. However, this technique usually suffers from large signal background due to the mismatch of the electrical resistance (R_e) of the oscillators to the impedance (50 ohm usually) of the cables for detection. The large signal background precludes the possibility of driving the device into self-sustaining oscillations using a phase-locked loop. We develop a reproducible method of minimizing the signal background in the magnetomotive reflection technique. A gold nanowire with a junction in the middle is fabricated on the top of a doubly-clamped SiNx nanobeam via e-beam lithography. By passing a large direct current through the nanowire, migration of the gold atoms around the junction is activated due to the heat dissipated. An analog feedback loop is designed to maintain a stable process of electromigration until the target R_e is reached. Initially, R_e is smaller than 500 ohm. The motional impedance of the nanowire shifts the total impedance closer to 500 ohm so that the resonance of the nanobeam appears as a dip on a large background in the amplitude spectrum. As R_e is increased to near 500ohm, the background reaches a minimum, and the resonance of the nanobeam turns into a peak. Self-sustaining oscillations of the nanobeam are successfully achieved via a phase-locked loop in this case. As R_e is further increased, the background becomes higher again. The dependence of the background signal on R_e agrees with calculations.

11:39AM M26.00003 In-situ electromechanical properties of suspended Poly-pyrrole (PPy) nanotube using metal coated AFM tip manipulations

SANG WOOK LEE, HAKSEONG KIM, SUNG HO JHANG, Konkuk University, NENM TEAM — Electromechanical properties of individual suspended poly-pyrrole (PPy) nanotube were investigated. PPy nanotubes were positioned and suspended using the ac electrophoresis and micro transfer method. The metal coated atomic force microscope tip was used as a pressure source of the suspended PPy tube and, at the same time, one of the contact electrodes for measuring in-situ current-voltage characteristics while the PPy tube is under stressed. The resistance of the PPy tube was decreased in electromechanical measurements with increasing pressure using a metal coated AFM tip. 1.36 GPa of maximum contact pressure on the tip-tube contact was estimated to reduce the contact resistance for making to 6.8 ohm cm in a lateral configuration.

This work was supported by NRF.

11:51AM M26.00004 GPU Accelerated Quantum Transport Modelling of Realistic Large Cross-Section Silicon Nanobeams

MOHAMMED HARBI, HONG GUO, McGill University — Understanding the quantum transport properties of silicon nano-beams or -wires is important for many practical applications. But for nanobeams with a cross section larger than 10 nm square or so, typical transport modelling techniques based on Green’s functions and atomistic DFT Hamiltonians become very computationally demanding. The computational burden becomes even greater when electron scattering with phonons is included. In this work we report hardware acceleration of the computational algorithm using a cluster of CPUs and GPUs working together in a heterogenous computing scheme. The GPU accelerated transport scheme is implemented for atomistic tight-binding Hamiltonian within the non-equilibrium Green’s function formalism. As examples, we calculate charge transport properties of realistic large cross-section Si nanobeams with several defect configurations, and report how local density of states can be significantly perturbed by the presence of the atomic impurity.
12:03PM M26.00005 Thermal properties of semiconductor nanowires using electromechanics . JOHN MATHEW, MANDAR DESHMUKH, Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai, India — We present low temperature measurements of thermal expansion and diffusivity of InAs nanowires using electromechanical response of the nanowire. To realize this, we fabricate InAs nanowire devices in doubly clamped, suspended field effect transistor geometry, and use direct radio frequency detection of the nanowire electromechanics. The resonant frequency of the nanowire is studied at different temperatures as a function of applied source-drain bias voltage. Due to Joule heating and the non-monotonic thermal expansion of InAs we observe positive and negative dispersion of the nanowire resonant frequency with applied bias. We also study dynamical response to heating to understand the thermal diffusivity in these sub-micron structures. We show that the resonant frequency of NEMS devices acts as a good indicator of thermal properties of semiconductor materials providing information on thermal conductivity, expansion and diffusivity.

12:15PM M26.00006 Optimizing electronic characteristics of SnO2 nanobelts for FET devices . TIMOTHY KEIPER, JORGE BARREDA, Department of Physics, Florida State University, JIM P. ZHENG, Electrical and Computer Engineering, FAMU/FSU College of Engineering, PENG XIONG, Department of Physics, Florida State University — Oxide semiconductors are attractive channel materials for nanoscale field effect transistors (FETs), especially for applications in chemical and biological sensing. Here we focus on optimizing the current-voltage relationship and gating response of SnO2 nanobelts (NB) FETs, a widely used sensor material. The NBs are grown by a physical vapor-liquid-solid process, with dimensions that are desirable for FET application, however the electrical characteristics of the as-grown materials are often not optimum for high-performance FETs. We have developed a multistep thermal annealing procedure in low vacuum ranging from 150 to 250 °C and oxygen environment at atmospheric pressure and 600 °C to increase the conductivity by more than 10^2. The multistep annealing process is necessary to consistently obtain FETs with low resistance, Ohmic contacts which differ by <5%. Utilizing a typical backgate geometry the device is transitioned from the on state to the off state over a gate voltage range of less than 30 V through a thick 250 nm SiO2 dielectric layer. The On/Off ratio is as large as 10^4. We surmise the oxygen annealing effectively activates the NBs while the vacuum annealing both helps clean the material and tune the carrier density at the surface, affecting metallization.

12:27PM M26.00007 Optoelectronic Properties of Hybrid Titania Nanotubes/Hematite Nanoparticles Structures . LILI WANG, EUGEN PANAITESCU, LATIKA MENON, Northeastern University — TiO2/Fe2O3 nanostructures are becoming promising alternatives for improving cost effectiveness (in $/W) of emerging photovoltaic devices such as dye sensitized or metal-insulator-semiconductor solar cells, combining the low cost, earth abundance and stability of the materials with the enhanced performance offered by the nanoscale architecture. We investigated novel, high quality titania/hematite composites, namely hematite nanoparticle decorated titania nanotube arrays, which were obtained by a simple, inexpensive and easily scalable two-step process, electrochemical anodization of titanium followed by forced hydrolysis. The titania nanotubular scaffold provides a large active surface area, while the iron oxide nanoparticles significantly broaden the light absorption range into the visible region. The morphological and structural characteristics of the samples were analyzed by scanning electron microscopy (SEM), X-ray diffraction (XRD) and transmission electron microscopy (TEM). The light absorption efficiency was measured by diffuse reflectance spectroscopy (DRS), and the optoelectronic behavior of the hybrid structures was analyzed by IV measurements under simulated solar illumination. The influence of the synthesis process and the structure design on the photovoltaic performance is currently investigated for optimal device prototyping.

12:39PM M26.00008 Structural and electronic properties of CdS/ZnS core/shell nanowires: A first-principles study . HYO SEOK KIM, YONG-HOON KIM1 , Korea Advanced Institute of Science and Technology — Carrying out density functional theory (DFT) calculation, we studied the relative effects of quantum confinement and strain on the electronic structures of II-IV semiconductor compounds with a large lattice-mismatch, CdS and ZnS, in the core/shell nanowire geometry. We considered different core radii and shell thickness of the CdS/ZnS core/shell nanowire, different surface facets, and various defects in the core/shell interface and surface regions. To properly describe the band level alignment at the core/shell boundary, we adopted the self-interaction correction (SIC)-DFT scheme. Implications of our findings in the context of device applications will be also discussed.

This work was supported by the Basic Science Research Grant (No. 2012R1A1A2044793), Global Frontier Program (No. 2013-073298), and Nano-Material Technology Development Program (2012M3A7B4049888) of the National Research Foundation funded by the Ministry of Education, Science and Technology of Korea.

1 corresponding author

12:51PM M26.00009 Surface States and Transport in Bismuth Nanowires with Strong Magnetic Field . SHIANG FANG, BERTRAND HALPERIN, EFTHIMIOS KAXIRAS, Department of Physics, Harvard University — Bismuth nanowires have attracted attention due to the enhancement of thermoelectricity in the one-dimensional geometry. Because of the large surface-bulk ratio and gapped bulk-like states, the transport in Bismuth nanowires is dominated by surface states, which may be probed by measurement in magnetic field ~14T. However, due to the spiral motion of electrons between various nanowire facets, the electron would bounce between multiple wire surface with different crystal orientations. Shubnikov-de Haas oscillations in magneto-resistance in transport encode the convoluted information for different surface states. To study these effects and the mechanism for transport in strong magnetic field, we employ a density functional theory calculation for the band structure. Maximally-Localized Wannier Functions are used to construct an empirical tight-binding model, which provides numerically accurate results at reduced computational cost. In this way, the surface states in a semi-infinite geometry can be obtained from the efficient iteration of Greens functions. The formation of Landau levels can also be studied by Peierls substitution.

Center for Integrated Quantum Materials, National Science Foundation DMR-1231319

1:03PM M26.00010 Transport through double quantum dots in Ge/Si core/shell nanowires . AZARIN ZARASSI, ZHAOEN SU, DHARMRAJ K. PATIL, SERGEY M. FROLOV, University of Pittsburgh, MOIRA HOCEVAR, Institute Neel CNRS, MINH NGUYEN, JINKYOUNG YOO, Los Alamos National Lab, SHADI A. DAYEH, University of California San Diego — In the studies of spin qubits long dephasing times are crucial. Qubits made of materials with low abundance of nuclear spin, group IV semiconductors, have shown long spin coherence times. On top of this, the predicted strong spin-orbit interaction in the valence band of Ge/Si makes it a good platform to electrically manipulate spin states. We have formed stable and tunable double quantum dot by confining holes with the help of bottom gate electrodes in Ge/Si core/shell nanowires. Hole transport through the dots exhibits excited hole states from Zeeman splitting of which g-factors can be extracted. We are searching for spin blockade in the transport between double dots, which can be used to readout spin qubits and study spin-orbit interaction.
1:15PM M26.00011 Intrinsic and extrinsic effects on electron-phonon coupling strength in individual ZnTe nanowires: The effects of laser annealing and metallic Te. JASON MARMON, Nanoscale Science Program, UNC-Charlotte, TAO SHENG, HAITAO ZHANG, Mechanical Engineering & Engineering Science, UNC-Charlotte, YONG ZHANG, Electrical & Computer Engineering, UNC-Charlotte — Electron-phonon coupling is typically studied as an intrinsic property for a given bulk material, and modifying the coupling has been explored in a nanostructure. We point out that the coupling strength can be easily perturbed both significantly and unintentionally. Nanowires, with their large surface-to-volume ratio, are more susceptible to extrinsic perturbations that affect coupling strength, although literature assumes that coupling is intrinsic. This work uses vibrational spectroscopy under a near resonant condition to probe the coupling strength of individual ZnTe nanowires. Using the intensity ratio of the first and second order Raman peaks, \( R = I_{1LO}/I_{2LO} \), as a measure of the electron-phonon coupling strength (proportional to the Huang-Rhys factor), we find that the ratio can change greatly when varying either the sample or measurement condition, for instance, the presence of defects in the as-grown sample and their removal though laser illumination.

1:27PM M26.00012 Single Schottky junction FETs based on Si:P nanowires with axially graded doping. JORGE BARREDA, TIMOTHY KEIPER, MEI ZHANG, PENG XIONG, Florida State University — Si nanowires (NWs) with a systematic axial increase in phosphorus doping have been synthesized via a vapor-liquid-solid method. Silane and phosphine precursor gases are utilized for the growth and doping, respectively. The phosphorus doping profile is controlled by the flow ratio of the precursor gases. After the as-grown product is ultrasonically agitated into a solution, the Si NWs are dispersed on a SiO\(_2\) substrate with a highly doped Si back gate. Individual NWs are identified for the fabrication of field-effect transistors (FETs) with multiple Cr/Ag contacts along the NW. Two-probe and four-probe measurements are taken systematically under vacuum conditions at room temperature and the contribution from each contact and each NW section between adjacent contacts is determined. The graded doping level, produced by a systematic reduction in dopant density along the length of the NWs [1], is manifested in the regular increases in the channel and contact resistances. Our Si NWs facilitate the fabrication of asymmetric FETs with one ohmic and one Schottky contact. A significant increase in gate modulation is obtained due to the single Schottky-barrier contact. Characterization details and the applicability for sensing purposes will be discussed.


1:39PM M26.00013 Fabry Perot phenomena in nanowire cavities, SHICHENG LU, JOSHUA VEAZEY, MENGCHEN HUANG, PATRICK IRVIN, Univ of Pittsburgh, HYUNGWOO LEE, SANGWOONG RYU, CHANG-BEOM EOM, Univ of Wisconsin-Madison, JEREMY LEVY, Univ of Pittsburgh — A solid-state geometry analogous to an optical Fabry-Perot cavity gives evidence for coherent transport on the order of microns through nanowires at the LaAlO\(_3\)/SrTiO\(_3\) (LAO/STO) interface. Conductive AFM lithography is used to create both the nanowires and the two confining barriers which define the cavity. These two barriers act as the primary scattering centers so that as the chemical potential is tuned through the conducting state of the device, partial reflections from the barriers interfere in the cavity, resulting in quasi-periodic oscillations of the conductance at low temperatures. Full and extended single-mode periodicity is not observed in all devices; however, the conductance oscillations are only observed in cavity structures, suggesting that the effects of the two manufactured barriers dominate over any random scattering sites from disorder. The conductance oscillations from interference of coherently scattered electrons give evidence for ballistic transport on much longer length scales than implied by mobility measurements in two-dimensional LAO/STO.

1:51PM M26.00014 Quantized conductance through reconfigurable 1D channels, SHICHENG LU, ANIL ANNADI, GUANGLIE CHENG, MICHELLE TOMCZYK, MENGCHEN HUANG, University of Pittsburgh, HYUNGWOO LEE, SANGWOONG RYU, CHANG-BEOM EOM, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, University of Pittsburgh — In recent years, a high mobility two-dimensional electron gas LaAlO\(_3\)/SrTiO\(_3\) (LAO/STO) system has become a model system to investigate various exotic ground states of condensed matter physics. This system can co-host superconductivity, magnetism, and strong spin-orbit coupling at 2D interfaces which led to predictions of exotic phenomena such as unconventional superconductivity, helical/chiral modes, and Majorana phases in these interfaces. In order to explore these exotic phases high quality 1D devices are desirable. We demonstrate the realization of a gate tunable quantum point contact (QPC) structure embedded in a LAO/STO nanowire created using conductive AFM lithography. We observe integer quantized conductance in the units of \( e^2/h \) at high magnetic fields (\( B = 9 \text{ Tesla}, T = 50 \text{ mK} \)), a signature of the existence of 1D quantum channels. Significantly, we observe quantized conductance for nanowires as long as 1 \( \mu m \), implying that transport is ballistic along the magnetic-field induced chiral edge states in these devices.

2:03PM M26.00015 Magnetoeconductance signatures of subband structure in semiconductor nanowires, GREGORY HOLLOWAY, CHRIS HAAPAMAKI, University of Waterloo, RAY LAPIERRE, McMaster University, JONATHAN BAUGH, University of Waterloo — Understanding the subband structure due to radial confinement in semiconductor nanowires can benefit technologies ranging from optical sensors to quantum information processing. An axial magnetic field couples to the orbital angular momentum, giving rise to non-trivial features in electronic transport as a function of magnetic field. Previous reports focused on conduction electrons confined to a thin shell near the nanowire surface, which lead to flux-periodic energies and conductance oscillations. Here, we calculate the eigenstates for more general radial potentials with moderate to low surface band bending such that electrons are distributed more uniformly across the nanowire cross-section. It is found that the energy spectrum becomes aperiodic in both gate voltage and magnetic field as the radial potential becomes flatter. The behavior of an energy level is dictated by its angular momentum, and this allows, in principle, each state to be identified based on its dependence on magnetic field and the chemical potential. We experimentally investigate a short-channel InAs nanowire FET in search of conductance features that reveal this subband structure. A qualitative measure for assigning conductance features to specific transverse states is introduced and applied to this device.


11:15AM M27.00001 Introduction, DAVID CHANDLER, Sandia National Laboratories —
3 of ice particles can be more than twice larger than the geometrical cross sections of these particles.

ozone hole where the polar stratospheric clouds play a key role in the ozone depletion process. The atmospheric cloud generation starts with the growing of

demand improved theoretical treatments which properly account for the interactions between different degrees of freedom: charge, electronic, vibrational, spin,

The field of molecular electronics has grown significantly since the first measurements of single molecule conductance. The

These new experimental advancements

Systems at the Atomic-Scale Resolutions of Time and Space

Funding from EPSRC (EP/G00224X and EP/L005913) is gratefully acknowledged.

12:03PM M27.00003 Earle K. Plyler Award: X-Ray and UV Studies of Molecular and Nano-

12:39PM M27.00004 Irving Langmuir Prize Lecture - A predictive theory of transition metal

1:15PM M27.00005 Electron Transport, Energy Transfer, and Optical Response in Single

In collaboration with Boris Fainberg, Faculty of Sciences, Holon Institute of Technology; Sergei Tretiak, Theoretical Division, Center for Integrated Nanotechnologies, Los Alamos National Laboratory; and Michael Galperin, Department of Chemistry and Biochemistry, University of California San Diego.

1:51PM M27.00006 First Steps in Atmospheric Particle Formation: Nucleation of the Smallest

Ice Snowflake

Clouds - role in atmospheric chemistry and climate. Perhaps the most famous example is the

Ozone hole

other layers in the middle atmosphere. This process

1 Grant agency of the Czech Republic, Grant No.: 14-08937S


157, 2012, 034304

12, 2010, 1218.


1 Funding from EPSRC (EP/G00224X and EP/L005913) is gratefully acknowledged.

References


157, 2012, 034304

112, 2014, 113401

115, 2013, 141.


1218.

1218.
2:03PM M27.00007 Probing Individual Atoms and Molecules on Pt(111) 1, ZHU LIANG, University of Illinois at Chicago, SURFACE AND INTERFACE SCIENCE LABORATORY, RIKEN, JAPAN COLLABORATION — A low-temperature scanning tunneling microscopy (LT-STM) is used to investigate the structure and reactivity of atomic nitrogen on Pt surfaces, which is important to a variety of catalytic processes. The adsorption of ammonia on an oxygen covered Pt surface leads to the formation of an NH1–O2 complex. Such a complex serves as a precursor to ammonia oxo-dehydrogenation, which produces an ordered atomic N layer on the surface when annealed to temperatures above 300 K. (√3 × √3)R30°-N and p(2 × 2)-N phases are found to coexist at temperatures between 360 and 400 K. After exposing the N-covered surface to hydrogen gas at 300 K, NH molecules are present as scattered molecules, as well as in dense islands. Mechanisms of dissociation of NH and lateral movement of H have been explored by examining the threshold energies and reaction rates. Measuring the response of the motion against applied bias voltages reveals the threshold energy, which is the energy of the vibrational mode that is responsible for activating a given motion. A theoretical model is used to fit the spectra, from which an estimate of reaction rate is obtained. ND dissociation and D hopping have also been investigated to role the role of hopping in these reactions.

Hyowon Kim, Hyun Jin Yang, and Junyeo Oh are acknowledged for their contributions to this work. Support and supervision by professor Yousoo Kim and professor Michael Trenary are gratefully acknowledged.

Wednesday, March 4, 2015 11:15AM - 2:15PM –
Session M28 GMAG DMP: Focus Session: Spin Liquids II 205 - Shigeki Onoda, RIKEN

11:15AM M28.00001 Numerical evidence of quantum melting of spin ice: quantum-classical crossover, YASUYUKI KATO, RIKEN Center for Emergent Matter Science, SHIGEKI ONODA, Condensed Matter Theory Lab., RIKEN; RIKEN Center for Emergent Matter Science — Unbiased quantum Monte-Carlo simulations are performed on the simplest case of the quantum spin ice model, namely, the nearest-neighbor spin-1/2 XXZ model on the pyrochlore lattice with an antiferromagnetic longitudinal and a weak ferromagnetic transverse exchange couplings, J and J⊥. On cooling across Tcsti ≈ 0.2J, the specific heat shows a broad peak associated with a crossover to a classical Coulomb liquid regime characterized by a remnant of the pinch-point singularity in longitudinal spin correlations as well as the Pauling ice entropy for |J⊥| ≪ J, as in classical spin ice. On further cooling, the entropy restarts gradually decaying to zero for J⊥ > J⊥c ≈ −0.10J, as expected for bosonic quantum Coulomb liquids. With negatively increasing J⊥ across J⊥c, a first-order transition occurs at a nonzero temperature from the quantum Coulomb liquid to an XY ferromagnet. Relevance to rare-earth pyrochlore oxides is discussed.

11:27AM M28.00002 Possible algebraic spin liquid in half-filled Hubbard model at intermediate U/t, XIANG LI, Institute for Advanced Study, Tsinghua University, Beijing, 100084, China, ZI YANG MENG, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, HONG YAO, Institute for Advanced Study, Tsinghua University, Beijing, 100084, China — Using large-scale fermion-sign-free projective Determinant Quantum Monte-Carlo (DQMC) method, we study the half-filled Hubbard model on the square lattice with staggered-flux. We calculate the single-particle gap, charge gap, as well as the improved dimensionless estimator of the antiferromagnetic (AF) order parameter, and map out the ground state phase diagram of this model spanned by U/t and staggered-flux. The lattice in our DQMC simulations has 2L×L sites with largest L=28. In the case of φ-flux, finite-size scaling analysis indicates a possible algebraic quantum spin liquid phase between the semi-metal phase at small U/t and the AF phase at large U/t. The algebraic spin liquid occurs in the arrange of 5.4 < U/t < 5.6. When the staggered-flux is smaller than the critical value of about \sqrt{φ}/10, the Fermi velocity in this system is largely anisotropic and it exhibits a direct transition from semi-metal phase to AF phase.

11:39AM M28.00003 Confinement–deconfinement transition in the algebraic RVB states, JI-QUAN PEI, SHAO-KAI JIAN, HONG YAO, Institute for Advanced Study, Tsinghua University — Deconfined algebraic spin liquids are usually expected when Gutzwiller projecting the non-interacting wave function of half-filled electrons on the square lattice with staggered flux φ. However, our large-scale variational Monte Carlo simulations show that there is the confinement-deconfinement transition at φ = φc, where φc ≈ 0.2 is the critical flux. When 0 < φ < φc, spinons are confined and the ground state develops an unexpected antiferromagnetic Neel ordering. From renormalization group analysis of anisotropic Dirac fermions coupled with U(1) compact gauge fields, we argue that the confinement of spinons in the Gutzwiller projected wave function might be due to the large anisotropy of Fermi velocity of Dirac fermions.

11:51AM M28.00004 ABSTRACT WITHDRAWN –

12:03PM M28.00005 Schwinger boson spin liquid states on square lattice: projective symmetry group study, XU YANG, FA WANG, Peking Univ — We will report our results on possible spin liquids on square lattice that respect all lattice symmetries and time-reversal symmetry within the framework of Schwinger boson (mean-field) theory. Such spin liquids have spin gap and emergent gauge field excitations. We classify them by the projective symmetry group method, and find six spin liquid states that are potentially relevant to the J1–J2 Heisenberg model. The properties of these states are studied under mean-field approximation and by projected wave functions on small lattices. Interestingly we find a spin liquid state that can go through continuous phase transitions to either Néel magnetic order or magnetic order of wavevector at Brillouin zone edge center. We propose that this state may be realized in J1–J2 Heisenberg model with ring exchange.

12:15PM M28.00006 Projective symmetry of partons in Kitaev’s honeycomb model1, PAULA MELLADO, Adolfo Ibañez University — Low-energy states of quantum spin liquids are thought to involve partons living in a gauge-field background. We study the spectrum of Majorana fermions of Kitaev’s honeycomb model on spherical clusters. The gauge field endows the partons with half-integer orbital angular momenta. As a consequence, the multiplicities reflect not the point-group symmetries of the cluster, but rather its projective symmetries, operations combining physical and gauge transformations. The projective symmetry group of the ground state is the double cover of the point group.

1We acknowledge Fondecyt under Grant No. 11121397, Conicyt under Grant No. 791112004, and the Simons Foundation (P.M.); the Max Planck Society and the Alexander von Humboldt Foundation (O.P.); and the US DOE Grant No. DE-FG02-08ER46544 (O.T.)
12:51PM M28.00007 Chiral spin liquid and emergent anyons in a Kagome lattice Mott insulator 
BELA BAUER, Microsoft Corp, LUKASZ CINCO, Perimeter Institute, BRENDAN P. KELLER, University of California, Santa Barbara, MICHELE DOLFI, ETH Zurich, GUIFRE VIDAL, Perimeter Institute, SIMON TREBST, University of Cologne, ANDREAS W. W. LUDWIC, University of California, Santa Barbara — One of the earliest proposals for a topological phase in a quantum spin system was the chiral spin liquid put forward by Kalmeyer and Laughlin in 1987 as the bosonic analogue of the fractional quantum Hall effect. Here, we examine a physically motivated model for a Mott insulator on the Kagome lattice with broken time-reversal (TR) symmetry that gives rise to a chiral spin liquid. We present unambiguous numerical identification and characterization of the universal topological properties of the phase, including ground state degeneracy, edge physics, and anyonic bulk excitations. To this end, we use a variety of powerful numerical probes, including the entanglement spectrum and modular transformations. We then discuss the phase diagram resulting from the competition of the TR symmetry breaking chiral term and a TR-symmetric Heisenberg term, which on the Kagome lattice has been argued to give rise to a TR-symmetric topological phase. In particular, we elucidate the dynamics of the chiral phase upon approaching the putative topological phase transition.

1:03PM M28.00008 Impact of non-Abelian anyons on criticality , MARC SCHULZ, FIONA BURNELL, Univ of Minn — Topological order provides an interesting playground to investigate criticality in phase transitions with no local order parameter where the condensing excitations interact statistically. We investigate the impact of these exchange statistics on critical properties by comparing two closely related models, which differ only by the presence or absence of such long-ranged statistical interactions for the condensed excitations:

1. The Ising string-net Hamiltonian, in which the transition is between a topologically ordered phase (with doubled Ising topological order) and a trivial phase. The excitations that condense across this transition are achiral non-Abelian anyons.

2. The Ashkin-Teller model on a triangular lattice, in which the transition is from a paramagnetic to a ferromagnetic phase.

We show that the non-Abelian excitations in the first model can be mapped onto the spin degrees of freedom of the second, and that the mapping captures all relevant features except the non-Abelian statistics. We derive the low-energy spectra of these models by means of high-order perturbation theory and exact diagonalization to study the resulting differences in their critical behavior.

1:15PM M28.00009 Variational Monte Carlo Study of a Non-Abelian Spin-1 Spin Liquid , JULIA WILDEBOER, N.E. BONESTEEL, NHMFL, Florida State University — Using variational Monte Carlo we analyze the properties of a non-Abelian spin-1 spin liquid state proposed in [1]. In this state the bosonic $\nu = 1$ Moore-Read Pfaffian wavefunction is interpreted as a wavefunction for a gas of bosons on a 2D square lattice with one flux quantum per plaquette. For this wavefunction the number of bosons on a given lattice site can be 0, 1 or 2, corresponding, respectively, to $S_z = -1$, 0 or 1 for a spin-1 degree of freedom on that site. Calculations are performed both in the planar geometry and on the torus. For the torus there are three distinct states corresponding to the three-fold degeneracy of the $\nu = 1$ bosonic Moore-Read state, and we show that the correlation functions in these states become identical in the limit of large system size. The Renyi entanglement entropy is also calculated for different system partitions in order to extract the topological entropy $\gamma = \ln D$ where $D$ is the total quantum dimension, predicted to be $D = 2$ for this state.


1:27PM M28.00010 Coherent Transmutation of Electrons into Fractionalized Anyons , MAISSAM BARKESHLI, Microsoft Station Q, EREZ BERG, Weizmann Institute, STEVEN KIVELSON, Stanford University — Electrons have three quantized properties — charge, spin, and Fermi statistics — that are directly responsible for a vast array of phenomena. Here we show how these properties can be coherently and dynamically stripped from the electron as it enters certain exotic states of matter known as a quantum spin liquid (QSL). In a QSL, electron spins collectively form a highly entangled quantum state that gives rise to emergent gauge forces and fractionalization of spin, charge, and statistics. We show that certain QSLs host distinct, topologically robust boundary types, some of which allow the electron to coherently enter the QSL as a fractionalized quasiparticle, leaving its spin, charge, or statistics behind. We use these ideas to propose a number of universal, conclusive experimental signatures that would establish fractionalization in QSLs.

1:39PM M28.00011 Chiral spin liquid in the frustrated XY model on the honeycomb lattice , TIGRAN SEDRAKYAN, Fine Theoretical Physics Institute, University of Minnesota and Physics Frontier Center, Joint Quantum Institute, University of Maryland — A honeycomb lattice allowing hops between nearest- and next-nearest neighbors hosts “moat” bands with degenerate energy minima attained along closed lines in Brillouin zone. If populated with hard-core bosons, a variety of unconventional ground states stabilizes. We argue that the degeneracy prevents Bose condensation, stabilizing novel spin liquid phases including composite fermion state and a chiral spin liquid. The latter stabilizes at half-filling, when the system is equivalent to $s = 1/2$ XY model at zero magnetic field. Absence of condensation means no spontaneous polarization in XY plane, however our consideration indicates formation of a state spontaneously breaking the time-reversal symmetry. This state has a bulk gap and chiral gapless edge excitations, and is similar to the one in Haldane’s “quantum Hall effect without Landau levels” in its topologically nontrivial sector with Chen number $C = \pm 1$. The applications of the developed analytical theory include an explanation of recent unexpected numerical findings and a suggestion of a chiral spin liquid realization in experiments with cold atoms in optical lattices.

Wednesday, March 4, 2015 11:15AM - 2:15PM –
Session M29 GMAG DMP FIAP: Focus Session: Spin-Torque Oscillators 206A - Igor Barsukov,
University of California, Irvine

11:15AM M28.00001 Time domain mapping of spin torque oscillators dynamics , JIEYI ZHANG, YUJIN CHEN, UC Irvine, GRAHAM ROWLANDS, Cornell University, ILYA KRIVOROTOV, UC Irvine, PATRICK BRAGANCA, JEFF CHILDRESS, BRUCE GURNEY, Hitachi Global Storage Technologies, UC IRVINE, HGST AND CORNELL UNIV COLLABORATION — Time domain measurements of spin torque oscillators (STOs) offer important insights into the magnetization dynamics under the action of spin torque. We use the time domain data to map statistical distributions of the STO free layer trajectories and analyze them in the framework of the Fokker-Planck effective energy approach. We make time-resolved measurements of the microwave voltage signal generated by an STO based on a 90 nm circular nanopillar patterned from IrMn/CoFe/CoFeGe/CoFe/Cu/CoFe/CoFeGe/CoFe multilayer. Based on our time domain data and the angular dependence of giant magneto-resistance of the device, we map out dynamic trajectories of the free layer. We then apply the Fokker-Planck approach to calculate spin torque dependent STO effective energy $E_{\text{eff}}$ from the experimentally measured statistical distributions of the free layer trajectories. We compare the measured $E_{\text{eff}}$ to that calculated in the macrospin approximation and discuss how such a comparison can be used for quantification of non-linear damping in the high-amplitude regime of STO operation.
11:27AM M29.00002 Tapered nanowire spin torque oscillator driven by spin orbit torques. LIU YANG, ANDREW SMITH, BRIAN YOUNGBLOOD, ZHENG DUAN, ILYA KRIVOROTOV, University of California, Irvine — We report microwave signal emission from a spin torque oscillator driven by spin orbit torques in a tapered Pt(7nm)/Py(5nm) ferromagnetic nanowire with 2 um long active region. The tapered nanowire oscillator exhibits lower spectral linewidth (<1 MHz) and higher integrated power (>1 nW) compared to a spin tube oscillator based on a nanowire with spatially uniform width. The tapered nanowire oscillator has two distinct regimes of the microwave signal emission: a low-current, low-amplitude regime with a soft onset of the microwave emission and a higher-current regime with a hard onset of large-amplitude oscillations. The existence of the two regimes arises from spatially non-uniform effective damping in the tapered nanowire geometry. The non-uniformity of the effective damping results in nucleation of magnetization self-oscillations at the narrow end of the nanowire and subsequent steady growth of the self-oscillatory region with increasing current throughout the low-power regime. The sudden turn on of the high-power regime takes place at a critical current, for which spatially averaged effective damping of the nanowire changes sign from positive to negative. Our work paves the way towards high-power spectrally pure spin torque oscillators driven by spin orbit torques.

11:39AM M29.00003 Spin Torque Oscillators with Highly Spin-Polarized Heusler Alloy. TAKESHI SEKI, TATSUYA YAMAMOTO, KOKI TAKANASHI, Institute for Materials Research, Tohoku University — An intriguing spin torque device is the spin torque oscillator (STO). An important issue for STOs from the viewpoint of practical use is to enhance the rf output power (Pout). Since Pout is roughly proportional to the square of the magnetoresistance (MR) ratio, a ferromagnetic material showing a large MR effect is a candidate for high-performance STO. In this study, we have developed high-power all-metal STOs with a full Heusler Co2Fe0.4Mn0.6Si (CFMS) showing a large MR effect. The present STOs consist of current-perpendicular-to-plane (CPP) giant magnetoresistance (GMR) stacks of CFMS | Ag | CFMS. A pillar-shaped STO showed clear auto-oscillation. The large Pout of 23.7 nW was obtained owing to its out-of-plane magnetization precession. Simultaneously, the oscillation linewidth showed the minimum value of 10 MHz. On the other hand, a point-contact-type STO showed auto-oscillation even at zero external magnetic field, and the oscillation mode was drastically changed as the bias current was increased. The large Pout for both STOs indicates the CPP-GMR devices with CFMS layers are promising for high performance STO.

11:51AM M29.00004 Linewidth reduction in spin–torque oscillators by delayed self-injection. JG thanks the European Research Council NanoBrain Grant 259068

12:03PM M29.00005 Spin wave beam mediated synchronization of nano-contact spin torque oscillators. AFSHIN HOUSHANG, EZIO IACOCCA, PHILIPP DURRENFELD, University of Gothenburg, SOHRAB SANI, New York University, JOHAN AKERMAN, RANDY DUMAS, University of Gothenburg — The synchronization of multiple nano-contact spin torque oscillators (NC-STOs) [1-3] is mediated by propagating spin waves (SWs). While it has been shown that the Oersted field generated in the vicinity of the NC can dramatically alter the emission pattern of SWs [4], its role in the synchronization behavior of multiple NCs has not been considered. We investigate the synchronization behavior in double NC-STOs oriented either vertically or horizontally, with respect to the in-plane component of the external field. Two NCs with nominal diameters of 100 nm and a center-to-center spacing of 300 nm are defined on top of an all metallic Co/Cu/NiFe pseudo spin valve. Synchronization is promoted (impeled) by the Oersted field strength when the NCs are oriented vertically (horizontally) due to the highly anisotropic SW propagation. The vertical positioning of the NCs gives rise to a unique magnetic field landscape that acts to localize SWs in a region just outside one of the NCs, as confirmed by micromagnetic simulations. [1] S. Kaka, et al., Nature 437, 389 (2005) [2] F.B. Mancoff, et al., Nature 437, 393 (2005). [3] S.R. Sani, et al., Nat. Comm. 4, 2731 (2013) [4] R.K. Dumas, et al., Phys. Rev. Lett. 110, 257202 (2013)

12:15PM M29.00006 Directional spin wave emission by the spin transfer torque oscillator into a nanomagnonic waveguide. VLADISLAV DEMIDOV, SERGEI DEMOKRITOV, Muenster University, SERGEI URAZHDIN, Emory University — Magnonics is based on signal transmission and processing by spin waves in a magnetic medium. Spin-torque nanooscillators (STNO) driven by dc electrical current can provide a local source of spin waves for nanomagnonics, but their spectral mismatch with the magnetic medium limits the spin wave emission efficiency. We have developed a nanomagnonic structure that combines a point-contact STNO with a dipolar field-induced nanowaveguide. We will describe our microfocus Brillouin light scattering microscopy measurements demonstrating efficient excitation of spin waves by the STNO and their directional propagation in the waveguide. Spectroscopic measurements and micromagnetic simulations indicate that efficient spectral matching between the waveguide and the STNO is achieved due the internal dipolar field of the nanopatterned waveguide. We show that the spin wave propagation length is increased compared to the extended films, due to their larger group velocity and the lack of wavefront spreading. Our results provide a simple and efficient route for the implementation of magnonic structures that integrate spin torque-based sources of spin waves and their processing via waveguiding structures.

12:27PM M29.00007 Coherent magnetization oscillation induced by nonlocal spin injection. SERGEI URAZHDIN, ANDREI ZHOLUD, Emory University, VLADISLAV DEMIDOV, SERGEI DEMOKRITOV, Muenster University — We experimentally demonstrate coherent magnetization oscillations induced by nonlocally injected pure spin current in a CoFe/Cu/Permальloy(Py) magnetic thin film heterostructure. The current injected into CoFe through a point contact is drained through the Cu spacer, while the spins diffusing from the CoFe/Cu interface to Py cause magnetic oscillations of the latter. Symmetry analysis and numeric calculations show that the current is negligible in the active region of the Py layer, and does not exceed 3 percent of the total current away from it. The oscillation frequency decreases with increasing current, and an additional spectral peak appears at large currents. Micro-focus Brillouin light scattering microscopy shows that the size of the oscillation region is larger than expected from the usual self-localization mechanism of auto-oscillation. Micromagnetic simulations suggest that the oscillation mode is localized by an effective potential well formed due to the local reduction of magnetization by the effects of spin current, providing a route for the development of spin-torque nano-oscillators with controllable spatial oscillation characteristics.

1 Supported by NSF ECCS-1305586.
12:39PM M29.00008 Noise-enhanced synchronization of stochastic magnetic oscillators1. JULIE GROLLIER, ALICE MIZRAHI, CNRS/Thales, Palaiseau, France, NICOLAS LOCATELLI, Institut d’Electronique Fondamentale, Orsay, France, ARTUR ACCIOLY, Instituto de Fisica, Univ. Federal do Rio Grande do Sul, Porto Alegre, Brazil, RIE MATSUMOTO, AKIO FUKUSHIMA, HITOSHI KUBOTA, SHINJI YUASA, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, VINCENT CROS, CNRS/Thales, Palaiseau, France, LUIGI GUSTAVO PEREIRA, Instituto de Fisica, Univ. Federal do Rio Grande do Sul, Porto Alegre, Brazil, DAMIEN QUERLOZ, JOO-VON KIM, Institut d’Electronique Fondamentale, Orsay, France — Due to their small magnetic volume the magnetization dynamics of spin-torque nano-oscillators is very sensitive to thermal fluctuations. The effect of thermal noise is large and can phase-lock the system to the thermal noise. Here we study how the thermal noise influences the phase-locking and the synchronization of a stochastic oscillator driven by spin-torque ferromagnetic resonance in YIG/Pt bilayers and the corresponding spatially-resolved spin-wave distribution are presented.

1We thank the European Research Council NanoBrain Stg Grant 250908.

12:51PM M29.00009 Terahertz Nano-oscillator using Antiferromagnet. RAN CHENG, DI XIAO, Carnegie Mellon University, ARNE BRATAAS, Norwegian University of Science and Technology — We present an analytical study on the current-induced dynamics of collinear antiferromagnets (AFs), and find that a sufficiently large current gives rise to terahertz auto-oscillation of the staggered order. For easy-plane AFs such as NIO, the acoustic and optical modes are well separated in frequency, and none of them exhibit chirality of precession. However, with increasing current-induced torque, the two modes become degenerate at a threshold, after which the chirality of precession is acquired. At a second threshold, the degenerate mode is driven into auto-oscillation with elliptical precession where the semi-major axis is 45 degree with respect to the easy-plane. The terahertz nano-oscillator is illustrated by X/AF/X heterostructures where X can either be a heavy metal or topological insulator.

1:03PM M29.00010 Nanoconstriction-based Spin Hall nanooscillator. ANDREI ZHOLUD, SERGEI URAZHODIN, Emory University, VLADISLAV DEMIDOV, SERGEJ DEMOKRITOV, University of Muenster — We experimentally demonstrate coherent magnetization oscillations induced in a bow tie-shaped Pt/Permalloy nanoconstrastion by pure spin current generated by the spin Hall effect. The devices generate microwave signals with a significant power and the spatial linewidth as low as 6.2 MHz at room temperature (RT). In contrast to the previously demonstrated spin Hall oscillators governed by the dynamical nonlinear self-localization mechanism, the localized oscillation mode is present in the thermal fluctuation spectrum even below the auto-oscillation onset and exhibits a significant redshift. These observations suggest that the localized auto-oscillation mode is formed due to the confinement in an effective potential well produced by a combination of the dipolar field of the magnetic nanoconstriction and the Oersted field of electrical current. The studied devices are characterized by a large oscillation area, minimizing the effects of thermal fluctuations and resulting in a narrow RT spectral linewidth without compromising the single-mode regime of autooscillation. Moreover, the simple structure of the proposed oscillators enables their cascading, which can be utilized to further improve the oscillation characteristics in mutually coupled devices.

1Supported by NSF grant DMR-0847159.

1:39PM M29.00013 Spin-transfer torque induced spin waves in antiferromagnetic insulators1. MATTHEW DANIELS, Carnegie Mellon University, WEI GUO, Fudan University, G. MALCOLM STOCKS, Oak Ridge National Laboratory, DI XIAO, Carnegie Mellon University, JIANG XIAO, Fudan University — We explore the possibility of exciting spin waves in insulating antiferromagnetic films by injecting spin-transfer torque, the two modes become degenerate at a threshold, after which the chirality of precession is acquired. At a second threshold, the degenerate mode is driven into auto-oscillation with elliptical precession where the semi-major axis is 45 degree with respect to the easy-plane. The terahertz nano-oscillator is illustrated by X/AF/X heterostructures where X can either be a heavy metal or topological insulator.


1:51PM M29.00014 Spin dynamics in patterned nanometer-thick yttrium iron garnet films1. MATTHIAS BENJAMIN JUNGLEISCH, WEI ZHANG, WANGJUN JIANG, STEPHEN M. WU, JOHN E. PEARSON, ANAND BHATTACHARYA, AXEL HOFFMANN, Argonne National Laboratory, JOSEPH SKLEWAR, JOHN B. KEITZER, Northwestern University, HOUCHEN CHANG, MINGZHONG WU, Colorado State University — We present experimental investigations on the propagation of spin-wave modes in micro-structured yttrium iron garnet (YIG) stripes.1 The stripes were patterned by photo-lithography from high-quality 40-nm-thick YIG films grown by sputtering.2 Magnetization dynamics is driven by the rf field of a shorted coplanar waveguide patterned onto the YIG stripes. The propagation of spin waves are detected by means of spatially-resolved Brillouin light scattering microscopy. The propagation distance of spin waves is determined in the linear regime, where an exponential decay of 10 µm is observed. The estimated Gilbert damping parameter extracted from the spin-wave decay length is 3 times larger than that obtained through ferromagnetic resonance measurements in unstructured films, which is possibly due to enhanced two-magnon scattering in the patterned films. Furthermore, studies on the spin dynamics driven by spin-torque ferromagnetic resonance in YIG/Pt bilayers and the corresponding spatially-resolved spin-wave distribution are presented.

1Supported by NSF grant DMR-0847159.

1:51PM M29.00014 Spin dynamics in patterned nanometer-thick yttrium iron garnet films1. MATTHIAS BENJAMIN JUNGLEISCH, WEI ZHANG, WANGJUN JIANG, STEPHEN M. WU, JOHN E. PEARSON, ANAND BHATTACHARYA, AXEL HOFFMANN, Argonne National Laboratory, JOSEPH SKLEWAR, JOHN B. KEITZER, Northwestern University, HOUCHEN CHANG, MINGZHONG WU, Colorado State University — We present experimental investigations on the propagation of spin-wave modes in micro-structured yttrium iron garnet (YIG) stripes.1 The stripes were patterned by photo-lithography from high-quality 40-nm-thick YIG films grown by sputtering.2 Magnetization dynamics is driven by the rf field of a shorted coplanar waveguide patterned onto the YIG stripes. The propagation of spin waves are detected by means of spatially-resolved Brillouin light scattering microscopy. The propagation distance of spin waves is determined in the linear regime, where an exponential decay of 10 µm is observed. The estimated Gilbert damping parameter extracted from the spin-wave decay length is 3 times larger than that obtained through ferromagnetic resonance measurements in unstructured films, which is possibly due to enhanced two-magnon scattering in the patterned films. Furthermore, studies on the spin dynamics driven by spin-torque ferromagnetic resonance in YIG/Pt bilayers and the corresponding spatially-resolved spin-wave distribution are presented.

1Supported by NSF grant DMR-0847159.

This work was supported by Department of Energy, Office of Science, Materials Science and Engineering Division, the Army Research Office, and National Science Foundation.

2:03PM M29.00015 Probing excitations in insulators by injecting spin currents. SHUBHAYU CHATTERJEE, SUBIR SACHDEV, Harvard University — Observation of fractional excitations in insulating spin-systems has been a long-sought goal in physics. In spite of promising evidence for observation of spin liquids, the exact nature of possible ground states, and in particular, the presence of a spin-gap is still unclear. Most experiments till this point have focused on thermodynamic measurements. We suggest a transport measurement as an alternate window into the nature of excitations of insulating spin systems. We couple a metal with a non-equilibrium spin-accumulation to an equilibrium insulating spin-system [1], and develop a general formalism to compute the spin current. We use this to calculate the current into ordered antiferromagnets as well as spin liquids, and note salient features in the spin conductance. [1] Takei et. al. Phys. Rev. B 90, 094408 (2014).
Preliminary electrical measurements on these devices show \( \sim \) transition from superparamagnetism to ferromagnetism-like, with ferromagnetism persisting at 300K. This transition is attributed to changes in both the amount of Ni \( \sim 10^{-25} \text{nm} \) and density \( \sim \) inside CNTs. Magnetometry results indicate that free-standing CS NPs and filled CNTs share a similar magnetic interaction mechanism. However, the overall magnetic moment in the graphene superlattice, helping to mediate the superexchange between the impurities. Depending on the choice of ion used, the interactions between the two ions can exhibit either a ferromagnetic or an antiferromagnetic behavior. These correlations indicate an RKKY-like behavior in the system. The effect of carrier doping, chemical modification at the edge, and finite temperature on the edge magnetism has been studied. The magnetic phase diagram with varied carrier doping, and on-site Coulomb interaction is found to be complex. Chemical modification of the edge atoms by hydrogen leads to partial quenching of local moments, giving rise to a richer phase diagram. We further report the influence of temperature on the long-range magnetic ordering at the edge using ab initio molecular dynamics. These findings will have important implications in controlling magnetism in graphene based low dimensional structures for technological purpose, and in understanding varied experimental reports.²

¹ We acknowledge support through Department of Science and Technology, India

¹¹¹AM 30.00004 ABSTRACT MOVED TO V1.00139

12:03PM M30.00005 Magnetic Interaction Study on Multi-Walled Carbon Nanotubes filled with Core/Shell Iron/Iron Oxide Nanoparticles

11:51AM M30.00004 ABSTRACT MOVED TO V1.00139

12:15PM M30.00006 Synthesis and properties of ferromagnetic nanostructures embedded within a high-quality crystalline silicon matrix
12:27PM M30.00007 Helical spin order in Fe nanoislands, SOO-HYON PHARK, Center for Activated Electron Systems, Institute for Basic Science, Seoul National University, Seoul, Korea. KOHJI NAKAMURA, Department of Physics Engineering, Me University, Japan. JASON FISCHER, MARCO CORBETTA, SAFIA OUZI, DIRK SANDER, JUERGEN KIRCHNER, Max-Planck-Institute of Microstructure Physics, Halle, Germany — We report a spin-polarized scanning tunneling microscopy and spectroscopy (SP-STM) using an atomic scale resolution, of individual nanostructures of biatomic-layer-high Fe on Cu[111]. SP-STM/S of the Fe nanoislands reveals a magnetic stripe phase with a period of 1.28 nm, which is identified as a one-dimensional helical spin order [1]. *Ab initio* calculations identify reduced-dimensionality-enhanced long range antiferromagnetic interactions as the driving spin-ordered phenomena [2,3]. In addition, electron-mapping provides a spatially-resolved and spin-dependent electronic structure of this helical spin order. The wave vector describing the spin order remains constant in the energy range -0.8 to +0.6 eV, whereas the spin contrast shows dissipation features around and sign change across the Fermi energy. We discuss the results in view of an energy gap opening associated with the non-collinear spin order. Our result identifies a novel aspect of SP-STM/S to characterize complex spin order with respect to the corresponding spin-dependent electronic band structure.


12:39PM M30.00008 Unconventional top down synthesis of FeNi core and C shell magnetic nanoparticles, RAKESH CHAUDHARY, ALI R. KOYMEN, Department of Physics, The University of Texas at Arlington — Carbon encapsulated FeNi nanoparticles were prepared by a top down approach using plasma in organic solvents. FeNi core-Carbon shell morphology of nanoparticles have been observed using transmission electron microscopy (TEM). FeNi nanoparticles prepared in toluene are of diameter 3-820 nm and encapsulated by a 3-60 nm shell. FeNi nanoparticles prepared in ethanol are of diameter 15-820 nm and encapsulated by a 4-34 nm shell. Using x-ray diffraction (XRD) the core crystal observed using transmission electron microscopy (TEM). FeNi nanoparticles prepared in toluene and ethanol showed a saturation magnetization of ∼1 emu/g and ∼3 emu/g and moderate coercivity ∼40 Oe and ∼10 Oe respectively at room temperature. We explore the uncommon and new, top down synthesis route of bimetallic nanoparticles of FeNi phase using plasma. These carbon-encapsulated FeNi nanoparticles could have potential applications in biomedicine, especially hyperthermia.

12:51PM M30.00009 Facile Synthesis of L10 FePt/Reduced-Graphene Oxide Nanocomposites, XIAOCAO HU, VASILIS TZITZIOS, University of Delaware, DAVID SELLMYER, University of Nebraska, GEORGE HADJIPANAYIS, University of Delaware — FePt nanoparticles (NPs) have attracted much attention recently for applications in high density recording media and catalysis. Usually the as-made FePt NPs are in the fcc phase and must be annealed at high temperatures to be converted to the L1(0) structure and because of this the particles agglomerate. In this paper, we used a novel fabrication method to directly prepare FePt NPs in fct phase on the surface of R-GO (Reduced Graphene oxide). A layered bimetallic precursor Fe(H2O)6[PtCl6] was mixed in water environment with exfoliated GO. The precipitates were annealed under a forming gas (5% H2 and 95% Ar)atmosphere at different temperatures varying from 500 °C to 950 °C. During the annealing process, the layered precursor [Fe(H2O)6][PtCl6] was reductively decompose directly to the L10 FePt crystal structure while the GO reduced by H2 atmosphere. Transmission electron microscopy (TEM) results showed that the FePt NPs have the L10 structure and a uniform size distribution with their average particle size in the range from 5 nm to 28 nm depending on the annealing temperature used. The fct particles had coercivity values in the range of 6 kOe-9 kOe. Furthermore, it is clear that the FePt nanoparticles are formed only on the surface of the graphene and no individual particles were observed off the graphene. The L10 FePt NPs are still isolated on the surface of the graphene and the particle size remains quite small (8 nm) even at annealing temperatures as high as 750 °C. Work supported by DOE-BES-DMSE (Grant No. DE-FG02-04ER4612).

1:03PM M30.00010 Ferromagnetic to antiferromagnetic transition in the Fe11/3(Ta1−x,Nbx)S2 layered dichalcogenides, CHIH-WEI CHEN, JESSE ADAMS, WILL HARDY, DOUGLAS NATELSON, EMILIA MOROSAN, Physics & Astronomy Department, Rice University — Fe11/3TaS2 is known to order ferromagnetically with Tc = 40 K, while the stoichiometric Nb compound orders antiferromagnetically below TN = 40 K. The Ta-Nb solid solution provides an opportunity to search for a quantum phase transition (QPT) as we tune the magnetic order in Fe11/3TaS2 by doping between T = Ta and T = Nb. We will analyze magnetization, specific heat, and resistivity data to search for signatures of a T = 0 transition. Additionally, we will compare the magnetoresistive effects in these Fe-intercalated TaS2 (T = Ta, Nb) and compare with our previous results on Fe11/3TaS2 (x = 0.25, 0.28). Small departures from the superstructure Fe compositions (x = 0.25, 0.33) in Fe11/3TaS2 resulted in two orders of magnitude increase in the magnetoresistance.

1:15PM M30.00011 Influence of interparticle interactions on the blocking temperature and high frequency permeability of Fe3O4 nanoparticle systems, M DHANSADAT, DAVID B. MAST, DONGLU SHI, University of Cincinnati, SERGEY L. BUD’KO, Ames Laboratory, Iowa State University — In Néel’s model of superparamagnetism, magnetization and relaxation dynamics depend on the magnetic anisotropy constant of the non-interacting, individual nanoparticle (NPs). However, NP interactions modify these dynamics in real systems. To investigate the influence of magnetic interactions on NP anisotropy, we compare the results from measurements of the blocking temperature of Fe3O4 NPs systems with very different average interparticle separations, one with uniformly dispersed NPs and the other with the NPs tightly confined in a polystyrene matrix. The blocking temperature for the confined NPs (263K) was substantially higher than for the uniformly dispersed NPs (131K), which we attribute to stronger dipolar interactions. The relaxation times are determined from peaks in the imaginary part of the complex permeability versus frequency from 10 MHz - 3 GHz. For uniformly dispersed Fe3O4 NP (in hydrocarbon carrier), the Néel relaxation and the gyromagnetic resonance were observed at 41 MHz and 1.2 GHz, respectively, which corresponds to an anisotropy constant of ~15 Kj/m3 compared to 12 Kj/m3 predicted by Néel’s relaxation model for 10 nm diameter Fe3O4 NPs. Details of this correlation between the blocking temperature and high frequency permeability will be discussed.

1:27PM M30.00012 Novel magnetic and electric properties of small pure gold clusters, LEI MA, RAMIRO MORO, BAIQIAN ZHANG, JOHN INDERGAARD, ILJA LARKIN, Georgia Institute of Technology, HANNU HÄKKINEN, Department of Physics Engineering, Me University, Japan. MAUSIT KINDBERG, Department of Physics, University of Jyväskylä, MATHEUS KINDBERG, Department of Physics, University of Jyväskylä, and the Center for Activated Electron Systems, Institute for Basic Science, Seoul National University, Seoul, Korea. — FePt nanoparticles (NPs) have attracted much attention recently for applications in high density recording media and catalysis. Usually the as-made FePt NPs are in the fcc phase and must be annealed at high temperatures to be converted to the L1(0) structure and because of this the particles agglomerate. In this paper, we used a novel fabrication method to directly prepare FePt NPs in fct phase on the surface of R-GO (Reduced Graphene oxide). A layered bimetallic precursor Fe(H2O)6[PtCl6] was mixed in water environment with exfoliated GO. The precipitates were annealed under a forming gas (5% H2 and 95% Ar)atmosphere at different temperatures varying from 500 °C to 950 °C. During the annealing process, the layered precursor [Fe(H2O)6][PtCl6] was reductively decompose directly to the L10 FePt crystal structure while the GO reduced by H2 atmosphere. Transmission electron microscopy (TEM) results showed that the FePt NPs have the L10 structure and a uniform size distribution with their average particle size in the range from 5 nm to 28 nm depending on the annealing temperature used. The fct particles had coercivity values in the range of 6 kOe-9 kOe. Furthermore, it is clear that the FePt nanoparticles are formed only on the surface of the graphene and no individual particles were observed off the graphene. The L10 FePt NPs are still isolated on the surface of the graphene and the particle size remains quite small (8 nm) even at annealing temperatures as high as 750 °C. Work supported by DOE-BES-DMSE (Grant No. DE-FG02-04ER4612).
1:39PM M30.00013 Effect of confinement on spin polarization and magnetism of Co$_2$Si nanoclusters$^1$, DAVID SELLMYER, BALAMURUGAN BALASUBRAMANIAN, PRIYANKA MANCHANDA, RALPH SKOMSKI, PINAKI MUKHERJEE, BHASKAR DAC, NCMN, University of Nebraska, Lincoln, NE 68588, GEORGE HADJIPANAYIS, University of Delaware, Newark, DE 19716 — Size-modified electronic structure and surface effects can lead to unusual magnetic ordering, modified ordering temperatures, and different spin structures in nanoclusters as compared to the corresponding bulk alloys. Thus nanoclusters can be used as building blocks to create new complex magnetic nanostructures for potential applications. We show room-temperature ferromagnetic ordering in Co$_2$Si nanoclusters with relatively large magnetic moments (0.49 $\mu_B$/Co at 300 K and 0.70 $\mu_B$/Co at 10 K) and magnetocrystalline anisotropy ($K_1 \approx 4$ Mergs/cm$^3$ at 10 K), as contrasted to very weak itinerant magnetism in bulk Co$_2$Si (0.001 $\mu_B$/Co at 300 K and 0.072 $\mu_B$/Co at 10 K). The DFT and analytical model calculations explain the size-dependence of the observed magnetic moments on the size of Co$_2$Si nanoclusters, which vary from 0.6 to 30 nm, by a surface-induced spin polarization of nanoclusters.

$^1$This research is supported by U.S. DOE-BES-DMSE (Grant No. DE-FG02-04ER46152) and NCMN.

1:51PM M30.00014 Magnetic properties of ternary and quaternary transition metal nanoclusters, JAIME SOUTO CASARES, JAMES CHELIKOWSKY, University of Austin at Texas — The magnetic properties of transition-metal nanostructures is a topic that has attracted much interest, mainly because of the dramatic difference that exists in comparison with the bulk. Without a proper knowledge of the fundamental mechanism behind the magnetic phenomena, it is hard to predict the properties of complex materials. We investigate the electronic and magnetic properties of nanoclusters made of ternary and quaternary compounds of transition metals (Fe, Co, and Ni) using PARSEC, a real-space implementation of pseudopotentials within density functional theory. Our code is well suited for the study of isolated structures because of its implementation of very efficient techniques for solving the Kohn-Sham equations. The real-space nature of PARSEC allows the use of proper boundary conditions, imposing the electronic wave functions to vanish outside a spherical domain. With these computational tools we can cover a wide spectrum of magnetic alloys and look for specific magnetic properties. This work is supported by NSF grant DMR 14-35219.


11:15AM M31.00001 Heat transport in the frustrated spin-ladder compound, BiCu$_2$PO$_6$$^1$, NARAYAN PRASAI, ALWYN REBELLO, JOSHUA L. COHN, University of Miami, SUELI H. MASUNAGA, JOHN J. NEUMEIER, Montana State University — We report measurements of thermal conductivity ($\kappa$) in the range 0.4 K $\leq T \leq$ 300 K for single-crystal BiCu$_2$PO$_6$, a recently discovered frustrated 2-leg spin-ladder compound. For heat flow both along and transverse to the spin ladders, $\kappa$ exhibits a broad maximum near 60 K, coinciding with a similar maximum reported in the magnetic susceptibility, and consistent with resonant phonon scattering from spin excitations with an energy scale 40-60 K. Anisotropy in $\kappa$, evidence for a spin contribution at low temperatures, and the influence of magnetic field will be discussed.

$^1$This material is based upon work supported by the U.S. Department of Energy Office of Basic Energy Sciences grant DE-FG02-12ER46888 (Univ. Miami) and the National Science Foundation under grant DMR-0907036 (Mont. St. Univ.).

11:27AM M31.00002 Evolution of magnetic excitations in BiCu$_2$PO$_6$ observed via magnetic suppression of phonon heat conduction, BYUNG-GU JEON, B., KOTESWARARAO, C.B. PARK, KEE HOON KIM, Seoul Natl. Univ., Korea, G.J. SHU, F.C. CHOU, Natl. Taiwan Univ., Taiwan, S.C. RIGGS, NHMFL, USA, S.B. CHUNG, IBS-CCES, Korea — We report the thermal conductivity of a frustrated spin ladder BiCu$_2$PO$_6$ under high magnetic field up to 30 T. At 0 T, strong suppression of the thermal conductivity is emerged around 15 K, leading a double-peak shape in the temperature-dependent thermal conductivity. Upon increasing the magnetic field, the suppression is further enhanced and shows a sharp dip in the magneto-thermal conductivity around the critical magnetic field. The anomalous, field-dependent thermal conductivity is interpreted as a resonance scattering of phononic heat carriers by magnetic excitations. From the analysis based on the transport theory, we successfully traced the magnetic field dependence of the magnetic excitation gaps up to 25 T.

11:39AM M31.00003 Stepwise orderings in anisotropically coupled spin ladders, SHUNSUKE FURUYA, THIERRY GIAMARCHI, Univ of Geneva — In low-dimensional quantum magnets, lowering the temperature, we can find phase transitions from lower to higher dimensional phases. The (unfrustrated) spin ladder is a good example to see such a change of the dimensionality because it occurs only under strong enough magnetic field. That is, the dimensionality in the coupled spin ladder system is controllable by means of the temperature and the magnetic field. In this presentation, we will discuss a cascade of the dimensionality from the 1D phase to the 3D ordered phase via a quasi-2D ordered phase and its interesting manifestation in stepwise temperature dependence of the order parameter. We presume two inequivalent interladder exchange interactions $J'_1$ and $J'_2$. The former connects spin ladders in a plane to form 2D layers and the latter connects those layers. For $0 < J'_2 \ll J'_1$, we would naively expect a very low critical temperature $T_c \rightarrow 0$ because quantum fluctuations prevents spontaneous breaking of continuous symmetries. However we would like to point out that it is not the case, that is, $T_c$ remains finite even for infinitesimal $J'_2$, leading to a sudden growth at a certain temperature $T_{cr}$ below $T_c$.
An extremely well-isolated 2D antiferromagnet

12:27PM M31.00005 An extremely well-isolated 2D antiferromagnet, CHRISTOPHER LAMDEE, NIZAR NAITLHO, Department of Physics, Clark University, M.M. TURNBULL, Carlson School of Chemistry, Clark University — We report on the synthesis, structure, and magnetic susceptibility of an extremely well-isolated rectangular Heisenberg, \( S = 1/2 \) antiferromagnet, \([\text{Cu}(pz)_2(4-\text{OHpy})_2](PF_6)_2\), where \( pz = \text{pyrazine} \) and \( 4-\text{OHpy} = 4\)-pyridine. The copper and pyrazine form nearly square layers of pyrazine-bridged copper(II) ions, with the pyridine molecules normal to the layers, coordinated to the copper sites by the oxygen. The distance between copper sites in adjacent layers is approximately 13 Å indicating a high degree of two-dimensionality. The magnetic susceptibility is best described by a model of an antiferromagnetic rectangle with the stronger and weaker interactions of 8.3 and 4.0 K, respectively. The compound is more symmetric than an analogous compound \([\text{Cu}(pz)_2(2\text{-OHpy})_2](\text{ClO}_4)_2\), reported previously [1].

12:27PM M31.00004 Temporal correlations in tunable Luttinger spin liquids, ANDREY ZHELudev, Laboratory for Solid State Physics, ETH Zurich, Switzerland — Landau’s theory of Fermi liquids, which is the cornerstone of our understanding of fermionic systems, breaks down in low dimensions. In one dimension, interacting fermions are in a quantum critical state with some fascinating universal thermodynamic properties and correlation functions. This particularly interesting case is quantitatively described by the so-called Luttinger liquid theory. The cleanest real-world realizations of this model are found in low-dimensional spin systems [1], such as in Heisenberg spin chain and ladder materials. The universal scaling relations in these Luttinger liquids have been studied both theoretically and experimentally. In this quest, neutron scattering has proven to be instrumental, as it provides direct access to spatial and temporal correlation functions. In classic previous studies [2,3], this technique has been employed to measuring finite-temperature scaling in the simplest spin chain models. The latter are described by Luttinger liquid theories with the so-called Luttinger parameter \( K=1/2 \), corresponding to a strong repulsion between particles. The new challenge is to investigate the scaling for other values of \( K \), particularly in systems with \( K>1 \) (attractive fermions). In experiments, \( K \) and other characteristics of Luttinger spin liquids can be, in principle, tuned continuously by the application of an external magnetic field. In practice, measurements under such conditions are extremely challenging due to several unexpected technical difficulties. Nevertheless, recent advances in neutron instrumentation, particularly at pulsed neutron sources, help overcome these obstacles. In my talk I shall review the most recent results of experimental studies of Luttinger liquid properties of low dimensional quantum magnets under high magnetic fields. I will cover spin chain materials where \( K \) is continuously tunable in the range \( 1/2< K <1 \), and the strong leg spin ladder compound DIMPY where \( K>1 \) was achieved for the first time [4-6]. I will also describe how residual 3-dimensional interactions, usually considered a nuisance for low-dimensional physics, can in certain cases be exploited to accurately measure the exact field-dependent values of all relevant one-dimensional Luttinger liquid parameters.

12:39PM M31.00006 Dynamics of a quasi-2D \( S = 1/2 \) spin-dimer Heisenberg antiferromagnet under hydrostatic pressure, GERARD PERREN, JOHANNES MOELLER, NSM group, ETH Zurich, Switzerland, DAN HUEVONEN, National Institute of Chemical Physics and Biophysics, Tallinn, Estonia, ANDREY ZHELudev, Oak Ridge National Laboratory, Oak Ridge, USA, ANDREY ZHELudev, NSM group, ETH Zurich, Switzerland — We present Inelastic Neutron Scattering measurements (INS) under hydrostatic pressure on a quasi-2D \( S = 1/2 \) spin-dimer Heisenberg antiferromagnet. At high pressure, the observed dynamic structure factor \( S(Q, \omega) \) features Goldstone modes, which is a key signature of long-range (magnetic) order. This is in good agreement with recent \( \mu\mathrm{SR} \) findings and the presence of a pressure-induced quantum critical point at a moderate pressure [1]. Furthermore, we suggest an explanation for an apparent contradiction with a previous INS study performed under similar conditions [2].

12:39PM M31.00004 Temporal correlations in tunable Luttinger spin liquids, ANDREY ZHELudev, Laboratory for Solid State Physics, ETH Zurich, Switzerland — Landau’s theory of Fermi liquids, which is the cornerstone of our understanding of fermionic systems, breaks down in low dimensions. In one dimension, interacting fermions are in a quantum critical state with some fascinating universal thermodynamic properties and correlation functions. This particularly interesting case is quantitatively described by the so-called Luttinger liquid theory. The cleanest real-world realizations of this model are found in low-dimensional spin systems [1], such as in Heisenberg spin chain and ladder materials. The universal scaling relations in these Luttinger liquids have been studied both theoretically and experimentally. In this quest, neutron scattering has proven to be instrumental, as it provides direct access to spatial and temporal correlation functions. In classic previous studies [2,3], this technique has been employed to measuring finite-temperature scaling in the simplest spin chain models. The latter are described by Luttinger liquid theories with the so-called Luttinger parameter \( K=1/2 \), corresponding to a strong repulsion between particles. The new challenge is to investigate the scaling for other values of \( K \), particularly in systems with \( K>1 \) (attractive fermions). In experiments, \( K \) and other characteristics of Luttinger spin liquids can be, in principle, tuned continuously by the application of an external magnetic field. In practice, measurements under such conditions are extremely challenging due to several unexpected technical difficulties. Nevertheless, recent advances in neutron instrumentation, particularly at pulsed neutron sources, help overcome these obstacles. In my talk I shall review the most recent results of experimental studies of Luttinger liquid properties of low dimensional quantum magnets under high magnetic fields. I will cover spin chain materials where \( K \) is continuously tunable in the range \( 1/2< K <1 \), and the strong leg spin ladder compound DIMPY where \( K>1 \) was achieved for the first time [4-6]. I will also describe how residual 3-dimensional interactions, usually considered a nuisance for low-dimensional physics, can in certain cases be exploited to accurately measure the exact field-dependent values of all relevant one-dimensional Luttinger liquid parameters.

12:51PM M31.00007 Magnetic phase diagram of the spatially anisotropic spin-1/2 zigzag ladder, MOHAMMAD SOLTANIEH-HA, ADRIAN FEIGUIN, Northeastern University — We study the magnetic phase diagram of a spatially anisotropic zigzag ladder with exchange interactions \( J_z \) and \( J_x^\prime \) along the legs. This system interpolates between the conventional \( J_1-J_2 \) chain, and the “sawtooth,” or “delta” chain, described by a linear arrangement of triangles. Both systems display dimerization in a region of the zero-field phase diagram, but the anisotropy leads to two excitations with different velocities. We study the magnetic phase diagram of the system as a function of \( J_z \) and \( J_x^\prime \) and find commensurate plateaus at \( m = 1/2 \) and \( m = 1/3 \), and study the competition between different orders, including incommensurate, chiral, polar, and two-component liquid phase.

1:03PM M31.00008 Symmetry protected topological states in antiferromagnets with magnetic field, SHINTARO TAKAYOSHI, National Institute for Materials Science, KEISUKE TOTSUKA, Yukawa Institute for Theoretical Physics, Kyoto University, AKIHIRO TANAKA, National Institute for Materials Science — A symmetry protected topological (SPT) phase is a short-range entangled state that cannot be adiabatically deformed into a direct product state under some symmetry. We show that magnetization plateau states of one-dimensional antiferromagnets in external magnetic field is in an SPT phase when \( S - m \) is odd, where \( S \) and \( m \) represent a spin quantum number and magnetization per site, respectively, if the system respects a bond-center inversion symmetry. We map the antiferromagnets into a field theory of a nonlinear sigma model with a Berry phase term which has a coefficient proportional to the quantity \( S - m \). This term appears in the functional form of the ground state wave function and dictates whether or not the system is in the SPT phase. We verify this prediction through numerical calculations of the entanglement spectra and an analysis using a matrix product state representation.

1:15PM M31.00009 Detailed analysis of critical points in coupled spin dimer systems, DOMINIK STRASSEL, Univ. of Kaiserslautern, PETER KOPIETZ, Univ. of Frankfurt, SEBASTIAN EGGERT, Univ. of Kaiserslautern — Spin dimer systems are a promising playground for the detailed study of quantum phase transitions. In many cases it is sufficient to use the magnetic field as the tuning parameter in order to reach interesting non-trivial critical points and observe a crossover from the characteristic scaling near the critical point to the behavior of a finite temperature phase transition. In order to quantitatively demonstrate those effects and inspired by recent experiments we have started large scale quantum Monte Carlo simulations in order to analyze several different physical quantities in spin dimer systems, namely the susceptibility, the magneto-caloric effect, and the spin stiffness. We discuss in detail how the phase transitions (quantum and finite temperature) are manifest in the characteristic scaling behavior near critical points by comparing them with interacting boson theories. For two dimensional systems the predicted logarithmic corrections cannot be observed, however.

Supported by OPTIMAS and the Deutsche Forschungsgemeinschaft via the SFB/TR49
1:27PM M31.00010 Magnetization Plateaux in a frustrated spin ladder, TAKANORI SUGIMOTO, Tokyo Univ of Science, MICHIMARU IGAMI, Japan Atomic Energy Agency, TAKAMI TOHYAMA, Tokyo Univ of Science, SADAMICHI MAEKAWA, Japan Atomic Energy Agency — Recently, successive phase transitions induced by magnetic field have been observed in BiCu\(_{2}\)PO\(_4\), whose effective spin model, a frustrated two-leg spin ladder, bridges between the frustrated spin chain and the non-frustrated spin ladder with one-half spins. According to theoretical studies, the frustrated spin chain exhibits one third plateau, although no plateau emerges in non-frustrated spin ladders. Therefore, a simple question arises as to whether the plateaux do appear in the frustrated spin ladder, or not. To clarify this question, we calculate the magnetic-field dependence of magnetization by using density-matrix renormalization-group method. In this calculation, we find some plateaux, which appear in neither the frustrated spin chain nor the non-frustrated spin ladder. Our study is useful to analyze experimental data of BiCu\(_{2}\)PO\(_4\).

1:39PM M31.00011 Fractional excitations in the square-lattice quantum antiferromagnet, H.M. RÖNNOW, EPFL Lausanne, M. MOURILGA, Georgia Institute of Technology, B. DALLA PIAZZA, EPFL Lausanne, N.B. CHRISTENSEN, Technical University of Denmark, G.J. NILSEN, Institut Laue-Langevin, T.G. PERRING, Rutherford Appleton Laboratory, M. ENDERLE, Institut Laue-Langevin, D.F. MCMORROW, University College of London, D.A. IVANOV, ETH Zurich and University of Zurich — The quantum square-lattice Heisenberg antiferromagnet (QSLHAf) exhibits a strongly anomalous magnetic spin spectrum. This question manifests itself in excitations propagating with the specific wavevector (\(\pi/2\),\(\pi\)). We used polarized neutron spectroscopy to fully characterize the magnetic fluctuations in the metal-organic compound Cu\(_4\)(DCCO\(_2\))\(_2\)\(4\)D\(_2\)O (CFTD), a known realization of the QSLHAF model. Our experiments reveal an isotropic excitation continuum at the anomaly, which we analyse theoretically using Gutzwiller-projected trial wave functions [1]. The excitation continuum is accounted for by the existence of pairs of fractional S = 1/2 quasiparticles that deconfine over intermediate length-scales. Away from the anomalous wavevector, these fractional excitations are bound and form conventional magnons. Our results reveal the existence of fractional quasiparticles in the high-energy spectrum of a quasi-two-dimensional antiferromagnet, even in the absence of frustration. [1] B. Dalla Piazza et al., to appear in Nature Physics (December 2014)

1:51PM M31.00012 Generalization of Magnetic Dimer Excitations, G. HOUCHINS, J.T. HARALDSEN, Department of Physics and Astronomy, James Madison University — Magnetic dimers commonly appear in the study of molecular magnets and quantum dots. Here, we discuss analytical representations for the inelastic neutron scattering excitation cross sections and static structure factor for the general S\(_2\)\(4\)\(_2\) dimeric system. Employing generalized Pauli matrices and the Kronecker tensor product to construct the matrix representation of the spin Heisenberg spin-spin Hamiltonian. After using exact diagonalization to determine the eigenstates of the spin Hamiltonian, we formulated an analytical solution to find the structure factor coefficients used in determining the inelastic neutron scattering excitation cross section from both the ground state and first excited state. We also detail a method for finding the S\(_2\) polarization constant within an applied field that may represent the presence of an external magnetic field. Furthermore, we provide a sample set of data and intensity plot generated from our results to illustrate experimental representations for split energy levels.

2:03PM M31.00013 ABSTRACT WITHDRAWN —

Wednesday, March 4, 2015 11:15AM - 2:15PM —
Session M32 GMAG DMP: Focus Session: Multiferroics II and Other 3d Transition Metal Oxides

11:15AM M32.00001 Imaging and characterization of conducting ferroelectric domain walls by photoemission electron microscopy, JAKOB SCHAAAB, ETH Zurich, INGO KRUG, TU Berlin, ZEWU YAN, EDITH BOURRET, Lawrence Berkeley National Laboratory, CLAUS SCHNEIDER, FZ Juelich, RAMAMOORTHY RAMESH, UC Berkeley, DENNIS MEIER, ETH Zurich — Unusual electronic properties arise at ferroelectric domain walls due to the low local symmetry and hypersensitivity of these natural oxide interfaces to electrostatics and strain. A major challenge is to expand the experimentally accessible parameter space in order to better understand these interfacial phenomena and ultimately exploit them to design domain-wall-based next-generation devices. Here, we show that ferroelectric domain walls can be visualized based on photo-induced charging effects using high-resolution X-ray photoemission electron microscopy (X-PEEM). We probe local variations in the electronic conductance in the ferroelectric semiconductor ErMnO\(_3\) contact-free and with nanometer resolution by mapping the kinetic energy distribution of photoelectrons. We find a pronounced domain-wall contrast which we assign to the local conductivity by a direct comparison with scanning probe microscopy data. Our experiments reveal a new and non-destructive pathway for element-specific studies of electronic and chemical domain-wall structures in ferroelectric and multiferroic bulk systems.

11:27AM M32.00002 Magnetochiral dichroism resonant with electromagnons in a chiral-lattice magnet Cu\(_2\)OSeO\(_3\), YOSHIHIRO OKAMURA, Univ. of Tokyo, FUMITAKA KAGAWA, SHINICHIRO SEKI, MASASHI KAWASAKI, RIKEN Center for Emergent Matter Science (CEMS), YOSHINORI TOKURA, Univ. of Tokyo, UNIV. OF TOKYO TEAM, RIKEN CENTER FOR EMERGENT MATTER SCIENCE (CEMS) COLLABORATION, POWER ELECTRONICS R&D UNIT, ROHM CO., LTD. COLLABORATION — Multiferroics, in which magnetic and ferroelectric properties coexist and are entangled, is one of the most promising candidates for materials that are capable of the control of the magnetization (M) by an electric field and the electric polarization (P) by a magnetic field. One direct consequence of the strong magnetoelectric (ME) coupling in multiferroics is an intriguing spin excitation endowed with electric-dipole activity. This remarkable spin excitation, termed as electromagnon, is ubiquitously found in multiferroics. In this study, we performed broadband microwave spectroscopy under magnetic fields in Faraday geometry to study the ME resonant character of the electromagnon in a multiferroic chiral-lattice magnet Cu\(_2\)OSeO\(_3\). We successfully observed different transmittance for oppositely propagating microwaves upon the electromagnon—the behavior known as magnetochiral dichroism (MChD). By studying the MChD spectra for various configurations, we elucidate the relationship between the MChD spectra and the dynamics of M and P upon the electromagnon excitation. We also discuss the magnitude of the MChD within a quantum theory and find that the theory well reproduces the experiment.

11:39AM M32.00003 Giant thermal Hall effect in polar magnets (Zn,Fe)\(_2\)Mo\(_3\)O\(_8\), TOSHIYA IDEUE, TAKASHI KURUMAJI, HOSHO KATSURA, SHINTARO ISHIWATA, Univ. of Tokyo, NAOTO NAGAOSA, YOSHINORI TOKURA, Univ. of Tokyo, RIKEN CENTER for Emergent Matter Science (CEMS), DEPARTMENT OF APPLIED PHYSICS, UNIVERSITY OF TOKYO TEAM, DEPARTMENT OF PHYSICS, UNIVERSITY OF TOKYO COLLABORATION, RIKEN CENTER FOR EMERGENT MATTER SCIENCE (CEMS) COLLABORATION — Spin transport in magnetic insulators has been attracting much attention because of the fundamental and technological interest for future spintronics. Recently we have observed Hall effect of magnons in ferromagnetic insulators with pyrochlore and perovskite structures in terms of the thermal Hall effect. Observed thermal Hall conductivity can be well explained by the Berry curvature of magnons induced by the Dzyaloshinsky-Moriya spin-orbit interaction which reflects the lattice geometry, while the magnitude of the signal is small and Hall effects in other magnetic phases have been unknown. In this work, we have studied thermal Hall effect in magnetic insulators (Zn,Fe)\(_2\)Mo\(_3\)O\(_8\). (Zn,Fe)\(_2\)Mo\(_3\)O\(_8\) has the polar crystal structure and shows various magnetic phases by changing the composition ratio of Fe and Zn or by applying the magnetic field. We have observed giant thermal Hall effect in ferrimagnetic phase in which the thermal Hall conductivities are twenty times larger than those of the magnon Hall effect observed in the previous study. We discuss possible mechanism of the large thermal Hall effect in this systems.
12:39PM M32.00008 Carrier Mediated Ferromagnetism in Fe-doped SrTiO$_3$.

CHUN-LAN MA, School of Mathematics and Physics, Suzhou University of Science and Technology, Suzhou 215009, China, ROCIO CONTRERAS-GUERRERO, RAVI DROOPAD, Ingram School of Engineering, Texas State University, San Marcos, TX 78666, USA — The discovery of III-V dilute magnetic semiconductors (DMS) and the subsequent unsuccessful search for room temperature ferromagnetism in DMSs have motivated researches on alternate dilute magnetic systems. Recent progresses in thin film growth techniques of perovskite oxides suggest that dilute magnetic oxides (DMOs) can be viable candidates to improve the magnetic properties of DMSs. In this talk we present an ab initio study of Fe-doped SrTiO$_3$. We find that a ferromagnetic ordering among localized Fe $t_{2g}$ spins is mediated by itinerant Fe $e_g$ electrons. The exchange interaction between $t_{2g}$ and $e_g$ electrons depends on crystal field splitting, on-site electron-electron interaction, and the relative energy of Fe d-orbitals to oxygen p-orbitals. The exchange coupling and the majority-minority spin splitting decrease with decreasing carrier concentration, confirming that itinerant carriers mediate the ferromagnetism.

C. Ma is supported by NSF of China (Grant Nos. 11247023 and 11304218), Jiangsu Qing Lan Project, and Jiangsu Overseas Research & Training Program. R.-C.-G., and B.L. are supported by AFOSR, award number FA9550-10-1-0133.

12:51PM M32.00009 Spin waves and phonons in a paraelectric antiferromagnet EuTiO$_3$.

HUIBO CAO, JIANGWANG HONG, OLIVIER DELAIRE, STEVEN HAHN, GEORG EHLERS, SONGXUE CHI, VASILE GARLEA, JAIME FERNANDEZ-BACA, BRYAN CHAKOUMAKOS, JIAQIANG YAN, BRIAN SALES, Oak Ridge National Laboratory — Perovskite titanates ATiO$_3$ (A=Ba, Pb, Sr, Ca, Cd, or Eu) are widely studied for their interesting instabilities and broad applications. A ferroelectric (FE) transition occurs in Ba, Pb, and Cd titanates, but not in SrTiO$_3$ (STO) or EuTiO$_3$ (ETO). In the case of STO, fluctuations yield a quantum paraelectric state, but whether ETO is quantum paraelectric remains an open question.

Despite a number of similarities with well-studied STO, ETO is also unique owing to the magnetic Eu ions. By applying a tuning parameter, such as bi-axial tension, ETO can be turned into a FE ferromagnet, the ideal multiferroic. [J. H. Lee, et al., Nature 466, 954 (2010)]

Spin-phonon and spin-lattice couplings in ETO are of great interest not only from a fundamental standpoint, but also for technological applications. We successfully grew a large, high-quality isotopically-enriched ETO crystal for neutron scattering. The crystal and magnetic structures were characterized with single crystal diffraction at HB-3A at HFIR at ORNL and with neutron diffraction at ORNL. In this presentation, we will discuss structural instabilities, spin-spin interactions, and spin-phonon couplings in ETO.

This work was supported by Office of Basic Energy Sciences, U.S. Department of Energy.
1:03PM M32.00010 Changes in magnetic properties of cobalt-iron-titanium oxide due to temperature variations1. CAJETAN NLEBEDIM2, Ames Laboratory, U.S. Department of Energy, DAVID JILES1, Department of Electrical and Computer Engineering, Iowa State University. — It has been found that the magnetic properties of cobalt ferrite such as magnetization, Curie temperature, including the electrical and structural properties can be tailored in a remarkably linear pattern by substituting titanium and controlling its concentration. The dependence of magnetocrystalline anisotropy and coercivity on temperature variations was found to be different compared to previous studies on cation substitution in cobalt ferrite. For example, we found a competition between magnetocrystalline anisotropy and microstructure in controlling coercivity; one dominating at higher concentration of substitution and the other dominating at lower concentration. It was also found that, while magnetocrystalline anisotropy controls the temperature dependence of coercivity, obstruction to domain wall processes by pinning sites in the microstructure controls the compositional dependence of coercivity. The physics of magnetism controlling the observed properties and how those depend on temperature variations will be presented. Such understanding is necessary for the application of the material in device development.

1This work was supported by the USDOE, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. The research was performed at Ames Laboratory, operated for the U.S. DOE by Iowa State University (contract #DE-AC02-07CH11358).

2Also affiliated to Department of Electrical and Computer Engineering, Iowa State University

1:15PM M32.00011 The impact of small polaronics on the properties of rare-earth titanates1. CHRIS VAN DE WALL, LARS BJAALIE, BURAK HİMMETOĞLU, ANDERSON JANOTTI, Materials Department, Univ. of California - Santa Barbara. — Optical conductivity measurements are frequently applied to determine the band gaps of complex oxides, such as the rare-earth titanate (RTIO₃) Mott insulators. The onset of the measured spectra, in the range of 0.2-0.7 eV, is commonly interpreted as the Mott-Hubbard gap. However, first-principles calculations that take strong electron-electron interactions into account using either density functional theory (DFT) with a hybrid functional or DFT+U) produce band gaps close to 2 eV for GdTiO₃ and YTiO₃ [Hümmeroglu et al., Phys. Rev. B 90, 161102 (2014)]. This raises the question of the origin of the absorption below 2 eV observed in optical experiments. We attribute this signal to excitation of small hole polarons. The rare-earth titanates commonly exhibit unintentional p-type conductivity, and we show that hole localization in the form of small polarons is enabled by the combined electron-configuration-strains enable us not only to assess the peak in optical absorption, but also to model the lineshape. Good agreement with experiment indicates that the infrared absorption is indeed likely to be polaron-related in GdTiO₃. The results probably apply to other rare-earth titanates as well.

1Work supported by NSF, ARO and ONR.

1:27PM M32.00012 Twofold spin reorientation and field induced incomplete phase transition in single crystal Dy₀.₅Pr₀.₅FeO₃. SHIXUN CAO, WEI REN, XIAOLING QIN, BAOJUAN KANG, JINCAIZHANG, Shanghai University. — Recently, rare earth orthoferrites show emerging magnetoelectric effect, ultrafast optomagnetic effect, promising applications in multiferroics and ultrafast optomagnetic recording. All these properties come from its intrinsic coupling between R-4f and Fe-3d electrons, and strongly correlated with the spin reorientation (SR) transition. We report an intriguing twofold SR transition for the Fe magnetic sublattice near room temperature TSRI=77 K and TSR2=45 K in Dy₀.₅Pr₀.₅FeO₃ single crystal. Magnetic field-induced incomplete spin configuration transition was observed by measurement of magnetization as a function of temperature. The SR temperature of Dy₀.₅Pr₀.₅FeO₃ single crystal can be controlled by changing the magnitude of the applied magnetic field. We also show that SR between TSR2 and TSR1 can be induced by an applied magnetic field along c-axis. The origin of the magnetic behavior is ascribed to the anisotropic effective field whose strength is determined by the interactions with rare-earth spins and can be modified by the external applied magnetic field. It provides deeper insights into the R-4f and Fe-3d magnetic interaction which dominate the sophisticated magnetic phase transitions in the rare earth orthoferrites.

1This work is supported by the National Natural Science Foundation of China (NSFC, Nos. 51352149, 50932003, 11274222).

1:39PM M32.00013 A-site magnetic ordering in quadruple perovskite oxides, MASAYUKI TOYODA, CREST, Japan Science and Technology Agency, KUNIHKO YAMAUCHI, ISIR, Osaka University, TAMIO OGUCHI, CREST, Japan Science and Technology Agency. — In the crystal structure of perovskites AA'ₓBₓO₃ is comprehensively investigated by using first-principles calculations. The ideal crystal structure (Im3) is characterized by the square-planer oxygen coordination around A' cations as well as the a²+a⁴ type tilting of BO₆ octahedra. Owing to these structural features, the compounds can include transition-metal ions both at the A' and B sites. Consequently, there are two magnetic sublattices with different oxygen coordination. Unlike the B-site magnetism that has been investigated for decades, detailed mechanisms for the A'-site magnetism and A'-B intersublattice magnetism are still unclear. In insulating compounds such as CaₓLaₓGeO₃ and YₓMnₓAl₂O₁₂, it is found that the nearest-neighbor superexchange interaction between the A' sites determines the ground-state magnetic ordering. Furthermore, in our simulation, it is shown that magnetic phase transition from antiferromagnetism to ferromagnetism will occur along with insulator-to-metal transition in YMnₓAl₂O₁₂ by modulating the tilting of AlO₆ octahedra. Possible strategies are suggested to realize such a modulation, for example, by imposing chemical or physical pressure.

1:51PM M32.00014 Looking for multiferroics through oxygen deficiency in Sr₄₋ₓ(FeₓCoₓ)O₃₋₄₋δ, JUAN MANUEL FLOREZ, Technical University Federico Santa Maria (Chile) and MIT, MEHMET CENGIZ ON-BASLI, DONG HUN KIM, MIT (USA), SHYUE PING ONG, University of California at San Diego, GERBRAND CEDER, MIT (USA), PATRICIO VARGAS, Technical University Federico Santa Maria (Chile), CAROLINE A. ROSS, MIT (USA) — We present a theoretical/experimental study of Sr₄₋ₓ(FeₓCoₓ)O₃₋₄₋δ magnetic perovskites obtained by solid solution of Fe and Co into SrTiO₃. We focus on the role of the oxygen deficiency as the factor triggering both a change of the saturation magnetization and the appearance of a macroscopic electric polarization. The magnetization is analyzed by calculating the t₂g⁵e₈ occupations of the magnetic levels as well as the same for the electric polarization. The electric polarization is calculated through the noncentrosymmetric resulting structures generated by the intrinsic strain related to the oxygen holes and changes of the ions radii. The optical properties are quantified by calculating the total and projected density of states while we take into account all the possible configurations of the O-vacancies respect to the noncentrosymmetric resulting structures generated by the intrinsic strain related to the oxygen holes and changes of the ions radii. The optical properties are quantified by calculating the total and projected density of states while we take into account all the possible configurations of the O-vacancies respect to the noncentrosymmetric resulting structures generated by the intrinsic strain related to the oxygen holes and changes of the ions radii. The optical properties are quantified by calculating the total and projected density of states while we take into account all the possible configurations of the O-vacancies respect to the noncentrosymmetric resulting structures generated by the intrinsic strain related to the oxygen holes and changes of the ions radii.

2:03PM M32.00015 Electronic structure of Fe₃O₄ revealed by RIXS, HSIAO-YU HUANG, Doctor Program of Science and Technology of Synchrotron Light Source, National Tsing Hua University, Hsinchu 30011, Taiwan, RU-PAN WANG, Department of Chemistry, Utrecht University, Utrecht, Netherlands, CHIEN-TE CHEN, National Synchrotron Radiation Research Center, Hsinchu 30076, Taiwan, JIANSHI ZHOU, Department of Mechanical Engineering, Texas Material Institute, The University of Texas at Austin, Texas 78712, USA, FRANK DE GROOT, Department of Chemistry, Utrecht University, Utrecht, Netherlands, CHUN-CHU LAI, Department of Chemistry, National Synchrotron Radiation Research Center, Hsinchu 30076, Taiwan — Magnetite (Fe₃O₄) is a prototypical example of a mixed valence compound. At 125 K, Fe₃O₄ undergoes the Verwey transition associated with charge ordering. The valence electrons order themselves over the octahedral sites (B sites) to form a Fe⁴⁺ and Fe³⁺ superstructure in the insulating phase below the transition temperature. Here we report measurements of resonant inelastic x-ray scattering (RIXS) to unravel the electronic structures of Fe₃O₄. By the advantage of high energy-resolution (∆E ≈ 80 meV) of the RIXS spectra, we found two distinctive features of magnetic excitations, coming from octahedral Fe²⁺ and Fe³⁺ separately. These magnetic excitations are described well by a local ionic model. The dd excitations of the different Fe sites are also revealed in the RIXS spectra.
11:15AM M33.00001 Chemical Physics and Properties of ThPt$_2$, ANDREAS LEITHE-JASPER, MPI-CPfS Dresden, ROMAN GUMENIUK, MPI-CPfS Dresden and TU Bergakademie Freiberg, WALTER SCHNELLE, MICHAEL NICKLAS, YURI GRIN, MPI-CPfS Dresden — ThPt$_2$ crystallizes with a unique type of structure (space group $I4/mmm$, $a = 4.1690(2)$ Å, $c = 14.3678(6)$ Å), which belongs to the group of the close-packed tetragonal structures (Pearson symbol $I12$). An analysis of the chemical bonding by the electron density/electron localization approach reveals formation of two-dimensional platinum anions separated by the Th cations. Measurements of magnetic susceptibility, electrical resistivity and specific heat show ThPt$_2$ to be diamagnetic with good metallic conductivity ($\rho$($300 \text{ K}$) ≈ 8.5 µΩ cm). The properties are in good agreement with the calculated electronic structure with a low DOS ($N(E_F) = 0.92$ states eV$^{-1}$ fm$^{-3}$). The stability of the compound with respect to other possible structural modifications was studied theoretically.

11:27AM M33.00002 Entanglement changes and caloric effects in $RAI_2$ single crystals, NILSON ANTUNES DE OLIVEIRA, JULIETH CARO PATIÑO, PEDRO J. VON RANKE, Universidade do Estado do Rio de Janeiro — In this work we theoretically discuss the entanglement changes and the caloric effects in $RAI_2$ single crystals, which crystallize in the cubic symmetry and have large magneto crystalline anisotropy due to the crystal electric field. For this purpose, we use a model of interacting magnetic moments including a term to account for the crystal electric field. We apply the model to calculate the entropy changes and the magnetocaloric quantities in TmAl$_2$ and NdAl$_2$ by applying magnetic field variations in different crystallographic directions. Our calculations for the entropy changes in these compounds are in a reasonable agreement with the available experimental data for $\Delta S$ at $T = 10$ K. Further experimental data are necessary to compare with our theoretical predictions for the adiabatic temperature change. We also calculate the caloric quantities by fixing the magnitude of the magnetic field and rotating its direction. In this case, our calculations predict an anomaly (i.e. a change of sign) in the caloric quantities of TmAl$_2$ when a magnetic field of 3 T rotates from $< 100 >$ to $< 110 >$ direction. A similar behavior is also observed in NdAl$_2$. This very interesting fact, which is basically due to the magneto crystalline anisotropy, needs experimental data to be confirmed.

11:39AM M33.00003 First-principles molecular dynamics simulations of high-concentration deuterium implantation in liquid lithium, MOHAN CHEN, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ, 08544, USA, TYLER ABRAMS, MICHAEL JAWORSKI, Princeton Plasma Physics Laboratory, Princeton, NJ, 08543, USA, EMILY CARTER, Department of Mechanical and Aerospace Engineering, Program in Applied and Computational Mathematics, and the Andlinger Center for Energy and the Enviro — First-principles molecular dynamics (FPMD) is performed to study liquid lithium (Li) samples with high-concentration deuterium (D) implantation. First, we validate FPMD against experimental properties of solid and liquid Li and LiD. The calculated properties of both Li and LiD include relative stabilities and bulk moduli of several solid phases, melting temperatures, pair distribution functions, and bond angle distribution functions. Excellent agreement is obtained between FPMD and available experimental data. Next, we randomly implant D atoms at four different concentrations into liquid Li at different temperatures. Specifically, the ratios of D:Li atoms studied are 0.25, 0.50, 0.75 and 1.00, and the temperatures range from 400 to 1143 K. FPMD reveals several interesting properties of these liquid Li samples with implanted D atoms. For example, we observe fast nucleation of rock-salt structures of LiD for samples at temperatures lower than the melting point of LiD (960 K). We find that the pure Li component is quickly suppressed with increased concentration of D atoms, and that no D clusters form. Finally, because measured diffusivities of D in liquid Li vary by several orders of magnitude, we predict the diffusivities of both Li and D atoms in all samples.

11:51AM M33.00004 Spin-phonon interactions to control the thermal transport in uranium dioxide, K. GOFRYK, Idaho National Laboratory, S. DU, C.R. STANEK, J.C. LASHLEY, X.-Y. LIU, R.K. SCHULZE, J.L. SMITH, D.J. SAFAIRK, D.D. BYLER, K.J. MCCLELLAN, B.P UBERUAGA, B.L. SCOTT, D.A. ANDERSSON, Los Alamos National Laboratory — Despite more than sixty years of intense research of uranium dioxide, a thorough understanding is lacking for the microscopic processes that control its transport and thermodynamic properties. In particular, it is not clear how different degrees of freedom and quasiparticle excitations interact and what is the relationship to the thermal behavior. We report our new experimental and theoretical studies on oriented and well characterized single crystals of uranium dioxide. Our results indicate that strong spin-phonon coupling and resonant scattering are important for understanding the general thermal behavior, and also explains the observed anisotropy in thermal conductivity by coupling to the applied temperature gradient and breaking cubic symmetry. We will discuss implications of these results.

12:03PM M33.00005 Simulating Order Parameters for Phase Transitions in Alloys, RICHARD R. VANFLEET, CONRAD W. ROSENROCK, GUS L.W. HART, BRANTON J. CAMPBELL, Department of Physics and Astronomy, Brigham Young University Provo — When determining the structure of alloys using diffraction patterns, possible distortions that lower the symmetry of the parent phase can be limited by group-theoretical arguments as long as a group-subgroup relationship exists between the parent and distorted phases. Order parameters are vectors in representation space where each dimension corresponds to a specific superlattice vector in reciprocal space (e.g. $L = [0.5,0.5,0.5]$ or $X=[1,0,0]$); such order parameters determine the distortions that may arise during a phase transition. By measuring the Fourier transform of the structure at each relevant superlattice vector during a Monte Carlo simulation for CuPt$_2$, we were able to extract these thermodynamic order parameters and qualitatively confirm distortions in the L and X order parameters observed in experiment. The methodology presents a highly effective avenue for comparing simulated phase transitions with experimental results.

12:15PM M33.00006 Concentration Waves in High-Entropy Alloys - a new alloy design approach, PRASHANT SINGH, Ames Lab, DUANE D. JOHNSON, Ames Lab and Iowa State University — Chemical short-range order (SRO) in solid solutions can be interpreted as a “concentration wave” — a Fourier decomposition of nascent order — identified experimentally via Warren-Cowley SRO parameters. We present a rigorous thermodynamic theory to predict and uniquely interpret the SRO in N-component alloys. Based on KKR-CPA electronic structure, we implemented this method using thermodynamic linear-response to include all alloying effects, e.g., band-filling, hybridization, Fermi-surface nesting and van Hove instabilities. We apply this first-principles method to high-entropy alloys (HEAs), i.e., solid solutions with N > 4 that inhibit small-cell order due to large entropy competing against ordering enthalpy, as their properties are sensitive to SRO. We validated theory with comparison to experiments in A2 Nb-Al-Ti and A1 Cu-Ni-Zn. We then predict and analyze SRO and mechanical trends in Ni-Ti-Zr-Cu-Al and Co-Cr-Fe-Mn-Ni systems — showcasing this new first-principles-based alloy design method.
12:27PM M33.00007 Magnetic Landau free energy density for the bcc-hcp phase transformation , MAHDI SANATI, Texas Tech Univ, ROBERT C. ALBERS, TURAB LOOKMAN, AVADH SAXENA, Los Alamos National Lab. — We have studied the he bcc-hcp phase transformation in Fe and Co with the use of first-principles calculations. The complete energy surface as the system goes from the bcc to hcp structure is determined. The results are used to find an appropriate Landau free energy (LFE) density for describing this transformation. The Landau free energy consists of three order parameters: shear, shuffle, and magnetization. The coefficients of the Landau free energy density are obtained from first-principles energy fits. The stability of the bcc phase in both elements has been studied and the results are then extended to understand the stability of the bcc Fe-Co alloys with varying stoichiometry.

12:39PM M33.00008 Vibrational entropy changes the solid solubility of a random alloy at high temperatures1 , NINA SHULUMBA, Linköping University Sweden, OLLE HELLMAN, California Institute of Technology USA, ZAMANAAN RAZA, Linköping University Sweden, JENIFER BARRIRERO, FRANK MÜCKLICH, Saarland University Germany, IGOR A. ABRIKOSSOV, MAGNUS ODÉN, Linköping University Sweden — We have developed a method to accurately and efficiently determine vibrational entropy as a function of temperature and volume for substitutional alloys from first principles. Using Ti1−xAlxN metal alloy as a model system we calculate the isostructural phase diagram by minimization of the free energy, solving the original Gibbs problem of finding its global minimum corresponding to the true equilibrium state of the system. We demonstrate that the vibrational contribution to the free energy has a decisive impact on the calculated phase diagram of Ti1−xAlxN alloy, lowering the maximum temperature for the miscibility gap from 9000 K to 2400 K. The solubility limit of the predicted phase diagram is experimentally verified by local chemical composition measurements of thermally aged Ti50Al50N alloys.

1:03PM M33.00010 Excited-state electron-dynamics probed by Alg phonons in Bi, Sb, and Bi2Te3 , CRYSTAL BRAY, Stanford University, PULSE Institute, EAMONN MURRAY, Tyndall National Institute, Cork, Ireland, STEPHEN FAHY, Tyndall National Institute; University College Cork, Ireland, DAVID REIS, Stanford University, PULSE Institute — We report on dynamics of photo-excited electronic states in bismuth, antimony and bismuth telluride as a function of photon energy and carrier density using the coherent A1g phonon as a probe. Previous National Institute; University College Cork, Ireland, DAVID REIS, Stanford University, PULSE Institute — We report on dynamics of photo-excited electronic states in bismuth, antimony and bismuth telluride as a function of photon energy and carrier density using the coherent A1g phonon as a probe. Previous studies have shown that the coherent dynamics of these materials are strongly coupled to the A1g phonon modes. We have observed a variety of dynamical processes including interband transitions, intraband excited state interactions and phonon-assisted transitions. In this work we present a detailed analysis of the coherent phonon dynamics in Bi, Sb and Bi2Te3, focusing on the excited state electron dynamics probed by the coherent A1g phonon. The results are compared to theoretical calculations to understand the underlying physical mechanisms.

1:15PM M33.00011 Hydrodynamics of Dirac and Weyl materials , GUSTAVO MONTEIRO, ALEXANDER ABANOV, Stony Brook University, V. PARAMESWARAN NAIR, City College of New York — The study of transport in Weyl and Dirac metals should account for additional contributions to the electric current coming from the chiral anomaly, namely chiral magnetic and chiral vortical effects. These responses are non-dissipative and fully characterized by the chiral anomaly coefficient. In addition, they are believed to be robust even in a strongly interacting regime, due to the topological nature of the anomaly. The fundamental equations for the hydrodynamic limit of such transports were introduced in [1], in order to describe the quark-glue plasma in nuclear collision. Having these equations as starting point, we present a variational principle for them and discuss the canonical structure of the corresponding hydrodynamic modes [2].


1:27PM M33.00012 Electronic properties and electron-phonon interaction in complex, multi-component alloys in application to high-entropy alloys , GERMAN SAMOLYUK, Oak Ridge National Laboratory, MARKUS DAENE, Lawrence Livermore National Laboratory, GEORGE MALCOLM STOCKS, Oak Ridge National Laboratory, JOSE ALFREDO CARO, Los Alamos National Laboratory, JAGER STOLLER, Oak Ridge National Laboratory — High-entropy alloys (HEAs) have recently been developed as nontraditional alloy systems. They are composed of multiple elements at or near equiatomic ratios that form random solid solutions on simple underlying fcc or bcc lattices. In recent years HEAs have attracted significant attention due to their high strength, ductility and possible high radiation resistance. The complexity of the alloys results in very interesting electronic system behavior. Even in thermal equilibrium, disorder, especially extreme disorder, has important impacts on all electronic, atomic, and magnetic properties. In the current work we present results of first-principles investigation of the electronic and magnetic properties of Ni-based multicomponent concentrated alloys using the coherent potential approximation (CPA). The influence of electronic structure modifications on the electron mean free path and values of electron-phonon coupling are calculated, together with preliminary results on similar quantities obtained by Time Dependent DFT. We discuss possible effects of tuning the mean free path and energy dissipation mechanisms to defect production and recombination in HEAs under irradiation.


1 A work supported by the Semiconductor Research Corporation
In addition, the Casimir stiction considering both quantum and thermal fluctuations is found to be relieved compared with bulks.

is shown that the heat flux can be greatly enhanced and the accurate prediction may differ significantly from that of the geometry-based Derjaguin’s proximity nanostructures capable of supporting higher efficiency or greater heat flux than simple planar substances. In this work, efficient and delocalized radiative heat of near-field heat transfer in thermophotovoltaic devices, thermal imaging, thermal rectifiers, and local thermal management have motivated the search for.

XIANGLEI LIU, BO ZHAO, ZHUOMIN ZHANG, Georgia Institute of Technology — The promising applications inhomogenous boundary conditions is also discussed.

For a deformed strip and for two compact objects of arbitrary shape in terms of the free energy of a standard region (circular ring or flat strip) whose dimension forces between objects that couple to the underlying field. For two dimensional conformal field theories (CFT) we derive exact results for the Casimir interaction.

Technology, Physics Department, 77 Massachusetts Avenue Cambridge, MA 02139 — Thermal fluctuations of a critical system induce long-ranged Casimir Fisiche, Universita di Napoli Federico II, Complesso Universitario MSA, Via Cintia, I-80126 Napoli, Italy, MEHRAN KARDAR, Massachusetts Institute of

Programme (FP7/2007-2013) under REA grant agreement no. 302005.

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This work is supported by JQI-PFC.

The repulsive Casimir effect in Weyl semimetals1. Justin Wilson, Andrew Allocca, Victor Galitski, Univ of Maryland-College Park — Weyl semimetals are a proposed topological material with broken time-reversal symmetry. Due to this, they experience a particular bulk Hall effect as well as a weak longitudinal conductance. In such a situation, one can see a repulsive Casimir effect between two Weyl semimetals (similar to what has been studied for topological insulators and quantum hall materials), and the effect can be tuned from attractive to repulsive with chemical potential or magnetic field. We consider, separately, a simplified bulk description and a thin film geometry taking into account the band structure.

1 This work was supported by JQI-PFC.

Weak localization as a definitive test of diffusive models in the Casimir effect1. Andrew Allocca, Justin Wilson, Victor Galitski, Univ of Maryland-College Park — Results from many measurements of the Casimir effect suggest that the metallic plates in these experiments should be modeled with the plasma model of free electrons as opposed to the naive diffusive Drude model, while other experiments seem to indicate the exact opposite, with results more in line with a diffusive model. We study the Casimir effect at low temperatures between a thick disordered plate and purely two-dimensional disordered system where the Drude conductivity decreases logarithmically at low temperatures due to weak localization. This effect can be tuned with either temperature or applied magnetic field leading to a measurable change in the Casimir force. On the other hand, a ballistic model cannot experience such an effect and is only weakly dependent on temperature and magnetic field. As a result, we propose that an experiment would unambiguously differentiate between diffusive and ballistic models by measuring the effect at low temperatures with an applied magnetic field. Additionally, we calculate the impact that fluctuations in the disorder distribution have on the Casimir effect. Assuming the validity of a diffusive model, we find that the Drude model is a good approximation of a more exact treatment of disorder.

1 This work was supported by the DOE-BES (Grant No. DESC0001911) (A.A. and V.G.), the QJ-I-PFC (J.W.), and the Simons Foundation.

Is it plasma or Drude? Experimental answer using rotating engineered samples. Ricardo Decca, Indiana Univ-Purdue Univ Indianapolis — Measurements done between a Ni covered sphere and a Au coated rotating sample made of sectors of Au and Ni are presented. This approach follows the proposal made by G. Bimonte1 Many samples with different thicknesses t of the top Au film (t ∈ [20, 84] nm) were prepared to measure the interaction. The Ni-coated sapphire sphere was mounted on a sensitive mechanical torsional oscillator. Measurements were done for separations between the sphere and the Au-coated engineered sample in the {200–1000} nm range. With integration times ~1000 s and after accounting for a systematic, once-per-revolution impulsive signal from the air-bearing spindle, the error in the measurement is ~0.3 fN. In all cases it was observed that a plasma-like model provides good agreement with the experiment, while the Drude model is off by factors as large as 1000. The experimental apparatus and the potential source of errors will be briefly discussed.


Casimir effect and radiative heat transfer between Chern Insulators. Pablo Rodriguez Lopez, LPTMS, CNRS et Univ de Paris - Sud, Adolfo Grushin, Max-Planck-Institut für Physik komplexer Systeme, Wang-Kong Tse, Diego Dalvit, Theoretical Division MS B213, Los Alamos National Laboratory — Chern Insulators are a class of two-dimensional topological materials. Their electronic properties are different from conventional materials, and lead to interesting new physics as quantum Hall effect in absence of an external magnetic field. Here we will review some of their special properties and, in particular, we will discuss the radiative heat transfer and the Casimir effect between two planar Chern insulators sheets. Finally, we will see how to control the intensity and sign of this Casimir force and the requirements to observe a repulsive Casimir force in the lab with those materials.

The research leading to these results has received funding from the People Programme (Marie Curie Actions) of the European Union’s Seventh Framework Programme (FP7/2007-2013) under REA grant agreement no. 302005.

Conformal field theory of critical Casimir forces. Thorsten Emig, Massachusetts Institute of Technology, UMI Multi-Scale Materials Science for Energy and Environment, Physics Department, Giuseppe Bimonte, Dipartimento di Scienze Fisiche, Universita di Napoli Federico II, Complesso Universitario MSA, Via Cintia, 180126 Napoli, Italy, Mehran Kardar, Massachusetts Institute of Technology, Physics Department, 77 Massachusetts Avenue Cambridge, MA 02139 — Thermal fluctuations of a critical system induce long-ranged Casimir forces between objects that couple to the underlying field. For two dimensional conformal field theories (CFT) we derive exact results for the Casimir interaction for a deformed strip and for two compact objects of arbitrary shape in terms of the free energy of a standard region (circular ring or flat strip) whose dimension is determined by the mutual capacitance of two conductors with the objects’ shape; and a purely geometric energy that is proportional to conformal charge of the CFT, but otherwise super-universal in that it depends only on the shapes and is independent of boundary conditions and other details. The effect of inhomogeneous boundary conditions is also discussed.

Efficient near-field energy transfer and relieved Casimir stiction between sub-wavelength gratings. Xianglei Liu, Bo Zhao, Zhijun Zhang, Georgia Institute of Technology — The promising applications of near-field heat transfer in thermophotovoltaic devices, thermal imaging, thermal rectifiers, and local thermal management have motivated the search for nanostructures capable of supporting higher efficiency or greater heat flux than simple planar substances. In this work, efficient and delocalized radiative heat transfer between two aligned 1D sub-wavelength gratings is demonstrated based on the scattering theory using the rigorous coupled-wave analysis (RCWA). It is shown that the heat flux can be greatly enhanced and the accurate prediction may differ significantly from that of the geometry-based Derjaguin’s proximity approximation (PA). The underlying mechanism is attributed to the excitation of hyperbolic modes that increase the energy transmission by supporting propagation of waves with large parallel wavevectors and. Besides efficient energy transport, the performance is robust, insensitive to the relative lateral shift. In addition, the Casimir stiction considering both quantum and thermal fluctuations is found to be relieved compared with bulks.
12:27PM M35.00007 Possibilities of Verifying Dynamical Casimir Effect with Nonlinear Materials in Microwave Cavities, VIKTOR DODONOV, Institute of Physics, University of Brasilia — I evaluate the number of “Casimir quanta” that could be created in high-quality electromagnetic cavities containing materials with big third-order nonlinear optical coefficients, due to the parametric amplification of the microwave vacuum field, if the effective refractive index of the material is modulated by periodic high-intensity short laser pulses. The main result is that the expected total number of created microwave photons depends neither on the laser beam shape, nor on the duration or power of individual pulses, but it is determined by the total energy of all pulses, provided the duration of each pulse is much shorter than the period of field oscillations in the selected resonant mode. The experiment can be feasible in small cavities with high resonance frequencies. Possible spurious effects will be discussed, too.

12:39PM M35.00008 Electrostatic patch potentials in Casimir force measurements, JOSEPH GARRETT, DAVID SOMERS, JEREMY MUNDAY, University of Maryland — Measurements of the Casimir force require the elimination of the electrostatic force between interacting surfaces. The force can be minimized by applying a potential to one of the two surfaces. However, electrostatic patch potentials remain and contribute an additional force which can obscure the Casimir force signal [1-2]. We will discuss recent measurements of patch potentials made with Heterodyne Amplitude-Modulated Kelvin Probe Force Microscopy that suggest patches could be responsible for >1% of the signal in some Casimir force measurements, and thus make the distinction between different theoretical models of the Casimir force (e.g. a Drude-model or a plasma-model for the dielectric response) difficult to discern [3].

12:51PM M35.00009 Tunable Casimir-Polder Forces and Spontaneous Emission Rates, FELIPE ROSA, WILTON KORT-KAMP, FELIPE PINHEIRO, TARIK CYSENE, DIEGO OLIVER, CARLOS FARINA, Universidade Federal do Rio de Janeiro — We investigate the dispersive Casimir-Polder interaction between a Rubidium atom and a graphene sheet subjected to an external magnetic field B. We demonstrate that this concrete physical system allows for a high degree of control of dispersive interactions at micro and nanoscales. Indeed, we show that the application of an external magnetic field can induce a 80% reduction of the Casimir-Polder energy relative to its value without the field. We also show that sharp discontinuities emerge in the Casimir-Polder interaction energy for certain values of the applied magnetic field at low temperatures. In addition, we also show that atomic spontaneous emission rates can be greatly modified by the action of the magnetic field, with an order of magnitude enhancement or suppression depending on the dipole’s moment orientation.

1:03PM M35.00010 Suppression of chaos assisted stiction in Casimir oscillators due to surface roughness, WUJAN BROER, GEORGE PALASANTZAS, JASPER KNOESTER, Zernike Institute for Advanced Materials, University of Groningen, HOLGER WAALKENS, Johann Bernoulli Institute of Mathematics and Computer Science, University of Groningen, VITALY B. SVETOVOY, MESA-Institute for Nanotechnology, University of Twente — At separations below 100 nm, the Casimir force strongly influences the vibration dynamics of MEMS (Micro mechanical systems) in dry vacuum conditions. This theoretical analysis includes the effects of both the material response and that of surface roughness in an experimentally relevant way. Moreover, energy gains and losses during actuation are considered via driving and damping, respectively. We show that the system can exhibit chaotic motion for certain actuation parameter values due to the nonlinearity of the Casimir force. Surface roughness of the interacting components turns out to make the MEMS actuation less susceptible to chaotic motion than that of flat surfaces.

1:15PM M35.00011 Influence of dissipation on two-atom dispersion interactions, PABLO BARCELONA, STEFAN YOSHI BUHMANN, Albert-Ludwigs-University of Freiburg, Institute of Physics — We consider the dispersion interaction between two neutral, ground-state atoms at zero and finite temperatures by means of a dynamical approach. Our result differs from the previous ones obtained with time-independent perturbation theory because it correctly accounts for the influence of dissipation via the atomic decay rates. Modern measurements of Casimir force seem to suggest a suppressed influence of dissipation. Our new result shows similar features and can hence help resolve the Drude-plasma debate. We also consider the interaction between a ground-state atom and an excited atom. There are discordant results in the literature for the retarded potential: one oscillating and one monotonic. Our dynamical result uniquely leads to the oscillating result when taking into account the decay rates.

1This work was supported by the DFG (grant BU 1803/3-1)

1:27PM M35.00012 Giant vacuum forces via transmission lines, EPHRAIM SHAHMOON, Weizmann Institute of Science, IGOR MAZETS, Atominstitut, TU Wien, Vienna, Austria, GERSHON KURIZKI, Weizmann Institute of Science — Quantum electromagnetic fluctuations induce forces between neutral particles, namely, the van der Waals (vdW) and Casimir interactions. Here we show that these fundamental interactions can be enhanced by many orders of magnitude upon changing the character of the mediating vacuum photon-modes. We consider two dipoles in the vicinity of any standard electric transmission line and find analytically that the interaction scales non-trivially with the inter-dipolar distance, resulting in a strong and long-range interaction. This may have profound implications on the non-additivity of vdW and Casimir interactions in many-particle systems, and opens the door for Casimir Physics in 1d. We discuss the possibilities of realizing this effect, e.g. in a coplanar waveguide line.

In January 2015, my affiliation is supposed to change to “Department of Physics, Harvard University”

1:39PM M35.00013 ABSTRACT WITHDRAWN —

1:51PM M35.00014 Negative Casimir Entropies in Nanoparticle Interactions, KIMBALL MILTON, Univ of Oklahoma, ROMAIN GUEROUT, Laboratoire Kastler-Brossel, CNRS, ENS, UPMC, Case 74, F-75252 Paris, France, GERT-LUDWIG INGOLD, Institut fur Physik, Universitat Augsburg, Universitaetsstrasse 1, D-86135 Germany, ASTRID LAMCREHT, SERGE REYNAUD, Laboratoire Kastler-Brossel, CNRS, ENS, UPMC, Case 74, F-75252 Paris, France — Negative entropy has been known in Casimir systems for some time. For example, it can occur between two perfectly conducting spheres, between two electrically polarizable nanoparticles if there is sufficient anisotropy, between a perfectly conducting sphere and a conducting plate. The latter effect is most pronounced in the dipole approximation, which occurs when the size of the sphere is small compared to the separation between the sphere and the plate. Therefore, here we examine cases where negative entropy can occur between two electrically and magnetically polarizable nanoparticles or atoms, which need not be isotropic, and between such a small object and a conducting plate. Negative entropy can occur even between two perfectly conducting spheres, between two electrically polarizable nanoparticles if there is sufficient anisotropy, between a perfectly conducting sphere and a Drude sphere, and between a sufficiently anisotropic electrically polarizable nanoparticle and a transverse magnetic conducting plate.

1Supported in part by the Simons Foundation, the Julian Schwinger Foundation, and CNRS
2:03PM M35.00015 Probing the Casimir force with optical tweezers, PAULO MAIA NETO, DINEY ETHER, LUIS PIRES, YARENI AYALA, FELIPE ROSA, UFRJ, STEFAN UMRATH, GERT INGOLD, U. Augsburg, NATHAN VIANA, MOYSES NUSSENZVEIG, UFRJ — Optical tweezers (OT) are single-beam laser traps for neutral particles, usually applied to dielectric microspheres immersed in a fluid. The stiffness is proportional to the trapping beam power, and hence can be tuned to very small values, allowing one to measure femttonewton forces, once the device is carefully calibrated. We employ OT to measure the Casimir (or retarded van der Waals) force between polystyrene beads in ethanol, for distances between 50 nanometers and 1 micrometer. The spherical beads have diameters ranging from 3 to 7 micrometers. We find a rather large correction to the widely employed Proximity Force approximation (PFA), since the ratio between distances and sphere radii is much larger than the typical values probed in recent experiments. For the comparison with experimental data, we compute the Casimir force using the scattering approach applied to the spherical geometry, including the contribution of double-layer forces. We also present experimental results for the total force between a mercury microdroplet and a polystyrene bead immersed in ethanol, with similar distances and diameters. In short, we probe the Casimir force with different materials in a regime far from the validity of PFA, such that the spherical geometry plays a non-trivial role.


11:15AM M36.00001 Superfluidity in Strongly Interacting Spin-Polarized Fermi Gases, BEN A. OLSEN, MELISSA REVELLE, JACOB A. FRY, RANDALL G. HULET, Department of Physics & Astronomy and Rice Quantum Institute, Rice University, Houston, TX 77005, DANIEL E. SHEEHY, Department of Physics & Astronomy, Louisiana State University, Baton Rouge, LA 70803 — We report measurements of phase separation in a harmonically trapped, spin polarized two-component Fermi gas. The interactions in the gas are varied using a magnetically-tuned Feshbach resonance between the weakly-interacting BCS and strongly-interacting BEC regimes. Using spin-selective imaging, we measure the density profiles for the two lowest hyperfine levels of $^6$Li, with the superfluid phase being indicated by an unpolarized central core. We determine phase boundaries for the superfluid transition as a function of interactions and polarization, finding results that are consistent with earlier experimental results in the crossover regime. We also explore the BEC side of resonance, where we compare our measurements to Quantum Monte Carlo simulations and also the deep BCS regime, where few theoretical predictions are available.

1Supported by DARPA, NSF, ARO, and ONR
3G. Bertainia and S. Giorgini, PRA 79, 013016 (2009)

11:27AM M36.00002 Equation of State of One-Dimensional Fermions in Harmonic Traps, CASEY BERGER, The Ohio State University, ERIC ANDERSON, JOAQUIN DRUT, The University of North Carolina at Chapel Hill — We test a novel numerical method for computing the ground state energy of fermions in a harmonic trapping potential. The new technique combines hybrid Monte Carlo and a Gauss-Hermite discretization instead of a uniform lattice. Use of the harmonic oscillator basis and Gauss-Hermite points avoids the problem of edge effects and spurious copies that arise from periodic boundary conditions. This study sets the stage for calculations in higher dimensions, relying on non-uniform Fast Fourier Transform algorithms for acceleration. Based on this method we determine the ground-state energy of unpolarized few-body systems constrained to one-dimensional motion.

11:39AM M36.00003 Strongly interacting fermions in 1D, LI YANG, Department of Physics and Astronomy, Rice University, Houston, Texas 77251, USA, TIMING GUAN, Institute for Advanced Study, Tsinghua University, Beijing 100084, People’s Republic of China, HAN PU, Department of Physics and Astronomy, Rice University, Houston, Texas 77251, USA, DEPARTMENT OF PHYSICS AND ASTRONOMY, RICE UNIVERSITY, HOUSTON, TEXAS 77251, USA, TEAM, INSTITUTE FOR ADVANCED STUDY, TSINGHUA UNIVERSITY, BEIJING 100084, PEOPLE’S REPUBLIC OF CHINA TEAM — Under second order degenerate perturbation theory, we show that the physics of N fermions with arbitrary spin in one dimension in Tonks-Girardeau (TG) and super-Tonks-Girardeau(sTG) regions can be described by super-exchange interaction. An effective spin chain Hamiltonian (none-translational-symmetric Sutherland model) can be obtained from this procedure. For spin-1/2 particles, this model is the none-translational-symmetric Heisenberg model, where a transition between Heisenberg anti-ferromagnetic (AFM) and ferromagnetic (FM) states is expected to occur when the interaction strength is increased from TG to sTG limit. We show that the FM and AFM states can be distinguished in two different methods: the first is based on their distinct response to a spin-dependent magnetic gradient, and the second is based on their distinct momentum distribution. We examine the validity of the spin-chain model by comparison with results obtained from unbiased techniques such as exact diagonalization and TEBD.

11:51AM M36.00004 1D-3D Crossover in a Spin-Imbalanced Fermi Gas, MELISSA REVELLE, BEN A. OLSEN, JACOB FRY, RANDALL G. HULET, Department of Physics and Astronomy and Rice Quantum Institute, Rice University, Houston, TX 77005 — We experimentally study the phases of an ultracold two-component gas of atomic fermions ($^6$Li) confined to 1D tubes formed by a 2D optical lattice. The atoms are prepared in the lowest two hyperfine sublevels where their interactions are tuned by a Feshbach resonance. We previously observed phase separation into a partially-polarized superfluid core and either fully-paired or fully-polarized wings depending on the spin polarization in 3D. In 1D, the phase separation is inverted, such that the cloud center is fully paired and the wings are partially-paired. We investigate the transition from 1D to 3D gas by varying the lattice depth and interaction strength which changes the ratio of the tunneling rate between the tubes to the pair binding energy. We are exploring a region of parameter space that is believed to be the most promising region for the exotic FFLO superfluid phase.

1Supported by DARPA, NSF, and ONR

12:03PM M36.00005 Stability of Fulde-Ferrell-Larkin-Ovchinnikov states in ultracold atomic Fermi gases, JIBIAO WANG, QUIN CHEN, Zhejiang University — The elusive Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) states have attracted enormous attention in the condensed matter and AMO communities. They have not been observed experimentally in three-dimensional (3D) Fermi gases, largely due to their predicted small region in the phase space and very low temperature required. In this talk, we will discuss the stability of the FFLO states in 3D homogeneous Fermi gases, both in equal-mass and mass imbalanced systems, within a pairing fluctuation theory. We find that the effective mass of noncondensed pairs in the directions perpendicular to the FFLO wavevector is negative, leading to instability of the FFLO states previously predicted in the literature. Treatment beyond the T-matrix level and further symmetry breaking effects such as optical lattices and spin-orbit coupling may be necessary in order to find stable FFLO states.

1Supported by NSF, MOE and MOST of China
12:15PM M36.00006 Strong-coupling ansatz for the one-dimensional Fermi gas in a harmonic potential, MEERA PARISH, London Centre for Nanotechnology, JESPER LEVINSEN, Aarhus University, PIETRO MASSIGNAN, ICFO, GEORG BRUUN, Aarhus University — The 1D Fermi gas with repulsive short-range interactions provides an important model of strong correlations and is often amenable to exact methods. However, in the presence of confinement, no exact solution is known for an arbitrary number of strongly interacting fermions. Here, we propose a novel ansatz for generating the lowest-energy wavefunctions of the repulsive 1D Fermi gas in a harmonic potential near the Tonks-Girardeau limit of infinite interactions. We specialize to the case of a single impurity interacting with N majority particles, where we may derive analytic forms of the approximate wavefunctions. Comparing with previous work, we show that our ansatz becomes exact for many-body wavefunctions of fermions and the exact ones for the ground-state wavefunction for N ≥ 8. Moreover, the overlap for the ground-state wavefunction extrapolates to 0.9999 as N → ∞. Thus our ansatz is essentially indistinguishable from numerically exact results in both the few- and many-body limits.


¹This work was supported by NSF grant DMR-1151717

12:39PM M36.00008 Pseudogap phenomenon near the phase transition from $p_x$- to $p_x + ip_y$-wave Fermi superfluid, DAI SUKE INOTANI, YOJI OHASHI, Department of Physics, Keio University — We discuss an ultracold superfluid Fermi gas with a $p$-wave Feshbach resonance (FR). In this system, it has been predicted that the split of $p_x$- to $p_y$- and $p_z$-wave channels in the $p$-wave FR by a dipole-dipole interaction leads to multi-superfluid phases. While the $p_x$-wave state appears below $T_c$, the $p_x + ip_y$-wave state is expected to become more stable below a certain temperature ($\equiv T_{p_x+ip_y}^c < T_c$). In this talk, including the split of FR, as well as $p$-wave pairing fluctuations, within a $T$-matrix approximation, we find that, near $T_{p_x+ip_y}^c$, the $p_x$-phase, pairing fluctuations in the non-condensed $p_y$- and $p_z$-wave channels cause the pseudogap phenomenon in the nodal direction of the $p_x$-wave order parameter. This pseudogap is shown to continuously change into the $p_x + ip_y$-superfluid gap, as one goes away from the nodal direction. Since pairing fluctuations are soon suppressed below $T_c$ in the ordinary $s$-wave case, this pseudogap near $T_{p_x+ip_y}^c (< T_c)$ is a characteristic phenomenon of a $p$-wave Fermi superfluid with multi-superfluid phases. In this talk, we also discuss how this pseudogap develops, as one decreases the temperature from $T_c$ to $T_{p_x+ip_y}^c$.

12:51PM M36.00009 Quantum Monte Carlo Simulation of one dimensional SU(N) Fermion system, SHENGLONG XU, CONGJUN WU, University of California, San Diego — One dimensional interacting fermionic systems with SU(N) symmetry have been realized in ultracold atom systems. The interplay between the dimensionality and symmetry provides a platform to search for unconventional phenomena. Inspired by recent experiments, we use quantum Monte Carlo to explore the metallic phase, nature of the metal-insulator transition as well as possible exotic magnetic orders of such systems. The effects of trapping potential are also discussed.

1:03PM M36.00010 Stoner ferromagnetism of a strongly interacting Fermi gas in the quasipulsive regime, LIANYI HE, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, XIA-JI LIU, Centre for Quantum and Optical Science, Swinburne University of Technology, Melbourne 3122, Australia, XU-GUANG HUANG, Physics Department, Fudan University, Shanghai 200433, China, JOSEPH CARLS ON, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, HUI HU, Centre for Quantum and Optical Science, Swinburne University of Technology, Melbourne 3122, Australia — Recent advances in rapidly quenched ultracold atomic Fermi gases near a Feshbach resonance arise a number of interesting problems, in the context of observing the long-sought Stoner ferromagnetic phase transition. The possibility of experimentally obtaining a “quasipulsive” regime in the upper branch of the energy spectrum due to the rapid quench is currently debated and theoretically, the Stoner transition has mainly been investigated at zero temperature or high polarization, due to the limited theoretical approaches in the strongly repulsive regime. Here, we develop a nonperturbative large-N expansion theory for a quasipulsive Fermi gas near resonance and present a finite temperature phase diagram for its Stoner instability. Our results agree well with the known quantum Monte-Carlo simulations at zero temperature and recover the virial expansion prediction at high temperature for arbitrary interaction strengths. At resonance, we find that the unitary Fermi gas undergoes the Stoner transition at about 1.5TF, where TF is the Fermi degeneracy temperature.

1:15PM M36.00011 Three-Component Fermi Gases in Two Dimensions, THOMAS KIRK, MEERA PARISH, London Center Nanotechnology, CONDENSED MATTER AND MATERIALS PHYSICS TEAM — We study a three-component Fermi gas in two spatial dimensions using a two-channel model. We investigate both few- and many-body properties of the gas, and we construct the ground-state phase diagram as a function of the effective range and coupling strength. We discuss how such a system may be experimentally realisable in the context of cold-atomic gases.

1:27PM M36.00012 Spin susceptibility and effects of fluctuating Cooper pairs in the BCS-BEC crossover regime of a superfluid Fermi gas¹, HIROYUKI TAJIMA, RY O HANAI, YOJI OHASHI, Keio University — We theoretically discuss the spin susceptibility $\chi$ and effects of strong-coupling corrections in the BCS-BEC crossover regime of an ultracold Fermi gas. Using an extended $T$-matrix approximation, we calculate $\chi$ over the entire BCS-BEC crossover region, showing that this magnetic quantity is very sensitive to pairing fluctuations in both the normal and the superfluid phase. In the normal state, it is suppressed by preformed singlet Cooper pairs near $T_c$, being similar to the spin-gap phenomenon in high-$T_c$ cuprates. Below $T_c$, on the other hand, pairing fluctuations enhance $\chi$, in the sense that the suppression of this quantity by the superfluid order is weakened due to partial dissociation of Cooper pairs. From these, we determine the region where pairing fluctuations strongly affect spin excitations in the phase diagram of a Fermi gas with respect to the temperature and the strength of a pairing interaction. We also compare our results with the recent experiments on a $^{40}$K Fermi gas. Our results indicate that the spin susceptibility is a useful observable in understanding strong-coupling properties of an ultracold Fermi gas in the BCS-BEC crossover region.

¹H. T. was supported by Graduate School Doctoral Student Aid Program from Keio University.
1:39PM M36.00013 Exact Ground-state Properties of Atomic Fermi Gases in Two Dimensions

Hao Shi, Simone Chiesa, Shiwei Zhang, William & Mary Coll — Experimental realization of the interacting Fermi gas in three dimensions and the precise comparison it has allowed with theory and computation have lead to rapid advances in the study of strongly paired fermions. Two-dimensional systems are being realized and offer many new opportunities. We perform exact calculations on the two-dimensional strongly interacting, unpolarized Fermi gas with a zero-range attractive interaction. A new auxiliary-field approach is used which is exact and accelerates the sampling of imaginary-time paths by a force bias technique. The method allows calculations with long imaginary-time and large lattice sizes. We present the calculated equation of state, the contact parameter, the condensate fraction, and the pairing correlation function. The structure of the pairing wave function is determined as a function of $k_F a$, we will also discuss the effect of spin-orbit coupling.

1:51PM M36.00014 Absence of spin order in a two-dimensional orbital optical lattice

Zhenyu Zhou, George Mason University, University of Pittsburgh, Vincent Liu, University of Pittsburgh, Erhai Zhao, George Mason University — Mott insulators with both spin and orbital degeneracy are pertinent to a family of transition metal oxides. The intertwined spin and orbital fluctuations can lead to exotic phases such as quantum spin-orbital liquids. Here we consider two-component spin 1/2 fermionic atoms with strong repulsive interaction on the p-band of the square optical lattice. We derive the spin-orbital exchange for quarter filling of the p-band in the Mott limit, and show it frustrates the development of long range spin order. Exact diagonalization indicates a spin-disordered ground state with ferro-orbital order. The system dynamically decouples into individual Heisenberg spin chains, each realizing a Luttinger liquid accessible at higher temperatures compared to atoms confined to the s-band. Our model serves as an example of how orbital order enhances quantum fluctuations to prevent spin order and leads to dimension reduction in a quantum gas system.

2:03PM M36.00015 Intrinsic p-wave pair amplitude in a trapped ultracold s-wave superfluid Fermi gas

Yuki Endo, Daisuke Inotani, Ryo Hanai, Yoji Ohashi, Keio University — We theoretically discuss the possibility that an unconventional p-wave Cooper-pair amplitude is induced in the ordinary s-wave superfluid Fermi gas. Using a Hubbard model, we numerically show that such a phenomenon really occurs, when both the spatial and (pseudo) spin inversion symmetries of the system are broken. In an ultracold Fermi gas, this situation is shown to be realized, when two spin states (that describe two atomic hyperfine states contributing to s-wave Cooper pairs) feel different trap potentials. Thus, in this situation, when the s-wave pairing interaction is suddenly changed to a p-wave one by using the Feshbach resonance technique, at least just after this tuning, the p-wave superfluid Fermi gas is expected to be realized (which is characterized by the superfluid order parameter given by the product of the p-wave pair amplitude and the p-wave pairing interaction). In this talk, we also clarify the optimal condition to obtain the p-wave pair amplitude in the BCS-BEC crossover region, using the BCS-Leggett strong-coupling theory.

Wednesday, March 4, 2015 11:15AM - 2:03PM — Session M37 GQI: Focus Session: Quantum Optics and Photonic Architectures 212A - Alexey Gorshkov, Joint Quantum Institute

11:15AM M37.00001 Demonstration of Backward-wave Parametric Down-Conversion

Chih-Sung Chuu, Chun-Yao Yang, Jim Lin, Department of Physics and Frontier Research Center on Fundamental and Applied Sciences of Matters, National Tsing Hua University, Taiwan, Charlotte Liljestrand, Carola Canalias, KTH - Royal Institute of Technology, Sweden, Stephen Harris, Edward L. Ginzbrot Laboratory, Stanford University, USA — Ultrabright sources of temporally long and spectrally narrow photons are essential for efficient light-matter interaction at the single-atom level. To achieve high brightness, parametric single-down-conversion of the backward-wave type was proposed for single-mode generation of long biphonons [1]. In this talk I will describe the demonstration of backward-wave parametric down-conversion in a nonlinear crystal, of which the time-energy entanglement was characterized by the Franson interference. I will also discuss the possibility of realizing a miniature ultrabright biphonon source.


11:27AM M37.00002 Nanomechanical single-qubit gates and iSWAP gate of single-electron spins in a carbon nanotube

Heng Wang, Guido Burkard, University of Konstanz, Germany — A universal gate set for quantum computation can be built with one-qubit and iSWAP gates. We theoretically investigate mechanically-induced single-electron spin resonance in a quantum dot [1] and a phonon-mediated iSWAP gate of two separate single electron spins in two quantum dots on a suspended carbon nanotube which is driven by an external electric field. The intrinsic spin-phonon coupling between the spin and the mechanical mode is induced by the spin-orbit coupling. Arbitrary-angle rotations about arbitrary axes of the single electron spin can be achieved by varying the frequency and the strength of the external electric driving field. If two single-electron spins in two quantum dots couple to the same vibrational mode simultaneously, the two spins are indirectly coupled via phonon exchange. Both electron spin resonance and the iSWAP gate can be turned off by suppressing the spin-phonon coupling by electrostatically shifting the electron wave function on the nanotube. Combining iSWAP and single spin gates, maximally entangled states of two spins can be generated in a single step. [1] H. Wang and G. Burkard, Phys. Rev. B 90, 035415 (2014).

11:39AM M37.00003 Nanophotonic photon echo memory based on rare-earth-doped crystals

Tian Zhong, Jonathan Kindem, Evan Miyazono, Andrei Fararon, Caltech, Caltech Nano Quantum Optics Team — Rare earth ions (REIs) are promising candidates for implementing solid-state quantum memories and quantum repeater devices. Their high spectral stability and long coherence times make REIs a good choice for integration in an on-chip quantum nano-photonics platform. We report the coupling of the 883 nm transition of Neodymium (Nd) to a Yttrium Orthosilicate (YSO) photonic crystal nano-beam resonator, achieving Purcell enhanced spontaneous emission by 21 times and increased optical absorption. Photon echoes were observed in nano-beams of different doping concentrations, yielding optical coherence times $T_2 > 80$ μs that are comparable to unprocessed bulk samples. This indicates the remarkable coherence properties of Nd are preserved during nanofabrication, therefore opening the possibility of efficient on-chip optical quantum memories. The nano-resonator with mode volume of $1.6(λ/ n)^3$ was fabricated using focused ion beam, and a quality factor of 3200 was measured. Purcell enhanced absorption of 80% by an ensemble of $1 \times 10^9$ ions in the resonator was measured, which fulfills the cavity impedance matching condition that is necessary to achieve quantum storage of photons with unity efficiency.

11:51AM M37.00004 Photons in synthetic gauge fields

Mohammad Hafezi, Joint Quantum Institute — Electronic transport is localized in low-dimensional disordered media. The addition of gauge fields to disordered media leads to fundamental changes in the transport properties. We implement a synthetic gauge field for photons using silicon-on-insulator technology. By determining the distribution of transport properties, we confirm that waves are localized in the bulk and localization is suppressed in edge states. Furthermore, we measure corresponding topological invariants and investigate the chiral gauge anomaly in the context of Chern-Simons theory. Our system provides a new platform for investigating the transport properties of photons in the presence of synthetic gauge fields.
12:27PM M37.00005 Harnessing gauge fields for maximally entangled state generation. SEBASTIAN REYES, LUIS MORALES-MOLINA, MIGUEL ORSZAG, Pontificia Universidad Catolica de Chile, DOMINIQUE SPEHNHER, Univesite Grenoble Alpes — We study the generation of entanglement between two species of bosons living on a ring lattice, where each group of particles can be described by a d-dimensional Hilbert space (qudit). Gauge fields are exploited to create an entangled state between the pair of qudits. Maximally entangled eigenstates are found for well-defined values of the Aharonov-Bohm phase, which are zero-energy eigenstates of both the kinetic and interacting parts of the Bose-Hubbard Hamiltonian, making them quite exceptional. We propose a protocol to reach the maximally entangled state (MES) by starting from an initially prepared ground state. Also, an indirect method to detect the MES by measuring the current of the particles is proposed.

12:39PM M37.00006 ABSTRACT WITHDRAWN —

12:51PM M37.00007 What does it mean for half of an empty cavity to be full? . ERIC BROWN, University of Waterloo — It is well known that the vacuum state of a quantum field is spatially entangled. This is true both in free and confined spaces, for example in an optical cavity. The obvious consequence of this, however, is surprising and intuitively challenging. Namely, that in some sense half of an empty box is full. Formally this is clear, but what does this physically mean in terms of, say, measurements that can actually be made? In this contribution I will discuss a new and simple perspective that answers this question precisely and physically concretizes the phenomenon. In so doing I will also propose a simple experimental setup for the verification of, and indeed the efficient harvesting of, vacuum entanglement. Preprint: http://arxiv.org/abs/1409.4203

1:03PM M37.00008 Protocols for a quantum network based on single photons . SUSANNE BLUM, Theoretical Physics, Saarland University, Germany, CHRISTOPHER O’BRIEN, Department of Physics and Astronomy, Texas A&M University, DANIEL REICH, Theoretical Physics III, University of Kassel, Germany, NIKOLAI LAUK, Physics Department, University of Kaiserslautern, Germany, CHRISTIANE KOEL, Theoretical Physics III, University of Kassel, Germany, MICHAEL FLEISCHHAUER, Physics Department, University of Kaiserslautern, Germany, GIOVANNA MORIGI, Theoretical Physics, Saarland University, Germany — Two protocols for interfacing single optical photons with individual qubits are theoretically discussed. The first is a protocol which allows one to interface a single optical photon with a superconducting qubit. It makes use of a spin ensemble, where the individual emitters possess both an optical and a magnetic dipole transition. Reversible frequency conversion is realized by combining optical photon storage, for instance by means of EIT, with the controlled switching on and off the coupling of the magnetic dipole transition with a microwave cavity, which in turn couples to a superconducting qubit. We test various strategies and compare their efficiencies in terms of robustness and transfer time. The second protocol aims at achieving perfect absorption of a photon by a single trapped atom, or solid-state emitter, by means of optimal control theory. We make use of the Krotov algorithm for the purpose of identifying pulses driving the atom, that maximize the efficiency and fidelity of absorption in the setup of [Reiser et al., Nature 508, 237 (2014)]. These protocols contribute to the development of a toolbox for quantum networks using hybrid platforms.

1:15PM M37.00009 QNIX: A Linear Optical Architecture for Quantum Computing . MERCEDES GIMENO-SEGOVIA, PETER J. SHADBOLT, TERRY G. RUDOLPH, Department of Physics, Imperial College London, SW7 2AZ, UK, DAN E. BROWNE, Department of Physics and Astronomy, University of Oxford, OX1 3RH, UK, GABRIEL MENDOZA, NICHOLAS J. RUSSELL, JOSHUA W. SILVERSTONE, ALBERTO SANTAMATO, JACQUES CAROLAN, JEREMY O’BRIEN, Centre for Quantum Photonics, H.H. Wills Physics Laboratory & Department of Electronic and Electrical Engineering, University of Bristol, BS8 1UB, UK — There is currently a great deal of effort to develop a large-scale quantum computer, and one of the most promising platforms to do so is integrated linear optics. We present a proposal for a dynamical scheme for an integrated linear optics implementation of a one-way quantum computer. We go beyond the purely theoretical work and address practical issues in order to create a physically realistic design. We describe every step of cluster state construction and processing, showing the outstanding issues left to be addressed and our contributions to the different stages of the dynamical process. These include optimised interferometers for the generation of GHZ states, a universal and scalable architecture which requires entangled sources of no more than 3 photons with no active feed-forward, and loss-tolerant and fault-tolerant strategies specifically tailored to our proposed architecture. Our work demonstrates that building a linear optical quantum computer need be less challenging than previously thought, and brings large-scale switch-free linear optical architectures for quantum computing much closer to experimental realisation.

1:27PM M37.00010 ABSTRACT WITHDRAWN —

1:39PM M37.00011 Reshaping quantum wave packets through time-dependent absorption . ARSENI GOUSSEV, Northumbria University — The problem of control and reliable manipulation of quantum states finds importance in many areas of physics including quantum metrology and matter-wave interferometry. Here we propose a new approach to reshaping the spatial wave function of a quantum particle, e.g., an atom, by passing the latter through a time-dependent absorbing barrier. Experimentally, such a barrier can be realized by means of a sharply focused laser beam or a light sheet, with the radiation frequency chosen to make the passing atom undetectable, for instance, by ionizing the atom or changing its internal state. In particular, we show how the proposed method can be used to shift, squeeze, or split spatially-localized quantum wave packets.

1:51PM M37.00012 Correlated random walks induced by dynamical wavefunction collapse1 . DANIEL BEDINGHAM, University of Oxford — Wavefunction collapse models modify Schrödinger’s equation so that it describes the collapse of a superposition of macroscopically distinguishable states as a genuine physical process [PRA 42, 78 (1990)]. This provides a basis for the resolution of the quantum measurement problem. An additional generic consequence of the collapse mechanism is that it causes particles to exhibit a tiny random diffusive motion. Furthermore, the diffusions of two sufficiently nearby particles are positively correlated — it is more likely that the particles diffuse in the same direction than would happen if they behaved independently [PRA 89, 032713 (2014)]. The use of this effect is proposed as an experimental test of wave function collapse models in which pairs of nanoparticles are simultaneously released from nearby traps and allowed a brief period of free fall. The random displacements of the particles are then measured. The experiment must be carried out at sufficiently low temperature and pressure for the collapse effects to dominate over the ambient environmental noise. It is argued that these constraints can be satisfied by current technologies for a large class of viable wavefunction collapse models.

1Work supported by the Templeton World Charity Foundation

11:15AM M38.00001 Contextuality: a benchmark for “quantumness” in theory and experiment, MATTHEW PUSEY, Perimeter Institute for Theoretical Physics — An ontological model for a quantum experiment is a purported explanation for the probabilities we see. Non-contextual models are particularly compelling because they never offer two different explanations for the same observations. I will review these notions and argue that the impossibility of non-contextual models is a good way to rigorously define “genuine quantumness”. Two examples of phenomena whose “quantumness” have been debated are “anomalous weak values” and “logical pre- and post-selection paradoxes”. I will outline how their incompatibility with non-contextual models clarifies why both defy compelling classical explanation. A related idea is to use contextuality to certify that an experiment has achieved quantum coherence without requiring a full characterization. To this end I will present a simple yet robust non-contextuality inequality that can be violated with a single qubit. (The work on pre- and post-selection paradoxes was done in collaboration with Matt Leifer.)

11:51AM M38.00002 Ordering relations for quantum states1, IAN DURHAM, Saint Anselm College — It is often desirable to model physical states in an order-theoretic manner, e.g. as a partially ordered set. Classical states are known to possess a unique ordering relation corresponding to a neo-realist interpretation of these states. No such unique relation exists for quantum states. This lack of a unique ordering relation for quantum states turns out to be a manifestation of quantum contextuality vis-à-vis the Kochen-Specker theorem. It also turns out that this provides a link to certain large-scale thermodynamic processes. The suggestion that the ordering of quantum states leads to macroscopic thermodynamic processes is at least five decades old. The suggestion that the mechanism that drives the ordering is contextuality, is unique to this work. The argument is framed in the language of the theories of domains, categories, and topology.

1Financial support provided by FQXi.

12:03PM M38.00003 Advances in weak-values based metrology, ANDREW JORDAN, GERARDO VIZA, JUILLIÁN MARTÍNEZ-RINCÓN, University of Rochester, GABRIEL ALVES, Universidade Federal do Rio de Janeiro, JOHN HOWELL, University of Rochester, PAUL KWIAT, University of Illinois at Urbana-Champaign — We theoretically [1] and experimentally [2] describe the relative advantages of implementing weak-values-based metrology versus standard methods. To accomplish this, we measure small optical beam deflections both a weak-values-based technique, and a standard technique. By introducing controlled external modulations of the detector, and transverse beam-jitter, we quantify the mitigation of these sources in the weak values-based experiment versus the standard experiment. In all cases, the weak-values technique performs the same or better than the standard technique by up to two orders of magnitude in precision for our parameters. We further measure the statistical efficiency of the weak-values-based technique. By post-selecting on 1% of the photons, we obtain 99% of the available Fisher information of the beam deflection parameter. We also discuss ways to recycle the discarded events [3], obtaining much greater precision on a measured parameter.


12:15PM M38.00004 On the efficacy of weak measurements for tomography, JONATHAN A. GROSS, CHRISTOPHER FERRIE, NINNAT DANGNIAM, CARLTON M. CAVES, University of New Mexico, Center for Quantum Information and Control — Recently there has been a fascination with weak measurements in the field of tomography. We conduct a detailed analysis of two specific schemes: so-called “direct state tomography”, and another scheme marketed as outperforming “standard” tomography with respect to fidelity considerations. Through the application of generalized measurement theory we clearly identify what weak measurements contribute beyond “standard” projective measurements and what simple techniques the application of weak measurements obscures.

12:27PM M38.00005 Many Worlds, the Born Rule, and Self-Locating Uncertainty, SEAN CARROLL, Caltech — A longstanding issue in attempts to understand the Everett (Many-Worlds) approach to quantum mechanics is the origin of the Born Rule: why is the probability given by the square of the amplitude? Recently, Page has raised another puzzle: the Born Rule itself is insufficient in cases where the wave function includes multiple indistinguishable observers in the same branch. I will argue that both problems share a common solution, arising from a proper treatment of self-locating uncertainty (physical situations containing multiple copies of identical observers). This analysis gives a simple, physics-oriented derivation of the Born Rule, as well as a justification for the treatment of identical classical observers.

1:03PM M38.00006 Quantum phenomena modelled by interactions between many classical worlds, HOWARD WISEMAN, MICHAEL HALL, Centre for Quantum Dynamics, Griffith University, DIRK-ANDRE DECKERT, Ludwig-Maximilians-Universität München — [Ref. Phys. Rev. X 4 041013 (2014)] We investigate how quantum theory can be understood as the continuum limit of a mechanical theory, in which there is a huge, but countable, number of classical “worlds,” and quantum effects arise solely from a universal interaction between these worlds, without reference to any wave function. Here a “world” means an entire universe with well-defined properties, determined by the classical configuration of its particles and fields. In our approach each world evolves deterministically; probabilities arise due to ignorance as to which world a given observer occupies; and we argue that in the limit of infinitely many worlds the wave function can be recovered (as a secondary object) from the motion of these worlds. We introduce a simple model of such a “many interacting worlds” approach and show that it can reproduce some generic quantum phenomena—such as Ehrenfest’s theorem, wavepacket spreading, barrier tunneling and zero point energy—as a direct consequence of mutual repulsion between worlds. Finally, we perform numerical simulations using our approach. We demonstrate, first, that it can be used to calculate quantum ground states, and second, that it is capable of reproducing, at least qualitatively, the double-slit interference phenomenon.

1:15PM M38.00007 Does protective measurement imply the reality of the quantum state?, MATTHEW LEIFER, Perimeter Institute for Theoretical Physics, JOSHUA COMBES, University of Waterloo, CHRIS FERRIE, University of New Mexico, MATTHEW PUSEY, Perimeter Institute for Theoretical Physics — In 1993, Aharonov and Vaidman claimed that the quantum state of a single system could be measured in a scheme they called ‘protective measurement’ and hence that the quantum state must be a real property of a single system. Despite attracting considerable controversy, we do not think that the existing criticisms have put their finger on precisely what is wrong with this claim. We explain why we think that, in the protective measurement scheme, the vast majority of the information about the quantum state comes from the protection operation rather than from the state itself. We also give simple toy models of protective measurement which show that the protection operation effectively reprepares the system in an independent copy of the initial state. Thus determining the quantum state by protective measurement is conceptually no different from performing state tomography on an ensemble of independently prepared systems.
Finally, we give simple quantum circuits for the implementation of this protocol with qubits, including initialization, weak interaction and postselection. With this result, we further find the Fisher information of weak measurement can approximately reach the Heisenberg limit with the assistance of entanglement.

In this work, we study the optimization of weak measurement and propose an entanglement-assisted protocol for practical application of weak measurement. In this work, we present the microscopic derivation of the OQBM for a Brownian particle. Here, we present the microscopic derivation of the OQBM for a Brownian particle with two internal degrees of freedom. Examples of the dynamics for initial Gaussian and non-Gaussian distributions are presented.


1:27PM M38.00008 Most likely paths for quantum trajectories: multiple solutions and generalization to two-qubit case. AREEYA CHANTASRI, Rochester Theory Center, University of Rochester, New York, ANDREW JORDAN, Rochester Theory Center, University of Rochester, New York; Institute of Quantum Studies, Chapman University, Orange, California — We study trajectories of quantum states evolving under the quantum measurement. We further analyze and develop our recent approach for finding the most likely path for quantum trajectories between any two states at different times. Under certain conditions, we find that the most likely path can bifurcate and multiple solutions do exist. Two or more solutions can have comparably large probability weights associated with them, implying multiple likely paths for the state trajectories. In developing this approach, we go beyond a single qubit. In this work, we study the optimization of weak measurement and propose an entanglement-assisted protocol for it. We start from maximizing the postselection probability with a given weak value. The result shows the maximum postselection probability is proportional to the variance of the observable under the initial state of the system. As is known that the variance has different scaling under entangled or uncorrelated states, it inspired us to show using entanglement in the initial state of the system can increase the postselection efficiency beyond that with sequential use of systems. With this result, we further find the Fisher information of weak measurement can approximately reach the Heisenberg limit with the assistance of entanglement. Finally, we give simple quantum circuits for the implementation of this protocol with qubits, including initialization, weak interaction and postselection.


1:39PM M38.00009 Microscopic derivation of open quantum Brownian motion¹, FRANCESCO PETRUCCIONE, ILYA SINAYSKIY, University of KwaZulu-Natal and National Institute for Theoretical Physics (KZN), UKZN TEAM — Recently a model of open quantum Brownian motion (OQBM) [M. Bauer, D. Bernard, A. Tilloy, Phys. Rev. A 88 (2013) 062340] was introduced as a scaling limit of Open Quantum Walks (OQWs) [S. Attal, F. Petruccione, C. Sabot, I. Sinayskiy, J. Stat. Phys. 147 (2012) 832]. OQBM is a new type of quantum Brownian motion where the dynamics of the Brownian particle not only depends on the interactions with a thermal environment, but also depends on the state of the internal degrees of freedom of the Brownian particle. Here, we present the microscopic derivation of the OQBM for a Brownian particle with two internal degrees of freedom. Examples of the dynamics for initial Gaussian and non-Gaussian distributions are presented.

¹This work is based upon research supported by the South African Research Chair Initiative of the Department of Science and Technology and National Research Foundation.

2:03PM M38.00011 Pricing postselection: the cost of indecision in state discrimination, JOSHUA COMBES, Perimeter Institute for Theoretical Physics, CHRISTOPHER FERRIE, University of New Mexico — Postselection is the process of discarding outcomes from statistical trials that are not the event one desires. Postselection can be useful in many applications where the cost of getting the wrong event is implicitly high. However, unless this cost is specified exactly, one might formally conclude that discarding all data is optimal. Here we analyze the optimal decision rules and quantum measurements in a decision theoretic setting where a pre-specified cost is assigned to discarding data. Non-trivial solutions are found for even the simplest state discrimination problem of choosing between two nonorthogonal qubit states. Our solutions interpolate between the Helstrom measurement and the unambiguous state discrimination experiment.

Wednesday, March 4, 2015 11:15AM - 2:15PM — Session M39 GQI: Focus Session: Superconducting Qubits: Hybrid Systems 213AB -

11:15AM M39.00001 Towards hybrid quantum devices combining superconducting qubits to a spin-ensemble multi-qubit register. CECILE GREZES, CEA Saclay — Processing quantum information requires quantum-mechanical systems with long coherence times and that can be easily coupled together to perform logic operations. We report progress on hybrid quantum devices, in which an ensemble of spins provides a long-lived multi-qubit register for superconducting qubits. We design a memory protocol able to store and retrieve on demand the state of a large number of qubits in the spin ensemble [1]. Qubit states are written by resonant absorption of a microwave photon in the spin ensemble and read out of the memory by applying Hahn echo refocusing techniques to the spins. In a first experiment, we demonstrate the write step of the protocol by integrating on the same chip a superconducting qubit, a resonator with tunable frequency, and an ensemble of NV center spins in diamond [2]. In a second experiment, we demonstrate an important building block of the read step, which consists in retrieving multiple classical microwave pulses at the few photon level using Hahn echo refocusing techniques [3]. First experimental results will be presented in the direction of combining these two building blocks for retrieving a field in the quantum regime.


11:51AM M39.00002 Exploring the Physics of Semiconductor Quantum Dots using Circuit Quantum Electrodynamics, ANNA STOCKKLAUSER, VILLE MAISI, THOMAS IHN, KLAUS ENSSLIN, ANDREAS WALLRAFF, ETH Zurich — Semiconductor quantum dots and superconducting qubits both possess excitations in the microwave domain for which a wide range of novel approaches to create, store, manipulate and detect individual photons have been developed. A key ingredient are coplanar waveguide resonators in which the field energy of an excitation is distributed over a small mode volume. This feature creates sizable electromagnetic fields at the level of individual microwave photons mediating strong electromagnetic interactions with a variety of quantum systems. In an approach known as circuit quantum electrodynamics (QED) we both probe fundamental quantum optical effects and demonstrate basic features of quantum information processing. In this presentation, I will discuss experiments exploring the physics of semiconductor quantum dots in the context of circuit QED. We investigate the coherent dipole coupling of double dots to microwave photons [1,2] and detect radiation emitted from the dots in inelastic electron tunneling processes. This approach may allow us to explore quantum coherent interfaces between semiconducting and superconducting qubits.

12:03PM M39.00003 Improving the coherence time of a quantum system via a coupling with an unstable system, YUICHIRO MATSUZAKI, XIAOBO ZHU, KOSUKE KAKUYANAGI, HIRAKU TOIDA, NTT Basic Research Laboratories, TAKAAKI SHIMO-OKA, NORIKAZU MIZIOCHI, University of Osaka, KAE NEMOTO, National Institute of Informatics, KOJI SEMBA, National Institute of Information and Communications Technology, WILLIAM MUNRO, HIROSHI YAMAGUCHI, SHIRO SAITO, NTT Basic Research Laboratories — One of the promising candidates for the realization of quantum information processing is nitrogen-vacancy (NV) center. High controllability of NV centers has been achieved with the current technology, including reliable single qubit operations and quantum non-demolition measurements. However, NV center is affected by dephasing due to magnetic-field environmental noise, which limits the coherence time of the quantum states. In this talk, we propose a counter-intuitive way to improve the coherence time of an NV center where we use a coupling with an unstable system. If we couple a two-level system such as a superconducting qubit with a single NV center, then a dark state of the NV center naturally forms after the hybridization. We show that this dark state becomes robust against environmental fluctuations due to the coupling even when the coherence time of the two-level system is much shorter than that of the NV center.

12:15PM M39.00004 Spin-qubit inspired architectures for superconducting quantum computing, YUN-PIL SHIM, CHARLES TAHAN, Laboratory for Physical Sciences — In recent years, the superconducting qubit community has achieved single and two-qubit benchmarked gate fidelities approaching 99.9%, fast readout with novel superconducting amplifiers, distributed entanglement, and other milestones on the road to fault-tolerant quantum information processing. Obviously, this is a field that could use some help from the semiconductor qubit community! Here we present theoretical work on superconducting qubit systems inspired by our experience with semiconductor qubits. We discuss initialization, single- and two-qubit gate operations, and measurement schemes for an encoded qubit in a two-dimensional architecture. Our results motivate new ways of designing or operating superconducting quantum information processors.

12:27PM M39.00005 Superconducting qubits with semiconductor nanowire Josephson junctions, K.D. PETERSSON, T.W. LARSEN, F. KUEMMETH, T.S. JESPERSEN, P. KROGSTRUP, J. NYGÅRD, C.M. MARCUS, Center for Quantum Devices, Niels Bohr Institute, Denmark — Superconducting transmon qubits are a promising basis for a scalable quantum information processor. The recent development of semiconductor InAs nanowires with in situ molecular beam epitaxy-grown Al contacts presents new possibilities for building hybrid superconductor/semiconductor devices using precise bottom up fabrication techniques. Here, we take advantage of these high quality materials to develop superconducting qubits with superconductor-normal-superconductor Josephson junctions (JJs) where the normal element is an InAs semiconductor nanowire. We have fabricated transmon qubits in which the conventional Al-AlOx-Al JJs are replaced by a single gate-tunable nanowire JJ. Using spectroscopy to probe the qubit we observe fluctuations in its level splitting with gate voltage that are consistent with universal conductance fluctuations in the nanowire’s normal state conductance. Our gate-tunable nanowire transmons may enable new means of control for large scale qubit architectures and hybrid topological quantum computing schemes.

12:39PM M39.00006 Coherent control of a transmon qubit with a nanowire-based Josephson junction, T.W. LARSEN, K.D. PETERSSON, F. KUEMMETH, T.S. JESPERSEN, P. KROGSTRUP, J. NYGÅRD, C.M. MARCUS, Center for Quantum Devices, Niels Bohr Institute, Denmark — Transmon qubits[1] have taken great leaps towards realizing a quantum processor[2]. Here we present measurements on a novel, gateable transmon. By tuning the electron density in a semiconducting nanowire transmon, we can control the qubit frequency from ~3 GHz to ~8 GHz. The transmon was embedded in an aluminum coplanar waveguide cavity for readout and qubit control. In the resonant regime we observe strong cavity-qubit coupling. In the dispersive regime we demonstrate coherent control on the Bloch sphere. The life- and coherence times were measured to $T_1 \approx 2T_2 \sim \sim 1 \mu$s. The coherence time was measured to almost $1 \mu$s. Fast gate operations facilitate z-rotations as well as promising fast two-qubit operations in future multiple-qubit devices. These measurements open new possibilities for gateable superconducting qubits and promise a plausible system for Majorana hybrid devices.

12:51PM M39.00007 Fermion parity measurement and control in Majorana circuit quantum electrodynamics, ERAN GINOSSAR, Advanced Technology Institute and Department of Physics, University of Surrey, Guildford, United Kingdom GU2 7XH, CONSTANTIN YAVILBERG, EYTAN GROSFELD, Department of Physics, Ben-Gurion University of the Negev, Be’er-Sheva 84105, Israel — Combining superconducting qubits with mesoscopic devices that carry topological states of matter may lead to compact and improved qubit devices with properties useful for fault-tolerant quantum computation. Recently, a charge qubit device based on a topological superconductor circuit has been introduced where signatures of Majorana fermions could be detected. This device stores quantum information in coherent superpositions of fermion parity states originating from the Majorana fermions, generating a highly isolated qubit whose coherence time could be greatly enhanced. We extended the conventional semi-classical method and obtain analytical derivations in the strong coupling regime of the device to cavity photons. We study the effect of the Majorana fermions on the quantum electrodynamics of the device embedded within an optical cavity and develop protocols to initialise, control and measure the parity states. We show that, remarkably, the parity eigenvalue is revealed via dispersive shifts of the optical cavity in the strong coupling regime and its state can be coherently manipulated via a second order sideband transition.

12:57PM M39.00008 ABSTRACT WITHDRAWN —
1:15PM M39.00009 Photon-assisted tunnelling with nonclassical microwaves in hybrid circuit QED systems by JEAN-RENE SOUQUET, McGill Univ, MATTHEW WOOLLEY, University of New South Wales, JULIEN GABELLI, PASCAL SIMON, QED systems — Motivated by recent experiments where superconducting microwave circuits have been coupled to electrons in semiconductor nanostuctures [1-3], we study theoretically the interplay of non-classical light produced in a cavity with electron transport through a tunnel junction [4]. We demonstrate that this basic light-matter interaction is naturally characterized by non-positive definite quasi-probability distributions which are intimately connected to the Glauber-Sudarshan P-function. We further demonstrate that this negative quasi-probability has unequivocal signatures on the differential conductance that should be easily detectable in state of art experiments. This thus turns the tunnel junction into a non-trivial probe of the microwave state. We also present a rigorous extraction of the interaction current on the cavity.

1:27PM M39.00010 Novel quantum electro-optic transducer for quantum information processing using superconducting 3D qubits by H. PAIK, L. S. BISHOP, D. T. MCCLURE, S. FILIPIK, J. M. GAMBITTA, C. B. LIRAKIS, IBM T. J. Watson Research Center, C. A. RYAN, J. SCHLAFER, M. P. DA SILVA, M. SOLTANI, M. PATEL, Z. DUTTON, Raytheon BBN Technologies — We propose a novel electro-optic system, SQOT (Superconducting Qubit Optical Transducer) [1] which can directly exchange quantum information between optical photons at telecom frequencies and superconducting qubits. Our scheme is based on three-dimensional qubits directly on top of a ultra-high Q whispering gallery mode optical cavity. The optical cavity is itself made from an electro-optic material such that we obtain a direct microwave-optical interaction between the qubit and optical cavity. In this talk, we present recent progress in designing and building the SQOT device and some challenges such as fabricating Josephson junctions on the electro-optic material and cryogenic microwave losses and possible solutions. [1] H. Paik, U.S. Patent Submitted (2013)

1:39PM M39.00011 Manipulation of non-classical microwave states using parametric interactions by MANUEL CASTELLANOS-BELTRAN, NIST - Boulder, MICHAEL DEFEO, ADAM SIROIS, LEONARDO RANZANI, NIST - Boulder, University of Colorado - Boulder, RAYMOND SIMMONDS, JOHN TEUFEL, JOSE AUMENTADO, NIST - Boulder — A primary tool for research in quantum optics has been the generation of exotic quantum states – such as Fock states or superpositions of two coherent states. These states have served well in many basic tests of the foundations of quantum theory and the latter may eventually prove useful for quantum computing, communication, and metrology. One important requirement for the generation and use of these states is their precise control and manipulation. In this respect, c-QED is a very versatile tool. In the past decade there have been extensive improvements in the storage and retrieval of quantum states of light in this experimental platform and more recently in the manipulation of those states using parametric interactions. In this talk, I will discuss our progress toward the goal of efficiently generating a superposition of small-amplitude coherent states, as well as their detection. This follows from our attempt/goal to implement an “on-chip” optical table which utilizes parametric interactions for state preparation and measurement. I will also discuss how we use homodyne tomography to fully characterize the states prepared in our setup.

1:51PM M39.00012 Fast control and Floquet state dynamics of a strongly driven superconducting qubit by CHUNQING DENG, FEIRUO SHEN, JEAN-LUC ORGIAZZI, Univ of Waterloo, SAHEL ASHHAB, Qatar Environment and Energy Research Institute, ADRIAN LUPASCU, Univ of Waterloo — Floquet states are quasi-stationary solutions of the Schrödinger equation with a time-periodic Hamiltonian. They are the appropriate states for describing the dynamics of a qubit in the strong driving regime, where the rotating wave approximation is no longer valid. We performed experiments on strong driving of a superconducting flux qubit using pulses with sub-nanosecond duration. We explore driving strength up to 5.0 GHz, largely exceeding the qubit Larmor frequency of 2.2 GHz. Floquet state dynamics is visible in the appearance of fast oscillating components in the qubit evolution in the rotating frame. Using pulse shaping, we also demonstrate the control of adiabatic/nonadiabatic transitions between the Floquet states. The control of the Floquet states is relevant for high-fidelity single-qubit operations in the strong driving regime.

2:03PM M39.00013 Probing an ensemble of superconducting devices by ADAM SEARS, DAVID HOVER, THEODORE GUDMUNSDEN, JONILYN L. YODER, MIT Lincoln Laboratory, ARCHANNA KAMIL, FLEI YAN, SIMON GUSTAVSSON, Research Laboratory of Electronics, Massachusetts Institute of Technology, ANDREW KERNER, WILLIAM OLIVER, MIT Lincoln Laboratory — We present experimental results on a system in which we use a flux qubit to probe an ensemble of weakly coupled superconducting devices. We employ standard qubit metrology techniques to reveal global device properties. In addition, we discuss the connection with engineered environmental decoherence. This work is sponsored by the Assistant Secretary of Defense for Research & Engineering under Air Force Contract FA8721-05-0002. Opinions, interpretations, conclusions, and recommendations are those of the authors and are not necessarily endorsed by the United States Government.


11:15AM M41.00001 Driving with squeezed vacuum in strong dispersive circuit-QED by MATTHEW ELLIOTT, ERAN GINOSAR, Advanced Technology Institute and Department of Physics, University of Surrey, Guildford, Surrey GU2 7XH — Recent experiments have demonstrated that it is possible to achieve a significant interaction between a squeezed microwave state and a superconducting qubit. Motivated by the success of coherent driving in circuit-QED, we study the dynamics of a two-part system where the squeezed output of a degenerate Josephson parametric amplifier, is used to drive a cavity-qubit system. We develop a Gaussian mean field model to describe the cavity state in the strong-dispersive regime and use this to investigate its steady-state behaviour. We compare this to full numerical solutions of the master equation, allowing us to also consider transient dynamics. Despite the effect of the qubit non-linearity, we demonstrate that it is possible to generate a stable, highly squeezed intracavity field in a range of parameters where the qubit can be used to reconstruct the states of the cavity. These results are testable using current experimental set-ups. Additionally, we discuss possible applications in the characterisation of sources of itinerant squeezed vacuum.

11:27AM M41.00002 Measurement of an ac Stark shift in a superconducting qubit under strong Rabi drive by YOUNG CHONG, DONG-GWANG HA, JUNG HWAN PARK, WON SONG, Korea Research Institute of Standards and Science, GWAN YEOL PARK, SOON GUL LEE, Korea University — We present a measurement of an ac Stark shift in a superconducting 3D transmon qubit. The qubit is strongly coupled to a superconducting aluminum cavity in circuit QED architecture. We observed the ac Stark shift under strong Rabi drive and measured it from detuning behavior of the Rabi oscillations as a function of the Rabi frequency. We also confirmed the shift by the Butler-Townes splitting measurement as a function of the qubit drive power.
11:39AM M41.00003 Observation of Dark State in a Three-dimensional Transmon Superconducting Qutrit

YUHAO LIU, XINSHENG TAN, DONG LAN, PENG ZHAO, JIE ZHAO, MENGMENG LI, SHUDONG HUANG, HAIFENG YU, SHILIANG ZH, YANG YU, School of Physics, Nanjing University, China — Dark state refers to a particular state of a quantum system that cannot absorb or emit photons in driving fields. It has important applications in quantum information processing and quantum metrology. Here we report the observation of dark state in a three-dimensional transmon superconducting qutrit. The transmon qutrit, which has cascade three energy levels $|0\rangle$, $|1\rangle$ and $|2\rangle$, is embedded in the center of a rectangle waveguide cavity. When two tone microwaves are applied resonantly between $|0\rangle$, $|1\rangle$ and $|2\rangle$, the state of the system will evolve in time domain. However, if we initialize the qutrit in the coherent superposition state, it will not change with time for certain driving amplitudes. The observed relationship between the initial state and the amplitudes of the two tone microwaves agrees well with the results from numerical calculations.

1Work supported by the SKPBR of China (2011CB922104, 2011CB9200205) and NSFC (91021003, 91321310, 11274156).

11:51AM M41.00004 Resonance Fluorescence and Photon Correlations Produced by 1-10 Qubits in 1D Infinite or Semi-Infinite Waveguides

YAO-LUNG L. FANG, HARALD BARANGER, Duke University — We study multiple two-level systems (2LS) coupled to a 1D waveguide in which one end is open and the other is either open (infinite waveguide) or closed (semi-infinite). Resonance fluorescence and two-photon correlations are presented for weak coherent driving. We show that while for a single 2LS coupled to an infinite waveguide the reflected photons are initially anti-bunched, for a semi-infinite waveguide they become highly bunched. As the number of 2LS increases (up to 10), rapid oscillations build up in the correlations that persist for a long time. At the same time, incoherently reflected photons are mostly distributed within the photonic band gap when driven resonantly, accompanied by sharp side peaks. Our calculations can be explained using the poles of the Green function in the Markovian regime together with the notion of time delay. Finally, in the non-Markovian regime we demonstrate that a 2LS in a semi-infinite waveguide can no longer be decoupled by placing it at the node of the photonic field, in sharp contrast to a recent experimental finding in the Markovian regime using superconducting qubits.

Work supported by the U.S. NSF (PHY-14-04125)

12:03PM M41.00005 Electromagnetically induced transparency and coherent population trapping with a superconducting artificial atom

SERGEY NOVIKOV, University of Maryland, College Park, TIMOTHY M. SWEENEY, J.E. ROBINSON, Laboratory for Physical Sciences, BALADITYA SURI, University of Maryland, College Park, F.C. WELLSTOOD, QJI, CNAM, Dept. of Physics, University of Maryland, College Park, B.S. PALMER, Laboratory for Physical Sciences — We embed a superconducting Al/AlOx/Al transmon qubit that acts as an artificial atom in a three-dimensional copper microwave cavity at a temperature of 22 mK. By addressing the hybridized qubit-cavity levels with two microwave drives (probe and coupler), we are able to create a $\Lambda$-like system with highly asymmetric decay rates. We observe electromagnetically induced transparency, and use this feature to achieve coherent population trapping (CPT) by creating a superposition state with the two drives whose duration is much longer than any coherence times in the system. After the drives are turned off, the resultant CPT dark state is coherent for $T_{\mathrm{CPT}} \approx 7.4 \mu s$. We estimate the minimum fidelity of the dark state achievable in this system to be 60%. These results present a way of superposition and entanglement generation with CW tones in a superconducting system.

12:15PM M41.00006 Electromagnetically Induced Superluminal Light in a 3D Transmon Device

TIMOTHY M. SWEENEY, Lab. for Physical Sciences, BALADITYA SURI, University of Maryland, College Park, F.C. WELLSTOOD, QJI, CNAM, Dept. of Physics, University of Maryland, B.S. PALMER, Lab. for Physical Sciences — Quantum interference in a three level $\Lambda$-type system can result in non-linear optical effects such as electromagnetically induced transparency/absorption (EIT/EIA), slow, and fast light. We have created a $\Lambda$ system with an effectively metastable state by dispersively coupling an Al/AlOx/Al transmon qubit (T$_1$ = 4 us) to a 3D Cu microwave cavity (T$_1$ = 340 ns). By probing the transmission through the cavity while pumping a qubit-cavity sideband yields a large change in the dispersion. We observe group advances of up to 10 us for Gaussian pulses propagating through the system, corresponding to a group index of -176,000.

12:27PM M41.00007 A superconducting qubit coupled to propagating acoustic waves

MARTIN V. GUSTAFSSON, Columbia University (USA) and Chalmers University of Technology (Sweden), THOMAS AREF, ANTON FRISK KOCKUM, MARIA K. EKSTRÖM, GÖRAN JOHANSSON, PER DELSING, Chalmers University of Technology (Sweden) — Mechanical devices in the quantum regime have so far consisted mainly of suspended resonators, where standing modes can be populated with quanta of vibrational energy. We present a fundamentally different system, where the mechanical excitation is not restricted to a specific mode and location. Instead, we demonstrate strong non-classical coupling between propagating phonons and a superconducting qubit. The qubit is fabricated on a piezoelectric substrate, and is designed to interact with Surface Acoustic Waves (SAWs) in the gigahertz frequency range. A separate on-chip transducer allows us to launch SAWs toward the qubit from a distance and pick up SAW phonons that the qubit reflects and emits. In a series of experiments where the qubit is addressed both electrically and acoustically, we show that the qubit couples much more strongly to SAWs than to any electrical modes. The low speed of sound sets phonons apart from photons as a medium for transporting quantum information, and should enable real-time manipulation of propagating quanta. The short acoustic wavelength and strong piezoelectric coupling should also allow regimes of interaction to be explored which cannot be reached in photonic systems.

1Gustafsson et al., Science 346, 207 (2014)

12:39PM M41.00008 Strong qubit-phonon interactions in a superconducting 1D open space

POL FORN-DIAZ, JEAN-LUC ORGIAZZI, MARTIN OTTO, ALI YURTALAN, Institute for Quantum Computing, University of Waterloo, Waterloo, Canada, BORJA PEROPADRE, Department of Chemistry and Chemical Biology, Harvard University, Cambridge MA, USA, JUAN-JOSE GARCIA-RIPOLL, Instituto de Física Fundamental IFF-CSIC, Madrid, Spain, CHRISTOPHER WILSON, ADRIAN LUPASCU, Institute for Quantum Computing, University of Waterloo, Waterloo, Canada — The field of superconducting quantum circuits has seen much progress using many ideas formerly developed for atomic systems, while at the same time exploring new avenues unattainable in other quantum systems. A novel, promising architecture for fundamental studies of quantum electrodynamics in one dimension can be built by coupling a single superconducting qubit to a transmission line [1]. The qubit interacts with the modes of the transmission line, behaving like a single scatterer that can interfere strongly with propagating photons. The interaction between the qubit and the propagating modes of the line can be made ultrastrong, thus enabling a new domain of physics and applications to be investigated. We will present preliminary results on an experiment consisting in a flux qubit-transmission line system at different coupling strengths and its connection to existing models of spin-boson physics [2].

A interacting with a one-dimensional waveguide through a realistic minimal-coupling interaction. We show that the diamagnetic term

Manufacturing

IEEE JOURNAL OF QUANTUM ELECTRONICS, VOL. 24, NO. 8, AUGUST 1988

two collective cooperativity parameters.

We present spectroscopic quantum operations in hybrid quantum systems. As an example of the application, we determine their coupling to transmon qubits with different frequencies and we present a bi-chromatic scheme for entanglement and gate operations. In this calculation, we obtain a maximally entangled state with a fidelity $F = 95\%$. Our proposal is competitive with the achievements of other entanglement-gates with superconducting devices and it may offer some advantages: (i) There is no need for additional control lines and dephasing associated with the conventional frequency tuning of qubits. (ii) When our qubits are idle, they are far detuned with respect to each other and to the resonator, and hence they are immune to cross talk and Purcell-enhanced decay.


12:51PM M41.00009 Flux qubit ultrastrongly coupled to two resonators. A. BAUST, E. HOFFMANN, M. HAEBERLEIN, M.J. SCHWARZ, P. EDER, J. GOETZ, F. WULSCHNER, E. XIE, L. ZHONG, K. FEDOROV, E.P. MENZEL, F. DEPPE, A. MARX, R. GROSS, TU Muenchen, Nanosystems Initiative Munich and Walther-Meissner-Institut, Germany — Circuit quantum electrodynamics has not only become a versatile toolbox for quantum information processing, but is also a powerful platform for the investigation of light-matter interaction. The coupling strength between microwave resonators and qubits acting as artificial atoms can be tuned over several orders of magnitude and can even reach the regime of ultrastrong coupling. We present a recently developed gapless two-qubit setup coupling two qubits with a long superconducting resonator. We report the first observation of a strong coupling regime between microwave resonators and qubits acting as artificial atoms.

By minimal, we mean that sending just one photon two photons are generated through the qubit. In our calculations, the parameters are taken from the chip reported in a recent Science paper by the Wallraff group [van Loo et al, Science 342, 1494 (2013)].

1:03PM M41.00010 ABSTRACT WITHDRAWN —

1:15PM M41.00011 Circuit QED Photonics, DAVID ZUECO, EDUARDO Sánchez-BURILLO, Universidad de Zaragoza-CSIC, JUANJO GARCIA-RIPOLL, CSIC, LUIS MARTÍN-MORENO, Universidad de Zaragoza-CSIC — In this talk we report our theoretical results for the scattering of few photons against few two level systems. The photons travel through an open superconducting coplanar waveguide transmission line and the two level systems can be flux qubits or transmons. Several phenomena will be discussed: the linear and nonlinear behavior as a function of the ratio between the number of photons and number of qubits. For the case of flux qubits we discuss the cases of strong and ultrastrong line-qubits coupling. Different phenomena are found and described: Fano profiles, Raman scattering, photon generation and novel and non-perturbative qubit-qubit interecations through the line. Finally, we consider the case of transmon qubits. We theoretically demonstrate that driven transmons can be used as a minimal setup for doing up and downconversion. By minimal, we mean that sending just one photon two photons are generated through the qubit. In our calculations, the parameters are taken from the chip reported in a recent Science paper by the Wallraff group [van Loo et al, Science 342, 1494 (2013)].

1:27PM M41.00012 Light-matter decoupling and $A^2$ term detection in superconducting circuits. JUAN JOSE GARCÍA-RIPOLL, Instituto de Física Fundamental, IFF-CSIC, Madrid, BORJA PEROPADRE, Department of Chemistry and Chemical Biology, Harvard University, SIMONE DE LIBERATO, School of Physics and Astronomy, University of Southampton — We study the spontaneous emission of a qubit interacting with a one-dimensional waveguide through a realistic minimal-coupling interaction. We show that the diamagnetic term $A^2$ leads to an effective decoupling of a single qubit from the electromagnetic field. This effect is observable at any range of qubit-photon couplings. For this we study a setup consisting of a transmon that is suspended over a transmission line. Assuming a standard model of qubit-line interaction, we prove that the relative strength of the $A^2$ term is controlled with the qubit-line separation and show that, as a consequence, the spontaneous emission rate of the suspended transmon onto the line can increase with such separation, instead of decreasing.

1:39PM M41.00013 Beyond strong coupling in a massively multimode cavity, NEEREJA SUNDARESAN, YANBING LIU, DARIUS SADRI, LASZLO SZOCS, DEVIN UNDERWOOD, MOEIN MALEKAKHLAGH, HAKAN TÜRECİ, ANDREW HOUCK, Princeton University — We present experiments in a new regime of cavity quantum electrodynamics (cQED), the multimode strong coupling regime, in which the qubit-cavity coupling is comparable to the free spectral range, thus requiring the collective treatment of all modes along with the qubit. Here we show that this regime is accessible in circuit QED by coupling a 90MHz microwave cavity with a transmon qubit, resonant with the 75th harmonic with a coupling strength exceeding 30MHz. When driving this system, we observe multimode fluorescence consistent with cavity-enhanced sideband emission, with unexpected multi-photon processes and the emergence of ultra-narrow linewidths. This multimode coupling opens the door for a wide range of potential experiments, including studying the manifestation of complex many-body phenomena, the breakdown of the rotating wave approximation, and the bridge between discrete and continuous Hilbert spaces.

1:51PM M41.00014 Multi-frequency modes in superconducting resonators: Bridging frequency gaps in off-resonant couplings, CHRISTIAN KRAGLUND ANDERSEN, KLAUS MØLMER, Univ of Aarhus — A SQUID inserted in a superconducting waveguide resonator imposes current and voltage boundary conditions that make it suitable as a tuning element for the resonator modes. If such a SQUID element is subject to a periodically varying magnetic flux, the resonator modes acquire frequency side bands. We calculate the multi-frequency eigenmodes and these can couple resonantly to physical systems with different transition frequencies and this makes the resonator an efficient quantum bus for weak and strong coupling schemes.


2:03PM M41.00015 Amplitude Bistability in the Multimode Regime of Circuit-QED, MOEIN MALEKAKHLAGH, NEEREJA SUNDARESAN, YANBING LIU, DARIUS SADRI, ANDREW HOUCK, HAKAN TÜRECİ, Princeton University, MESOSCOPIC QUANTUM OPTICS GROUP TEAM, QUANTUM COMPUTING AND CONDENSED MATTER PHYSICS WITH MICROWAVE PHOTONS TEAM — In theory of dynamical systems, bistability refers to a situation where the system has two possible stable equilibrium states. For certain optical devices, it is possible to have two resonant transmission states that only differ in amplitude and is referred as “optical amplitude bistability.” This phenomenon occurs due to nonlinear nature of light-matter interaction where the light absorption or blockade by the absorber strongly depends on the drive strength. The transition between these two bistable solutions happens when the absorber is saturated and no longer capable of blocking light. In this talk, we study the dynamics of a transmon qubit coupled to a large number of modes of a long superconducting resonator and driven by an external microwave drive. We introduce a generalized theory of multimode amplitude bistability first discussed by C.M. Savage and H.J. Carmichael [1] for a resonant single mode cavity. We will demonstrate that bistability is a characteristic of the entire system including the qubit and all modes of the resonator and can be characterized analytically by the knowledge of two collective cooperativity parameters.


Wednesday, March 4, 2015 11:15AM - 2:15PM –
Session M43 DPOLY FIAP: Focus Session: Industry Day: Applied Polymer Physics in Advanced Manufacturing 214C - Brent Neal, Milliken & Company
Elasticity and Extensibility Determine Printability and Spinnability of Polymer Solutions. Jelena Dinić, Leidy Nallely Jiménez, Vicky Mei Yiran Zhang, Vivek Sharma. Chemical Engineering, University of Illinois Chicago. Many advanced manufacturing technologies like inkjet printing, 3D printing, nano-fiber spinning, gravure printing and nano-imprint lithography involve complex free-surface flows, where both shear and extensional rheology affect processability. In applications that involve progressive thinning and break-up of a fluid column or sheet into drops, the dominant flow within the filament is extensional in nature. Polymer fluids exhibit a much larger resistance to flow in an elongational flow field than Newtonian fluids with same shear viscosity. Characterizing the filament thinning and break-up kinetics in jetting, dripping and stretching liquid bridge provides invaluable insight into the interplay of elastic, viscous, capillary and inertial stresses relevant for these applications. In this talk, we elucidate how polymer composition, flexibility, and molecular weight determine the kinematics of capillary-driven thinning and pinch-off in our experiments. Both effective relaxation time and transient extensional viscosity are found to be strongly concentration dependent even for dilute solutions. Further, we show how fragile extensibility of polymers dramatically changes the kinematics from elastocapillary to visco-capillary under strong extensional flow fields that can lead to coil-stretch transition.

Controlling Fiber Morphology in Simultaneous Centrifugal Spinning and Photopolymerization. Yichen Fang, Austin Dulaney, Christopher Ellison. University of Texas at Austin - McKetta Department of Chemical Engineering. Current synthetic fiber manufacturing technologies use either solvent or heat to transform a solid preformed polymer into a liquid before applying a force to draw the liquid into fiber. While the use of solvent poses concerns regarding process safety and environmental impact, the use of heat may also lead to polymer degradation and excessive energy consumption. To address these critical challenges, here we present an alternative fiber manufacturing method that encompasses extruding a monomer solution through an orifice, drawing it using centrifugal Forcespinning and polymerizing the monomer jet into solid fiber in flight using UV initiated thiol-ene chemistry. This method not only negates the use of both heat and solvent, but also produces fibers that are highly crosslinked, mechanically robust, and thermally stable. In this process, the balance between curing kinetics, fiber flight time, and solution viscoelasticity is essential. Studies were conducted to quantitatively investigate the effect of these factors on fiber formation and morphology. An operating diagram was developed to show how the intricate interplay of these factors led to the formation of smooth fibers and other undesirable fiber defects, such as beads-on-string, fused fibers, and droplets.

Engineering the Crystalline Morphology of Polymer Thin Films at a Molecular Level via Matrix Assisted Pulsed Laser Evaporation. Hyuncheol Jeong, Craig Arnold, Rodney Priestley. Princeton University. Controlling the crystalline morphology of polymeric thin films at a molecular level has been increasingly important due to their potential as the active layer in organic electronics. Typically, the crystalline morphology in films is achieved via thermal annealing or melt-crystallization of spin-cast polymers. This approach often leads to a spherulitic morphology where the crystalline lamellae grow in all directions. Here, we introduce an alternative approach to make crystalline polymer films via Matrix Assisted Pulsed Laser Evaporation (MAPLE). Using polyethylene oxide (PEO) as a model polymer, we show that the preferential orientation of polymer crystals can be controlled during the film growth. By laser-ablatting a frozen dilute solution of the desired polymer, MAPLE provides a non-destructive means for the deposition of polymer films. Due to the liquid nature of as-deposited polymers confined in nanodroplets, this technique can exploit the substrate effect on the crystal nucleation and growth of nano-confined polymers during the film growth. Mimicking the epitaxial growth of metallic films, this novel polymer deposition technique may enable the engineering of film properties in a way not achievable in bulk.

Coupling frontal photopolymerization and surface instabilities for a novel 3D patterning technology. Alessandra Vitale, Matthew Hennessy, Omar Matar, Imperial College London. Patterning of soft matter provides an exceptional route for the generation of micro/nanostructured and functional surfaces. We describe a new 3D fabrication process based on coupling frontal photopolymerization (FPP) with precisely controlled, yet spontaneous, interfacial wrinkling. FPP is a complex spatio-temporal process that can lead to well-defined propagating fronts of network formation, both stable and unstable. We investigate this process focusing on the interfacial monomer-to-polymer conversion profile and its wave propagation. A simple coarse-grained model is found to describe remarkably well the planar frontal logarithmic kinetics, capturing the effects of UV light exposure time (or dose) and temperature, as well as the front position. In defined conditions, surface instabilities are introduced and interfere with wave planarity, resulting in the formation of "minimal" surfaces with complex 3D geometries. Building on this understanding on the propagation of wavefronts of network formation during photopolymerization, we demonstrate the design and fabrication of 3D patterned polymer materials with tunable shapes with optical and surface functionality.

Improving information density in ferroelectric polymer films by using nanoimprinted gratings. Daniel E. Martínez-Tong, Département de Physique, Faculté des Sciences, Université libre de Bruxelles (ULB), Boulevard du Triomphe, 1050 Brussels, Belgium. The development of polymer non-volatile memories depends on the effective fabrication of devices with high information density. Well-defined low aspect ratio nanogratings on thin films of poly(vinylidene fluoride–trifluoroethylene) copolymers can be fabricated by using Nanoimprint Lithography (NIL). By using these nanogratings, an improved management of writing and reading information can be reached as revealed by Piezoresponse Force Microscopy (PFM). Structural investigation by means of Grazing Incidence X-ray (GX) scattering techniques indicates that the physical confinement generated by nanoimprint promotes the development of smaller and edge-on oriented crystals. Our results evidence that one-dimensional nanostructuring can be a straightforward approach to improve the control of the polarization in ferroelectric polymer thin films.
mobilities, \( P \) can be used to reveal additional structure in the MBL phase, and to make progress on otherwise intractable theory problems. I also show how this “spectral perspective” is far more robust than the conventional “eigenstate” perspective. Eigenstates thermalize upon functions of local operators, evaluated in arbitrary states. This perspective reformulates the standard theory in terms of (in principle) experimentally measurable quantities. Moreover, this “spectral” perspective on MBL is far more robust than the conventional “eigenstate” perspective. Eigenstates thermalize upon arbitrary weak coupling to an external environment, but the correlation functions (which are the physical observables) continue to show signatures of MBL as long as the coupling to the environment is weaker than the characteristic energy scales in the system Hamiltonian. I explain how MBL can be reformulated without invoking exact eigenstates or perfect isolation. I introduce a way to think about MBL in terms of correlation functions. I study a two-level system controlled in a discrete feedback loop, modeling both the system and the controller in terms of stochastic Markov processes. We find that the extracted work, which is known to be bounded from above by the mutual information acquired during measurement, has to be compensated by an additional energy supply during the measurement process itself, which is bounded by the mutual information from below. Our results confirm that the total cost to operate an information engine is in full agreement with the conventional second law of thermodynamics. We also consider the efficiency of the information engine in the finite-time case.

The standard theory of many body localization (MBL) is framed in terms of exact eigenstates of perfectly isolated quantum systems. Has shown that human pluripotent stem cells differentiated in 3D environments are mature and possess high degree of biological function necessary for them to function in vivo. 3D Printing of Personalized Organs and Tissues, KAIMING YE, SUNY Binghamton — A wide variety of systems exhibiting spatiotemporal chaos have been shown to be extensive, in that their fractal dimensions grow linearly with volume. Ruelle argued that this extensivity is evidence that these systems can be viewed as a gas. We have tested this hypothesis by performing large-scale computational studies of spatiotemporal chaos in the 1D complex Ginsburg-Landau equation, and we have found that aspects of the coarse-grained system are well-described not only as a gas, but as an equilibrium gas. This result not only supports Ruelle’s picture but also suggests that the coarse-grained behavior of this far-from-equilibrium system might be understood using equilibrium statistical mechanics.

How to detect many body localization in experiments, RAHUL NANDKISHORE. The standard theory of many body localization (MBL) is framed in terms of exact eigenstates of perfectly isolated quantum systems. However, exact eigenstates can neither be prepared nor measured in the laboratory, and perfectly isolated quantum systems are equally unrealizable. In this talk I explain how MBL can be reformulated without invoking exact eigenstates or perfect isolation. I introduce a way to think about MBL in terms of correlation functions of local operators, evaluated in arbitrary states. This perspective reformulates the standard theory in terms of (in principle) experimentally measurable quantities. Moreover, this “spectral” perspective on MBL is far more robust than the conventional “eigenstate” perspective. Eigenstates thermalize upon arbitrarily weak coupling to an external environment, but the correlation functions (which are the physical observables) continue to show signatures of MBL as long as the coupling to the environment is weaker than the characteristic energy scales in the system Hamiltonian. I also show how this “spectral perspective” can be used to reveal additional structure in the MBL phase, and to make progress on otherwise intractable theory problems.

Kinetics of Brownian Maxima, ELI BEN-NAIM, Los Alamos National Laboratory, PAUL KRAPIVSKY, Boston University — We study extreme-value statistics of Brownian trajectories in one dimension. We define the maximum as the largest position to date and compare maxima of two particles undergoing independent Brownian motion. We focus on the probability \( P(t) \) that the two maxima remain ordered up to time \( t \), and find the algebraic decay \( P \sim t^{-\beta} \) with exponent \( \beta = 1/4 \). When the two particles have diffusion constants \( D_1 \) and \( D_2 \), the exponent depends on the mobilities, \( \beta = \frac{1}{4} \arctan \sqrt{D_2/D_1} \). We also use numerical simulations to investigate maxima of multiple particles in one dimension and the largest extension of particles in higher dimensions.
12:27PM M44.00007 Attaining local temperatures close to absolute zero in a nonequilibrium quantum system. ABHAY SHASTRY, CHARLES STAFFORD, University of Arizona — We consider a question motivated by the third law of thermodynamics: Can there be a local temperature arbitrarily close to absolute zero in a nonequilibrium quantum system? We consider ballistic quantum conductors with the source reservoir held at finite temperature and the drain held at or near absolute zero, a problem outside the scope of linear response theory. We compute the local temperature by numerically solving a nonlinear system of equations describing equilibration of a scanning thermoelectric probe with the system, and obtain excellent agreement with analytic results derived using a method analogous to the Sommerfeld expansion.

12:39PM M44.00008 Local temperature of an interacting quantum system far from equilibrium. CHARLES STAFFORD, University of Arizona — A theory of local temperature measurement of an interacting quantum electron system far from equilibrium via a floating thermoelectric probe is developed [1]. A number of relations are derived relating the probe temperature (and chemical potential) to the local properties of the nonequilibrium system, including a fluctuation-dissipation relation [2]. It is shown that the measured local electron temperature of a steady-state system far from equilibrium is consistent with the zeroth, first, second, and third laws of thermodynamics, provided the probe-system coupling is weak and broad band (ideal temperature measurement). For general probe-system couplings, there are corrections to the zeroth and first laws that are higher-order in the Sommerfeld expansion. The corrections to the zeroth and first laws are related, and can be interpreted in terms of the error of a non-ideal temperature measurement. [1] C. A. Stafford, arXiv:1409.3179; [2] J. Meari, J. P. Bergfield, C. A. Stafford, Ph. Jacquod, Phys. Rev. B 90, 035407 (2014)

12:51PM M44.00009 Thermodynamics of Maximum Transition Entropy for Quantum Assemblies. DAVID ROGERS, University of South Florida — We present one possible unifying framework for the statistics of driven quantum systems in terms of a stochastic propagator for the density matrix. Its classical limit [Rogers, Beck and Rempe, J. Stat. Phys 145:385, 2011] takes the form of a Langevin equation with an associated large-deviation functional intimately related to the partition function of statistical mechanics. Surprising results of this quantum theory are that work is a measurable quantity, and that a precise form of the second law of thermodynamics can be stated for dynamical systems. Numerical results are presented for the time-course of work and heat production for trapped 1D particles. Properties of the large deviation functional are discussed in the context of the quantum measurement problem.

1:03PM M44.00010 Entropy Production in Isolated Quantum Many-Body Systems. EDGARDO SOLANO CARRILLO, ANDREW MILLIS, Columbia University — Beginning with the Liouville-von Neumann equation for the density matrix of an isolated quantum many-body system, and applying well-known projection-operator techniques, we derive an equation of motion for the rate of change of the thermodynamic entropy, valid to arbitrary order in the perturbation deviating the system from equilibrium. To lowest order, a balance equation is obtained which coincides with the one defining the entropy production in irreversible thermodynamics. A connection with fluctuation theorems is mentioned, as well as an application of the results to clarify the “thermalization problem” in the Jaynes-Cummings model.

1:15PM M44.00011 ABSTRACT WITHDRAWN —

1:27PM M44.00012 Spin Noise Spectroscopy Beyond Thermal Equilibrium and Linear Response. NIKOLAI SINITSYN, Theoretical Division, Los Alamos National Laboratory, PHILIPP GLASENAPP, Experimentelle Physik, Technische Universität Dortmund, D-44221 Dortmund, Germany, DIBYENDU ROY, Experimentelle Physik, Technische Universität Dortmund, D-44221 Dortmund, Germany, LUYI YANG, SCOTT CROOKER, National High Magnetic Field Lab, Los Alamos National Laboratory, D. G. RICKEL, National High Magnetic Field Lab, Los Alamos National Laboratory, ALEX GREILICH, M. BAYER, Experimentelle Physik, Technische Universität Dortmund, D-44221 Dortmund, Germany, LUYI YANG, SCOTT CROOKER, National High Magnetic Field Lab, Los Alamos National Laboratory — Per the fluctuation-dissipation theorem, the information obtained from spin fluctuation studies in thermal equilibrium is necessarily constrained by the systems linear response functions. However, by including weak radio frequency magnetic fields, we demonstrate that intrinsic and random spin fluctuations even in strictly unpolarized ensembles can reveal underlying patterns of correlation and coupling beyond linear response, and can be used to study nonequilibrium and even multiphoton coherent spin phenomena. We demonstrate this capability in a classical vapor of 41K alkali atoms, where spin fluctuations alone directly reveal Rabi splittings, the formation of Mollow triplets and Autler-Townes doublets, ac Zeeman shifts, and even nonlinear multiphoton coherences.

1:39PM M44.00013 Finite N corrections to Vlasov dynamics and the range of pair interactions. ANDREA GABRIELLI, Institute of Complex Systems (ISC) - CNR (Italy), MICHAEL JOYCE, JULES MORAND, LPNHE - Univ. Paris VI "Pierre et Marie Curie" (France) — We explore [1] the conditions on a pair interaction for the validity of the Vlasov equation to describe the dynamics of an interacting N particle system in the large N limit. Using a coarse-graining in phase space of the exact Klimontovich equation for such a system, we evaluate the scalings with N of the terms describing the corrections to the Vlasov equation for the coarse-grained one particle phase space density. Considering an interaction with radial pair force $F(r) \sim 1/r^d$, regulated to a bounded behavior below a "softening" scale l, we find that there is an essential qualitative difference between the cases $a<d$ (i.e. the spatial dimension) and $a>d$, i.e. depending on the the integrability at large distances of $F(r)$. For $a<d$ the corrections to the Vlasov dynamics for a given coarse-grained scale are essentially insensitive to the softening parameter l, while for $a>d$ the corrections are directly regulated by l, i.e. by the small scale properties of the interaction, in agreement with the Chandrasekhar approach [2]. This gives a simple physical criterion for a basic distinction between long-range $(a<d)$ and short range $(a>d)$ interactions, different from the thermodynamic one $(a<d-1)$ or $(a>d-1)$. This alternative classification, based purely on dynamical arguments, is relevant notably to understanding the conditions for the existence of so-called quasi-stationary states in long-range interacting systems.

1:51PM M44.00014 Molecular dynamics study on a nonequilibrium motion of a colloidal particle driven by an external torque, DONGHWAN YOO, Myongji University, YOUNGKyun JUNG, KISTI, CHULAN KWON, Myongji University — We investigate the motion of a colloidal particle driven out of equilibrium by an external torque. We use the molecular dynamics simulation that is alternative to the simulation based on the Langevin equation and is expected to mimic an experiment more realistically. We choose a heat bath composed of about a thousand particles interacting to each other through the Lenard-Jones potential and impose the Langevin thermostat to maintain it in equilibrium. We prepare a colloidal particle to interact with the particles of the heat bath also by the Lenard-Jones potential while any dissipative force and noise are not employed explicitly. We study the stochastic properties of the nonequilibrium fluctuation for work and heat produced incessantly in the steady state. We accurately confirm the fluctuation theorem for the work production. We also investigate the motion beyond the overdamped limit by varying the mass of the particle. We compare our result with a previous theoretical result in the overdamped limit based on the Langevin equation.


2:03PM M44.00015 Transient Orthogonality Catastrophe in a Time Dependent Nonequilibrium Environment, MARCO SCHIRO, CNRS and CEA-Saclay, ADITI MITRA, NYU, 0 TEAM — We study the response of a highly-excited time dependent quantum many-body state to a sudden local perturbation, a sort of orthogonality catastrophe problem in a transient non-equilibrium environment. To this extent we consider, as key quantity, the overlap between time dependent wave-functions, that we write in terms of a novel two-time correlator generalizing the standard Loschmidt Echo. We discuss its physical meaning, general properties, and its connection with experimentally measurable quantities probed through non-equilibrium Ramsey interferometry schemes. Then we present explicit calculations for a one dimensional interacting Fermi system brought out of equilibrium by a sudden change of the interaction, and perturbed by the switching on of a local static potential. We show that different scattering processes give rise to remarkably different behaviors at long times, quite opposite from the equilibrium situation. In particular, while the forward scattering contribution retains its power law structure even in the presence of a large non-equilibrium perturbation, with an exponent that is strongly affected by the transient nature of the bath, the backscattering term is a source of non-linearity which generates an exponential decay in time of the Loschmidt Echo, reminiscent of the standard Loschmidt Echo. The main points of our approach are: (i) The use of a generating function formalism, (ii) The derivation of simple equations for the moments of these clusters.

We discuss the intimate connection between network symmetry and cluster synchronization. We apply computational group theory to reveal the clusters and determine their stability. In complex networks the symmetries can number in the millions, billions, and more. The connection between symmetry and cluster synchronization is experimentally explored using an electro-optic polarization modulator to observe and explain a new dynamical state in which acluster of pendulums loses synchrony while leaving others connected to them synchronized. We show the isolated desynchronization is intimately related to the decomposition of the group of symmetries into subgraphs. The results could guide the design of new power grid systems or lead to new understanding of the dynamical behavior of networks ranging from neural to social.

Wednesday, March 4, 2015 11:15AM - 2:03PM - Session M45 Focus Session: Emerging Topics in Network Synchronization: Patterns, Stability, and Transitions 216AB - Takashi Nishikawa, Northwestern University

11:15AM M45.00001 Symmetries, Cluster Synchronization, and Isolated Desynchronization in Complex Networks, LOUIS PECORA, Naval Research Laboratory — Many networks are observed to produce patterns of synchronized clusters, but it has been difficult to predict these clusters in general or understand the conditions for their formation. We show the intimate connection between network symmetry and cluster synchronization. We apply computational group theory to reveal the clusters and determine their stability. In complex networks the symmetries can number in the millions, billions, and more. The connection between symmetry and cluster synchronization is experimentally explored using an electro-optic polarization modulator to observe and explain a new dynamical state in which a cluster of pendulums loses synchrony while leaving others connected to them synchronized. We show the isolated desynchronization is intimately related to the decomposition of the group of symmetries into subgraphs. The results could guide the design of new power grid systems or lead to new understanding of the dynamical behavior of networks ranging from neural to social.

11:51AM M45.00002 Chimera states: limits and open questions, DANIEL ABRAMS, Northwestern University, MARK PANAGGIO, Northwestern University and Rose Hulman Institute of Technology — ‘Chimera states’ are surprising patterns that can be found in systems of identical coupled oscillators, where synchrony and incoherence seem to stably coexist in a spatially asymmetrical state. The existence and stability of chimera states in a variety of settings relevant to real-world systems remains an active topic of research. Here I summarize what is known and present preliminary results for interesting limits including small and large-N, small and large coupling lag, as well as near-local and near-global coupling.

12:03PM M45.00003 Cluster dynamics of pulse coupled oscillators, KEVIN O’KEEFFE, STEVEN STROGATZ, Cornell University, PAUL KRAPIVSKY, Boston University — We study the dynamics of networks of pulse coupled oscillators. Much attention has been devoted to the ultimate fate of the system: which conditions lead to a steady state in which all the oscillators are firing synchronously. But little is known about how synchrony builds up from an initially incoherent state. The current work addresses this question. Oscillators start to synchronize by forming clusters of different sizes that fire in unison. First pairs of oscillators, then triplets and so on. These clusters progressively grow by coalescing with others, eventually resulting in the fully synchronized state. We study the mean field model in which the coupling between oscillators is all to all. We use probabilistic arguments to derive a recursive set of evolution equations for these clusters. Using a generating function formalism, we derive simple equations for the moments of these clusters. Our results in good agreement simulation. We then numerically explore the effects of non-trivial connectivity. Our results have potential application to ultra-low power “impulse radio” & sensor networks.

12:15PM M45.00004 Driven Synchronization in Random Networks of Oscillators, JASON HINDES, CHRISTOPHER R. MYERS, Cornell University — Synchronization is a universal phenomenon found in many non-equilibrium systems. Much recent interest in this area has overlapped with the study of complex networks, where a major focus is determining how a system’s connectivity patterns affect the types of emergent behavior that it can produce. Thus far, modeling efforts have focused on the tendency of networks of oscillators to mutually synchronize themselves, and largely neglected the effects of external driving, even though both effects are present, and often compete, in many naturally occurring systems. In this work we study the interplay between mutual and forced synchronization in networks of phase oscillators, and in particular resolve how the structure and emergence of these states depends on the underlying network topology for simple random networks with a given contact distribution. We provide a bifurcation analysis, centering on the unfolding of a Takens-Bogdanov-Cusp singularity, which naturally separates homogeneous and heterogeneous network behavior, and determines the number, stability, and appearance of entrained and mutually synchronized states as a function of a few system parameters.

12:27PM M45.00005 Mode-Locking Behavior of Ihizikevich Neuron Under Periodic External Forcing, AMIRALI FAROKHNIAEE, EDWARD LARGE, Department of Physics, University of Connecticut — In this study we obtained the regions of existence of various mode-locked states on the periodic-strength plane, which are called Arnold Tongues, for Izhikevich neurons. The study is based on the new model for neurons by Izhikevich (2003) which is the normal form of Hodgkin-Huxley neuron. This model is much simpler in terms of the dimension of the coupled non-linear differential equations compared to other existing models, but excellent for generating the complex spiking patterns observed in real neurons. Many researchers have studied both of these cases, but the brain must encode amplitude variations of a periodic signal. These neurons under periodic stimulation display rich dynamical states including mode-locking and chaotic responses. Periodic stimuli such as sinusoidal waves and amplitude modulated (AM) sounds can lead to various forms of n : m mode-locked states, similar to mode-locking phenomenon in a LASER resonance cavity. Obtaining Arnold tongues provides useful insight into the organization of mode-locking behavior of neurons under periodic forcing. Hence we can describe the construction of harmonic and sub-harmonic responses in the early processing stages of the auditory system, such as the auditory nerve and cochlear nucleus.
12:39PM M45.00006 Synchronization On Hanoi Networks, SHANSHAN LI, STEFAN BOETTCHER, Emory University — Synchronization of coupled oscillators has been intensively studied on a variety of structures. It is believed that the dynamics is deeply associated with its structure. To explore this relation, we study the synchronization of coupled oscillators on Hanoi networks. We analyze the evolution of coupled units over time, and characterized the convergence to the global synchronized state. For this state, the results show a close connection to the spectrum of connectivity matrix. Inspired by this connection, we try to show a dynamical pattern that describes the entire synchronization process from the onset to the final state. This may unveil the unique hierarchical structure of these self-similar Hanoi networks. Our goal is to map the dynamics to the spectrum of the connectivity matrix that encodes significant information about the structure of the underlying system. This exploration may have implications on designing networks that synchronizes coupled units efficiently.

1Supported through NSF grant DMR-1207431

12:51PM M45.00007 Synchronization in growing populations of coupled oscillators and excitable elements, WEN YU, Graduate Student Research Assistant, Univ of Michigan - Ann Arbor, KEVIN WOOD, Assistant Professor, Univ of Michigan - Ann Arbor — In biological systems, synchronized dynamics often exist in growing populations. We show here that population growth can have significant effects on collective synchronization in discrete phase models of coupled oscillators or excitable elements. Using numerical simulations, mean field theory, and linear stability analysis, we demonstrate that coupling between population growth and synchrony can lead to a wide range of dynamical behavior, including extinction of synchronized oscillations, the emergence of asynchronous states with unequal state (phase) distributions, bistability between oscillatory and asynchronous states or between two asynchronous states, and modulation of the frequency of bulk oscillations.

1:03PM M45.00008 A Simple Kuramoto-like Circuit, ZHUWEI ZENG, DAVID MERTENS, Dickinson College — The toy model for spontaneous collective synchronization is the Kuramoto model, a model of nonlinear coupled phase oscillators. Although it is a popular theoretical tool, the Kuramoto model is too simple to accurately characterize the dynamics of any experimental collection of oscillators. In this talk, we present a simple electronic oscillator design similar to the Wien bridge design of Temirbayev et al. Although the oscillator is not strictly modeled by the Kuramoto model, it can be quantitatively modeled by a more generic phase oscillator model. The coefficients governing the oscillator’s behavior can be directly extracted from the voltage time series of the oscillator. We find that, in practice, only a handful of coefficients are necessary to quantitatively describe the behavior of the oscillators, making precise theory tractable.

1Dickinson Woodside Student-Faculty Research Fund

1:15PM M45.00009 A rule for coarse graining phase oscillator models, DAVID MERTENS, Dickinson College — The Kuramoto model is often studied as a paradigm for synchronization. Among phase oscillator models, the Kuramoto model exhibits unique properties that simplify the analysis, and call into question whether or not results from the Kuramoto model are applicable to other phase oscillator models. Instead of focusing on the Kuramoto model, I show how a coarse graining procedure can be applied to generic phase oscillator models with global coupling, providing an alternative method for analyzing their critical behavior. In particular, I discuss a simple geometrically motivated rule that is crucial for the coarse graining approximations.

1:27PM M45.00010 Phase patterns in finite oscillator networks with insights from the piecewise linear approximation, DANIEL GOLDSTEIN, Brandeis Univ — Recent experiments on spatially extend arrays of droplets containing Belousov-Zhabotinsky reactants have shown a rich variety of spatio-temporal patterns. Motivated by this experimental set up, we study a simple model of chemical oscillators in the highly nonlinear excitable regime in order to gain insight into the mechanism giving rise to the observed multistable attractors. When coupled, Zhabotinsky reactants have shown a rich variety of spatio-temporal patterns. Motivated by this experimental set up, we study a simple model of chemical oscillators in the highly nonlinear excitable regime in order to gain insight into the mechanism giving rise to the observed multistable attractors. When coupled, these two attractors have different preferred phase synchronizations, leading to complex behavior. We study rings of coupled oscillators and observe a rich array of oscillating patterns. We combine Tuning analysis and a piecewise linear approximation to better understand the observed patterns.

1:39PM M45.00011 Improving the Network Structure can lead to Functional Failures, TIAGO PEREIRA, Imperial College London, PHILIPP PADE, Humboldt University — In many real-world networks the ability to synchronize is a key property for their performance. Examples include power-grid, sensor, and neuron networks as well as consensus formation. Recent work on undirected networks with diffusive interaction revealed that improvements in the network connectivity such as making the network more connected and homogeneous enhances synchronization. However, real-world networks have directed and weighted connections. In such directed networks, understanding the impact of structural changes on the network performance remains a major challenge. Here, we show that improving the structure of a directed network can lead to a failure in the network function. For instance, introducing new links to reduce the minimum distance between nodes can lead to instabilities in the synchronized motion. This counter-intuitive effect only occurs in directed networks. Our results allow to identify the dynamical importance of a link and thereby have a major impact on the design and control of directed networks.

1:51PM M45.00012 Observability and Controllability of Nonlinear Networks: The Role of Symmetry, STEVEN SCHIFF, ANDREW WHALEN, SEAN BRENNAN, Penn State University, TIMOTHY SAUER, George Mason University — Observability and controllability are essential concepts to the design of predictive observer models and feedback controllers of networked systems. For example, noncontrollable mathematical models of real systems may have subspaces that influence model behavior, but cannot be controlled by an input. Such subspaces are difficult to determine in complex nonlinear networks. Since most of the present theory was developed for linear networks without symmetries, here we present a numerical and group representation framework, to quantify the observability and controllability of nonlinear networks with explicit symmetries that shows the connection between symmetries and measures of observability and controllability. We numerically observe and theoretically predict that not all symmetries have the same effect on network observation and control. We find that the presence of symmetry in a network may decrease observability and controllability, although networks containing only rotational symmetries remain controllable and observable. These results alter our view of the nature of observability and controllability in complex networks, change our understanding of structural controllability, and affect the design of mathematical models to observe and control such networks.

2National Academies - Keck Futures Initiative, NSF grant DMS 1216568, and Collaborative Research in Computational Neuroscience NIH grant 1R01EB014641.
11:15AM M46.00001 Soft Electronics for the Human Body, JOHN ROGERS, University of Illinois — Biology is soft, curvilinear and transient; modern silicon technology is rigid, planar and everlasting. Electronic systems that eliminate this profound mismatch in properties will lead to new types of devices, capable of integrating non-invasively with the body, providing function over some useful period of time, and then dissolving into surrounding bioloids. Recent work establishes a complete set of materials, mechanics designs and manufacturing approaches that enable these features in a class of electronics with performance comparable to that of conventional wafer-based technologies. This talk summarizes the key ideas through demonstrations in skin-mounted ‘epidermal’ monitors, advanced surgical tools and biodegradable electronic bactericides.

11:51AM M46.00002 The Physics of Food, DAVID WEITZ, Harvard University — This talk will describe some experiences gained from an introductory physics course at Harvard University, developed several years ago as part of the general education curriculum. The course is entitled “Science and Cooking: From Haute Cuisine to Soft Matter Science,” and has become a popular course for non-science majors. It has also been successful in outreach, to help develop interest in science for the general public. This talk will describe how the course uses cooking to teach concepts of soft matter science. It will include a description of course and the learnings about how to excite non-science majors in science through the use of a theme in which they are interested. It will also include some demos used in the course and in outreach lectures for the general public.

12:27PM M46.00003 Picasso at the Nanoscale: The Art of Using Cutting-Edge Science to Understand Cultural Heritage1, VOLKER ROSE, Argonne National Laboratory — Scientists are using high-energy X-ray instruments to solve mysteries behind art masterpieces, including artwork by Picasso. Learn how Argonne National Laboratory is working with major art institutions, such as The Art Institute of Chicago and Smithsonian Institution, to unlock groundbreaking information about art, the artist, and our cultural heritage. A deep connection to our past and shared cultural heritage must be preserved to foster a balanced society where all humanity can thrive. This talk will describe the analysis of paint materials used by Pablo Picasso at the nanoscale, as only possible at the brightest synchrotron sources. It will highlight how new imaging techniques can reveal the invisible, bringing to light underlying compositions of old master’s paintings. This in turn enables the writing of new art history and provides important material clues that can assist with attribution and authentication. We will explain how the use of new technology can lead to new discoveries, which, in turn, can change the public’s and the specialists’ perception of great works of art. In collaboration with scientists from The Art Institute of Chicago we have teamed up to study the chemical make up of zinc oxide pigments used in artworks by Pablo Picasso. We will show how highly focused X-ray beams with nanoscale spatial resolution and trace element sensitivity have helped to determine that Picasso has used conventional house paint in some of his paintings. Surprisingly, the study gives also new insights into the pigment material zinc oxide, which has also great potential in applications such as in spintronics or as transparent electrodes in solar panels.

1Work at the Advanced Photon Source and the Center for Nanoscale Materials was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under contract DEAC02-06CH11357.

1:03PM M46.00004 A molecular compass for bird navigation1, PETER HORE, University of Oxford — Migratory birds travel spectacular distances, navigating and orienting by a variety of means, most of which are poorly understood. Among them is a remarkable ability to perceive the intensity and direction of the Earth's magnetic field. Biologically credible mechanisms for the sensing of such weak fields (25-65 microtesla) are scarce and in recent years just two proposals have emerged as frontrunners. One involves biogenic iron-containing nanoparticles; the other relies on the magnetic sensitivity of short-lived photochemical intermediates known as radical pairs. The latter began to attract attention following the proposal 15 years ago that the necessary physics and chemistry could take place in the bird's retina in specialized phototactic proteins called cryptochromes. The coherent dynamics of the electron-nuclear spin systems of pairs of photo-induced radicals is conjectured to form the basis of the sensing mechanism even though the interaction of an electron spin with the geomagnetic field is six orders of magnitude smaller than the thermal energy. The possibility that slowing decohering, entangled electron spins could form the basis of an important sensory mechanism has qualified radical pair magnetoreception for a place under the umbrella of “Quantum Biology.” In this talk, I will introduce the radical pair mechanism, comment on the roles of entanglement and quantum coherence, outline some of the experimental evidence for the cryptochrome hypothesis, and summarize what still needs to be done to determine whether birds (and maybe other animals) really do use a chemical compass to find their way around.

1This work was supported by grants from DARPA, AFOSR, ERC and the EMF Biological Research Trust.

1:39PM M46.00005 The Physics of Data: Can your degree in condensed matter theory get you a job at Google? , JEFF M. BYERS, Materials and Sensors Branch, Naval Research Laboratory, Washington, DC — All around us data is being collected by governments, corporations and individuals in staggering amounts. Entire industries are emerging to collect and process this Big Data with the expectation that more is better. But is more better and what can actually be learned? Interestingly, physics confronted this problem more than 150 years ago and developed many important concepts and computational tools within statistical mechanics to address these issues. A great deal of this apparatus has been exported into statistics and computer science to form a heterogeneous conglomeration called machine learning that is leading the charge into the Big Data problem. A brief tour through this world shows how statistical mechanics has been abstracted from its physical origins and transformed into a collection of powerful data processing tools. However, machine learning has interesting things to tell physics as well and can amply re-pay its intellectual debts. The reason for this emerges from the different relationships of physics and machine learning to their respective data. In physics, data is collected by arguably the best experimentalists in the world that attempt to isolate the physical processes so that a direct theoretical analysis is possible. In machine learning, the data is usually an uncontrolled accretion of nearly random instances with limited knowledge of the underlying structure that generated it. Poor data quality forces the analysis tools to acquire powerful new capabilities not usually required in physics. These analysis strategies, in turn, can be valuable to physicists tackling complex phenomenon not amenable to traditional approaches. Examples from biology and astronomy will be used to illustrate the point.


11:15AM M47.00001 Computing the properties of ferroelectrics and magnetoelectrics in applied electric fields, DAVID VANDERBILT, Rutgers University — The technology for computing properties of insulators in a finite electric field \( \hat{E} \), based on the coupling of \( \hat{E} \) to the Berry-phase polarization \( P \), has been available for over a decade and is currently implemented into several standard code packages. I will give an overview of recent developments in the extension of these methods and their applications to studies of ferroelectrics and multiferroics. I will first discuss the extension to allow calculations at fixed electric displacement field \( D \), emphasizing its advantages for calculations on superlattice and ultrathin capacitor geometries. I will also discuss the qualitative differences, as evidenced by their distinct electric equations of state (\( P \) vs. \( \hat{E} \), \( P \) vs. \( D \), or \( D \) vs. \( \hat{E} \)), for ordinary ferroelectrics, improper ferroelectrics, and “hyperferroelectrics.” The latter constitute a new class of proper ferroelectrics that polarize even when the depolarization field is unscreened, i.e., even at fixed displacement field \( D \). I will then turn to magneto-electric effects, which can be computed by studying the change in magnetization as an electric field is applied. A particularly subtle component is the one that comes from the change of orbital magnetization. This is found to have an isotropic component, the so-called “axion coupling,” that takes the form of an integral of a Chern-Simons three-form over the three-dimensional BZ, as well as anisotropic components that can be expressed in a more conventional Kubo-Greenwood form. I will end with some comments on current and future challenges.
11:51AM M47.00002 The quantum nature of skyrmions and half-skyrmions in Cu2OSeO3.
JEROEN VAN DEN BRINK, IFW Dresden — The Skyrme-particle, the skyrmion, was introduced over half a century ago in the context of dense nuclear matter. But with skyrmions being mathematical objects—special types of topological solitons—they can emerge in much broader contexts. Recently skyrmions were observed in helimagnets, forming nanoscale spin-textures. Extending over length scales much larger than the interatomic spacing, they behave as large, classical objects, yet deep inside they are of quantum nature. Penetrating into their microscopic roots requires a multi-scale approach, spanning the full quantum to classical domain. We performed such an approach for the first time in the skyrmionic Mott insulator Cu2OSeO3. We show that its magnetic building blocks are strongly fluctuating Cu4 tetrahedra, spawning a continuum theory that culminates in 51 nm large skyrmions, in striking agreement with experiment [1]. Another consequence is the presence of two distinct types of modes: a low-energy manifold that includes a gapless Goldstone mode and a set of weakly dispersive high-energy magnons [2]. Using high-field electron spin resonance with a terahertz free-electron laser and pulsed magnetic fields up to 64 T we identified these modes [3], corroborating the presence of fluctuating Cu4 tetrahedra. We also show that the emerging electric polarization P is governed by quadrupolar spin contributions from symmetry inequivalent bonds and to calculate the induced P in different crystallographic directions as a function of the orientation of an applied magnetic field, which are confirmed by experiment [2]. One so far untested prediction that ensues is the temperature-dependent decay of skyrmions into half-skyrmions.

12:27PM M47.00003 Electric polarization of Sr0.5Ba0.5MnO3: a multiferroic Mott insulator. REZA NOURAFKAN, Département de Physique and RQMP, Université de Sherbrooke, Sherbrooke, Québec, Canada — Multiferroics, materials which display simultaneous magnetic and ferroelectric orders, are interesting both for their rich physics and for their promising practical applications. The search for multiferroic materials with strong-magnetoelectric coupling is challenging and requires an understanding of how the magnetic order, or more specifically the correlations, influence the electric polarization and vice versa. A calculations of the electric polarization in the paramagnetic (PM) insulating phase of multiferroics is essential to address this mutual influence. Ab initio calculations of the electric polarization are based on the modern theory of polarization, which is a single-electron theory. Thus, a correlation driven insulating state is beyond the scope of this approach. Here we show that combining correlated band structure calculations (DFT+DMFT) with a formula for the electric polarization of interacting insulators, expressed in terms of the full Green and vertex functions, allows for the first time to reliably calculate the polarization in the PM phase. We focus on the Mott insulator Sr0.5Ba0.5MnO3, in which both magnetic and ferroelectric instabilities are related to the Mn ions. We predict a ferroelectric polarization of \( \approx 16.5 \, \mu C/cm^2 \) in the high temperature paramagnetic phase and recover the measured value of \( \approx 13.3 \, \mu C/cm^2 \) in the low temperature antiferromagnetic phase. Our calculations reveal that the the driving force behind the ferroelectric distortion comes from the tendency of Mn \( g \) states to establish a stronger covalency with the surrounding oxygens. This covalency is reduced by correlations, in particular by Hund coupling. On the other hand, the half-filled Mn \( t_2g \) orbitals give rise to the magnetic ordering which decreases the ionic displacement, hence its contribution to the polarization. For fixed ionic displacement, the magnetic order also slightly decreases the electronic contribution to the electric polarization. For fixed ionic displacement, the magnetic order also slightly decreases the electronic contribution to the electric polarization.

1NSERC, CRC, CFI, CC, CQ, FRQNT, and CIFAR

1:03PM M47.00004 Mott Multiferroics and Ferroelectric Metals from Dynamical Mean-Field Theory combined with Density-Functional Theory. MASSIMO CAPONE, International School for Advanced Studies (SISSA) and CNR-IOM, Trieste — Multiferroic materials, in which ferroelectricity and long-range magnetic ordering coexist, are natural candidates for applications. In this perspective, the most promising compounds are those in which the two phenomena do not simply coexist, but they influence each other through a magnetoelastic coupling. We present different applications of Density Functional Theory combined with Dynamical Mean-Field Theory in which electron-electron correlation effects are crucial in the stabilization of multiferroic behavior and in the magnetoelectric coupling. Within this wide family we can distinguish different cases. In \( \text{Sr}_3\text{Ba}_2\text{Mn}_5\text{O}_{12} \), the ferroelectric behavior is associated with a Mott insulating state in which the Mn half-filled \( t_2g \) orbitals are responsible for the magnetic properties and the value of the polarization is strongly affected by the magnetic state [1]. \( \text{LiOsO}_3 \) shares the same electronic configuration with half-filled Os \( t_2g \) orbitals. Despite this configuration enhances the effect of electron-electron interactions, the material remains metallic and represents a peculiar ferroelectric metal [2]. We propose however how to turn this non-magnetic polar metal into a multiferroic through the design of a superlattice, which increases the degree of correlation, leading to Mott localization of the Os orbitals [3]. In completely different systems, such as organic crystals like \( (\text{TMTTF})_{2}\text{X} \), strong correlations can lead to multiferroicity in organic crystals such as \( (\text{TMTTF})_{2}\text{X} \), where charge ordering promotes a polarization which is favored by an antiferromagnetic spin ordering [4]. We finally discuss how strong correlations can play a major role away from half-filling when the Hund’s coupling is sizable in compounds with a nominal valence of, e.g., two electrons in the three \( t_{2g} \) orbitals. Such “Hund’s metals” are correlated despite being far from Mott localization.

This physical regime can be a fertile ground to obtain other ferroelectric materials.

This work is supported by ERC/FP7 through the Starting Grant SUPERBAD (Grant Agreement 240524)

1:39PM M47.00005 Electric field effects in transition metal oxides, their surfaces and heterostructures. KARSTEN HELD, Vienna University of Technology — Modern computational tools such as density functional theory and its merger with dynamical mean field theory are nowadays inevitable for the modeling and understanding of oxides, their heterostructures and surfaces. In this talk, I will concentrate on the impact of electric fields, how they affect the physical properties and how to make use of them. Substantial internal electric fields are created at polar surfaces, and even for an isolator-interface the electronic reconstruction can lead to a charge transfer and hence a dipole field [1]. Such internal fields can be employed to efficiently separate electrons and holes in a oxide solar cell [2]. Even if the polar dipole field is compensated by a surface reconstruction, a local surface potential remains, and makes SrTiO3 (110) the arguably simplest 2 dimensional electron gas (2DEG) [3]. External electric fields, on the other hand, can trigger "gigantic" responses, since correlated oxides are prone to small perturbations. For example, a field-effect Mott transistor can be realized in a few layers of \( \text{SrVO}_3 \), where ideal on-off (metal-insulator) switching properties [4], and interfacing a ferroelectric, \( \text{BaTiO}_3 \), plus a 2DEG with large spin-orbit coupling, BaO_{0.5}, allows for a giant switchable Rashba effect.


3Support by the ERC through grant agreement n.306447 is gratefully acknowledged.
11:15AM M49.00001 Double helix configuration of lyotropic chromonic liquid crystals in cylindrical capillaries with homeotropic anchoring

We acknowledge the support from the U.S. Office of Basic Energy Sciences, Department of Energy: grant DE-SC 0001412.

11:27AM M49.00002 Director distortion reduces molecular order of lyotropic chromonic liquid crystal on large scales

This work is supported by DMS-1434185.

11:39AM M49.00003 Observation of large nematic domains of discotic liquid crystals

11:51AM M49.00004 Nucleation and Growth of Discotic Liquid Crystals

12:03PM M49.00005 Reconstruction of the surface of freely suspended films of heptyloxybenzylidene heptylanilines
12:15PM M49.00006 Tension and Rupture Dynamics of Freely-Suspended Bent-Core Liquid Crystalline Fibers, OLIVER KRESS, SEYYED MUHAMMAD SALILI, Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State University, Kent, OH 44242 USA, TANYA OSTAPENKO, Institute of Experimental Physics, Otto-von-Guericke-Universit"at, Universitatsplatz 2 39106 Magdeburg, Germany, CHRISTOPHER BAILEY, Leidos, 3745 Pentagon Blvd., Beavercreek, OH 45431, ALEXEY EREMIN, RALF STANNARIUS, Institute of Experimental Physics, Otto-von-Guericke-Universit"at, Universitatsplatz 2 39106 Magdeburg, Germany, ANTAL JÁKLI, Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State University, Kent, OH 44242 USA, JÁKLI LAB TEAM, ABTEILUNG NICHTLINEARE PHÄNOMENE, DEPARTMENT OF NONLINEAR PHENOMENA, PROF. RALF STANNARIUS TEAM — Euler buckling, a physical mechanism which classically describes deformations in an elastic beam, has been expanded to describe the recoil of viscoelastic liquid crystalline filaments. Rupture of the freely suspended filaments resulted in a buckling instability that propagated through the filament. A characteristic wavelength and a time constant emerge as the filament recoils. Tensions of the suspended filaments were measured by induced mechanical deflection. The analysis of the results reveals a temperature dependent competition between surface and bulk effects that distinguishes these viscoelastic filaments from classical elastic beams.

1 http://www.uni-magdeburg.de/anp/

12:27PM M49.00007 Dynamics of Stable and Metastable Structures of Liquid Crystal and Lipid Systems at Interfaces, LAWRENCE HONAKER, Liquid Crystal Institute, Kent State University, PIOTR POPOV, ELIZABETH MANN, Department of Physics, Kent State University, EDGAR KOOLMAN, Department of Biological Sciences, Kent State University, ANTAL JÁKLI, Liquid Crystal Institute, Kent State University — Due to the amphiphilic structure and character of liquid crystal molecules, they tend to align in a planar fashion at a boundary with water and homeotropically at a boundary with air. However, the introduction of heteromolecules with long aliphatic tails, such as phospholipids, into the system promotes alignment, a conformational change which is easily visually observable. It can be expected that the presence of these lipids induces a uniformly homeotropic texture in the liquid crystalline system, but experimental observations show otherwise. Studies of the textures and features that arise in such systems are presented here with an emphasis on the study of the metastable hybrid textures that develop, their stability, the characteristics of their alignment, and factors that influence their presence.

12:39PM M49.00008 Self-assembly of DNA origami particles in suspension of non-absorbing depleting polymers, MAHSA SIAVASHPOURI, MARK ZAKHARY, Brandeis University, CHRISTIAN WACHAUF, HENDRIK DIETZ, Technische Universität München, ZVONIMIR DOGIC, Brandeis University — The connection between the macroscopic properties of a liquid crystalline material and the microscopic features of the constituent molecules is the essential theme that permeates the field of liquid crystals. Previous studies have shown that monodisperse rod-like colloids such as filamentous bacteriophage self-assemble into 1D twisted ribbons in presence of attractive interactions mediated by non-absorbing polymers. The microscopic properties of the colloidal particles play an important role in determining the physical properties of these mesoscopic assemblies. Using structural DNA nanotechnology, we present the design and structure of DNA origami six-helix bundles with tunable microscopic properties, which can be used as a new building block for the self-assembly of rod-like colloidal particles. We demonstrate that formation of higher order structures from the assembly of colloidal rods is universal. By tuning the chirality, aspect ratio and flexibility of the DNA origami particles we can control the physical properties of the entire self-assembled structures.

12:51PM M49.00009 Dynamic Theory for Polydomain Structures in Liquid-Crystal Elastomers1, AYHAN DUZGUN, JONATHAN SELINGER, Kent State Univ - Kent — Liquid-crystal elastomers are remarkable materials that combine the elastic properties of cross-linked polymer networks with the anisotropy of liquid crystals. Any distortion of the polymer network affects the nematic order of the liquid crystal, and, likewise, any change in the magnitude or direction of the nematic order influences the shape of the elastomer. When elastomers are prepared without any alignment, they develop disordered polydomain structures as they are cooled into the nematic phase. To model these polydomain structures, we develop a dynamic theory for the isotropic-nematic transition in elastomers. In this theory, the local nematic order is coupled to the strain tensor, which satisfies the constraint of elastic compatibility. If the system is rapidly cooled into the nematic phase, a polydomain state with a characteristic length scale can emerge. This polydomain state may eventually become uniform, or it may be locked in by quenched impurities.

1 This work was supported by NSF Grant DMR-1409658.

1:03PM M49.00010 Novel confinement of liquid crystals in Janus droplets1, WEI-SHAO WEI, JOONWOO JEONG, University of Pennsylvania, Department of Physics and Astronomy, PETER J. COLLINGS, Swarthmore College, Department of Physics and Astronomy, TOM C. LUBENSKY, A. G. YODH, University of Pennsylvania, Department of Physics and Astronomy — In this work we create and investigate Janus droplets composed of liquid crystal (LC) and polymer. The Janus droplets are formed when homogeneous droplets of LC-polymer-solvent phase separate into LC and polymer regions during solvent evaporation through aqueous continuous phase. This scheme enables us to realize unique confinement geometries for LCs such as spherical caps and bowls, which are difficult to be achieved via other systems. The morphologies and surface anchoring conditions can be controlled by changing the size of droplets, the volume ratio between LC and polymer, and the type/concentration of surfactants in aqueous background phase. We explore a variety of defects in these novel confined geometries including dislocations and focal conic defects of smectic LCs. Nematic and cholesteric LCs are also explored. Models that balance the energetics of bulk elasticity and surface anchoring determine the director configurations of confined liquid crystals (LCs).

1 This work is funded by NSF Grant DMR-1205463, NSF MRSEC Grant DMR-1120901, and NASA Grant NNX08AO6G.

1:15PM M49.00011 Microlenses of smectic flowers1, FRANCESC A SERRA, MOHAMED-AMINE GHARBII, Dept. Physics and Astronomy, CBE, LRS M, University of Pennsylvania, IRIS B. LIU, YIMIN LUO, NATHAN D. BADE, Chemical and Biomolecular Engineering, University of Pennsylvania, RANDALL D. KAMEN, Dept. Physics and Astronomy, University of Pennsylvania, SHU YANG, LRS M, University of Pennsylvania, KATHLEEN J. STEBE, Chemical and Biomolecular Engineering, University of Pennsylvania — The search for new and tunable optical components finds suitable candidates in liquid crystals, which have both reconfigurability and unique optical properties. Here we discuss smectic liquid crystals arranged in focal conic domains (FCDs), which can work as gradient-refractive index microlenses. We exploit this property to create an assembly of microlenses that resembles an insect compound eye. The system consists of a thin layer of smectics on a substrate patterned with microposts. The smectic film is pinned at the microposts, creating a curved interface that induces a hierarchical assembly of FCDs called the “flower pattern”: each FCD resembles the petal of a flower around the micropost. The arrangement of FCDs, with the largest eccentricity, only work as microlenses for one direction of light polarization.

1 We thank the MRSEC NSF grant DMR11-20901.
1:27PM M49.00012 Phototropic liquid crystal materials containing naphthopyran dopants. MARIACRISTINA RUMI, Seth CAZZELL, Air Force Rsch Lab - WPAFB, TAMAS KOSA, LUDMILA SUKHOMLINNOVA, BAHMAN TAHERI, Alpha Micron Inc., TIMOTHY BUNNING, TIMOTHY WHITE, Air Force Rsch Lab - WPAFB — Dopant molecules dispersed in a liquid crystalline material usually affects the order of the system and the transition temperature between various phases. If the dopants undergo photosomerization between conformers with different shapes, the interactions with the liquid crystal molecules can be different for the material in the dark and during exposure to light of appropriate wavelength. This can be used to achieve isothermal photoinduced phase transitions (phototropism). With proper selection of materials components, both order-to-disorder and disorder-to-order photoinduced transition have been demonstrated. Isothermal order-increasing transitions have been observed recently using naphthopyran derivatives as dopants. We are investigating the changes in order parameter and transition temperature of liquid crystal mixtures containing naphthopyrans and how they are related to exposure conditions and to the concentration and molecular structure of the dopants. We are also studying the nature of the photoinduced phase transitions, and comparing the behavior with that of azobenzene-doped mixtures, in which exposure to light leads to a decrease, instead of an increase, in the order of the system.

1:39PM M49.00013 A Simple Method For The Determination of High-Accuracy Refractive Indices of Liquid Crystals via High-Resolution Birefringence Data. SENAY USTUNEL, ERLIN KUTLU, MEHMET CAN CETINKAYA, HALUK OZBEK, Istanbul Tech Univ — We proposed a simple procedure to determine extraordinary (n_e) and ordinary refractive indices (n_o) of LCs both in the N and Sm A phases based on the high-accuracy birefringence measurements. We show that, apart from the birefringence data, the procedure needs only a single value for the refractive index which is the value of that in the isotropic (I) phase just above the N-I transition temperature. By checking the consistency of our approximation model using the criteria found in the literature, we then conclude that our proposal is self-consistent. Additionally, we show that the temperature variation of refractive indices is well portrayed by the fit expression presented here for the first time contrary to the Haller extrapolation method. Furthermore, we then show that, without addressing density measurements, the proposed method allows one to obtain the temperature dependence of normalized molecular polarizabilities for extraordinary and ordinary rays, and the effective geometry parameter.

1:51PM M49.00014 Liquid Crystal Based Sensor to Detect Beta-Sheet Formation of Peptides. MONIROSAUT SADATI, University of Chicago, ASLIN IZMITLI APIK, NICHOLAS L. ABBOTT, University of Wisconsin, Madison, JUAN J. DE PABLO, University of Chicago and Argonne National Laboratory — Protein aggregation into amyloid fibrils is involved in the progression of Alzheimer’s, typeII diabetes, MONIROSADAT SADATI, University of Chicago, ASLIN IZMITLI APIK, NICHOLAS L. ABBOTT, University of Wisconsin, Madison, JUAN J. DE PABLO, University of Chicago and Argonne National Laboratory — Protein aggregation into amyloid fibrils is involved in the progression of Alzheimer’s, typeII diabetes and Huntington’s diseases. Although larger aggregates remain important for clinical determination, small oligomers are of great interest due to their potentially toxic nature. It is therefore crucial to develop methods that probe the aggregation process at early stages and in the vicinity of biological membranes. Here, we present a simple method that relies on liquid crystalline materials and a Langmuir monolayer at the aqueous-liquid crystal (LC) interface. The approach is based on the LC’s specific response to β-sheet structures, which abound in amyloid fibrils. When the system is observed under polarized light, the fibrils formed by amyloidogenic peptides give rise to the formation of elongated and branched structures in the LCs. Moreover, the PolScope measurements prove that the LCs are predominantly aligned along the fibrils when exposed to a β-sheet forming peptide. In contrast, non-amyloidogenic peptides form ellipsoidal domains of irregularly tilted LCs. This method is capable of reporting aggregation at lipid-aqueous interfaces at nanomolar concentrations of the peptide, and much earlier than commonly used fluorescence-based techniques.

We thank Prof. Oleg D. Leventovich and Young-Ki Kim from the Liquid Crystal Institute of Kent State University for the use of their PolScope instrument. This work was primarily supported by the Swiss National Science Foundation (P300P2_151342).

2:03PM M49.00015 Liquid Crystalline Compositions as Gas Sensors. PETR SHIBAEV, JOHN MURRAY, ANTHONY TANTILLO, MADISON WENZLICK, Fordham University, JORDAN HOWARD-JENNINGS, Bronx Science High School — Droplets and films of nematic and cholesteric liquid crystalline materials were studied as promising detectors of volatile organic compounds (VOCs) in the air. Under increasing concentration of VOC in the air the detection may rely on each of the following effects sequentially observed one after the other due to the diffusion of VOC inside liquid crystalline matrix: i. slight changes in orientation and order parameter of liquid crystal, ii. formation of bubbles on the top of the liquid crystalline droplet due to the mass transfer between the areas with different order parameter, iii. complete isotropisation of the liquid crystal. All three stages can be easily monitored by optical microscopy and photo camera. Detection limits corresponding to the first stage are typically lower by a factor of 3-6 than detection limits corresponding to the beginning of mass transfer and isotropisation. The prototype of a compact sensor sensitive to the presence of organic solvents in the air is described in detail. The detection limits of the sensor is significantly lower than VOC exposure standards. The qualitative model is presented to account for the observed changes related to the diffusion, changes of order parameter and isotropisation.

Wednesday, March 4, 2015 11:15AM - 2:15PM — Session M51 DCMP: Invited Session: Topological Superconductivity in Ferromagnetic Metal Chains Grand Ballroom C1 - Allan MacDonald, University of Texas at Austin

11:15AM M51.00001 Topological Superconductivity with Magnetic Atoms. LEONID GLAZMAN, Departments of Physics and Applied Physics, Yale University, New Haven, CT 06511, USA — Chains of magnetic impurities embedded in a conventional s-wave superconductor may induce the formation of a topologically non-trivial superconducting phase. If such a phase is formed along a chain, then its ends carry Majorana fermions. We investigate this possibility theoretically by developing a tight-binding Bogoliubov-de Gennes description, starting from the Shiba bound states induced by the individual magnetic impurities. While the resulting Hamiltonian has similarities with the Kitaev model for one-dimensional spinless p-wave superconductors, there are also important differences, most notably the long-range (power-law) nature of hopping and pairing as well as the complex hopping amplitudes. We develop an analytical theory, complemented by numerical approaches, which accounts for the electron long-range pairing and hopping along the chain [1], inhomogeneous magnetic order in the chain of embedded impurities or spin-orbit coupling in the host superconductor, and the possibility of direct electron hopping between the impurity atoms. This allows us to elucidate the domain of parameters favoring the formation of a topological phase and to find the spatial structure [2] of Majorana states appearing in that phase.

This talk is based on joint work with F. von Oppen, Falko Pientka, and Yang Peng.

11:51AM M51.00002 Observation of Majorana fermions in ferromagnetic atomic chains on a superconductor

STEVAN NADJ-PERGE, Princeton University, USA — Majorana fermions are zero-energy excitations predicted to localize at the edge of a topological superconductor, a state of matter that can form when a ferromagnetic system is placed in proximity to a conventional superconductor with strong spin-orbit interaction. With the goal of realizing a one-dimensional topological superconductor, we have fabricated ferromagnetic iron atomic chains on the surface of superconducting lead [1]. Using high-resolution spectroscopic imaging techniques, we show that the onset of superconductivity, which gaps the electronic density of states in the bulk of the chains, is accompanied by the appearance of zero-energy end-states. This spatially resolved signature provides strong evidence, corroborated by other observations and theoretical modeling [2], for the formation of a topological phase and edge-bound Majorana states in this system. Our results demonstrate that atomic chains are viable platform for future experiments to manipulate Majorana bound states [3] and to realize other related 1D or 2D topological superconducting phases. [1] S. Nadj-Perge, I. K. Drozdov, J. Li, H. Chen, S. Jeon, J. Seo, A. H. MacDonald, B. A. Bernevig, and A. Yazdani, Science 346, 602 (2014). [2] Jian Li, Hua Chen, Ilya K. Drozdov, A. Yazdani, B. Andrei Bernevig, A.H. MacDonald, ArXiv:1410.3453 (2014). [3] Jian Li, Titus Neuert, B. Andrei Bernevig, Ali Yazdani, ArXiv:1404.4058 (2014).

This work has done in collaboration with Ilya K. Drozdov, Jian Li, Hua Chen, Sangjun Jeon, Jungpil Seo, Allan H. MacDonald, B. Andrei Bernevig and Ali Yazdani. We acknowledge ONR, NSF-MRSEC, ARO-MURI, NSF-DMR and EU Marie Curie for support.

12:27PM M51.00003 Theory of Topological Superconductivity in Ferromagnetic Metal Chains on Superconducting Substrates

HUA CHEN, University of Texas at Austin — Recent experiments have provided evidence that one-dimensional (1D) topological superconductivity based on transition metal atom chains formed on a superconducting substrate can be realized experimentally when the chain behaves like a ferromagnetic macrospin [1]. In this talk I will address the structural and bonding considerations which determine whether or not a particular atom chain will have magnetic and electronic properties favorable for topological superconductivity. By using a Slater-Koster tight-binding model to account for important features of transition metal electronic structure, I conclude that topological states are common for ferromagnetic chains on superconductors and that they are nearly universal when ferromagnetic transition metal chains form straight lines on superconducting substrates. The proximity induced superconducting gap on the chain is ~ \Delta E_{so}/J where \Delta is the s-wave pair-potential on the chain, E_{so} is the spin-orbit splitting energy induced in the normal state chain bands by hybridization with the superconducting substrate, and J is the exchange-splitting of the ferromagnetic chain d-bands. Because of the topological character of the 1D superconducting state, Majorana end modes appear within the gaps of finite length chains. I will specifically discuss the spatial decay length of the Majorana end modes which can be much shorter than the coherence length from the induced \gamma-wave gap on the chain due to its strong coupling to the three-dimensional superconducting substrate, in agreement with experimental results [2]. Pb is a particularly favorable substrate material for ferromagnetic chain topological superconductivity because it provides both strong \gamma-wave pairing and strong Rashba spin-orbit coupling, but there seems to be considerable scope to optimize the 1D topological superconductivity by varying the atomic composition and structure of the chain. [1] S. Nadj-Perge, I. K. Drozdov, J. Li, H. Chen, S. Jeon, J. Seo, A. H. MacDonald, B. A. Bernevig, and A. Yazdani, Science 346, 602 (2014). [2] J. Li, H. Chen, I. K. Drozdov, A. Yazdani, B. A. Bernevig, and A. H. MacDonald, ArXiv:1410.3453.

The authors acknowledge support from the Office of Naval Research under grant ONR-N00014-14-1-0330.

1:03PM M51.00004 Experimental progress on Majoranas in semiconductors

LEO KOUVENHOVEN, Delft Univ of Tech — Majoranas in semiconductor nanowires can be probed via various electrical measurements. Tunnel spectroscopy reveals zero-bias peaks in the differential conductance. These zero-bias peaks have a particular dependence on magnetic field (amplitude and direction) and electron density. This dependence allows to falsify many alternative theories for the observations. New challenges include a direct demonstration of topological protection, which is provided by a parity protection: How stable is the system’s occupation in terms of an even or an odd number of quasi-particles? We demonstrate that the quasi-particle parity in a superconducting Cooperpair box can be stable over timescales of minutes. To demonstrate this protection for Majoranas it is crucial that the induced superconducting gap has negligible sub-gap states. To obtain such “hard gaps” under Majorana conditions currently forms the most important challenge. We report on progress in optimizing materials and measurement techniques.

1:39PM M51.00005 Fermionic and Majorana Bound States in Hybrid Nanowires With Rashba and Synthetic Spin-Orbit Interactions


We acknowledge support from the Harvard Quantum Optical Center, the Swiss NSF, and NCCR QIST.


11:15AM M52.00001 Entanglement Hamiltonians in Fermion Systems and the Riemann-Hilbert problem

ISRAEL Klich, University of Virginia — In this talk, I will discuss work on entanglement in fermion systems. I will describe recent results on effective entanglement hamiltonians in conformal quantum field theories, and how the free fermion entanglement Hamiltonian in 1d can be obtained by solving a Riemann-Hilbert problem. I will also show how finite size corrections to the Hamiltonian may be obtained by perturbing around the Riemann-Hilbert solutions, as well as explore subtle difference between the Neveu-Schwarz and Ramond sectors of free fermion fields.
11:51AM M52.00002 Entanglement Scaling Laws and Eigenstate Thermalization in Many-Particle Systems, KUN YANG, Florida State University — While entanglement entropy of ground states usually follows the area law, violations do exist, and it is important to understand their origin. In 1D they are found to be associated with quantum criticality. Until recently the only established examples of such violation in higher dimensions are free fermion ground states with Fermi surfaces, where it is found that the area law is enhanced by a logarithmic factor. In Ref. [1], we use multi-dimensional bosonization to provide a simple derivation of this result, and show that the logarithmic factor has a 1D origin. More importantly the bosonization technique allows us to take into account the Fermi liquid interactions, and obtain the leading scaling behavior of the entanglement entropy of Fermi liquids. The central result of our work is that Fermi liquid interactions do not alter the leading scaling behavior of the entanglement entropy, and the logarithmic enhancement of area law is a robust property of the Fermi liquid phase. In sharp contrast to the fermionic systems with Fermi surfaces, quantum critical (or gapless) bosonic systems do not violate the area law above 1D (except for the case discussed below). The fundamental difference lies in the fact that gapless excitations live near a single point (usually origin of momentum space) in such bosonic systems, while they live around an (extended) Fermi surface in Fermi liquids. In Ref. [2], we studied entanglement properties of some specific examples of the so called Bose metal states, in which bosons neither condense (and become a superfluid) nor localize (and insulate) at T=0. The system supports gapless excitations around “Bose surfaces,” instead of isolated points in momentum space. We showed that similar to free Fermi gas and Fermi liquids, these states violate the entanglement area law in a logarithmic fashion. Compared to ground states, much less is known concretely about entanglement in (highly) excited states. Going back to free fermion systems, in Ref. [3] we show that there exists a duality relation between ground and excited states, and the area law obeyed by ground state turns into a volume law for excited states, something widely expected but hard to prove. Most importantly, we find in appropriate limits the reduced density matrix of a subsystem takes the form of thermal density matrix, providing an explicit example of the eigenstate thermalization hypothesis. Our work [3] explicitly demonstrates how statistical physics emerges from entanglement in a single eigenstate.


12:27PM M52.00003 Entanglement and Stability of Quantum Matter: from Spin-liquids to Many Body Localization, TARUN GROVER, Kavli Institute for Theoretical Physics, Univ of California - Santa Barbara — Quantum entanglement often serves as a fruitful order parameter to characterize quantum phases and phase transitions. However, recent developments have lead to a completely new role for quantum entanglement: the nature of quantum entanglement also plays strong constraints on the structure of phase diagrams itself. Specifically, the universal part of entanglement provides a natural ordering for critical systems whereby a critical, scale-invariant phase can be unstable only if the instability reduces entanglement. In this talk, I will elucidate implications of the aforementioned general relation between entanglement and critical phases for a wide variety of challenging problems in condensed matter physics. I will first discuss general arguments on why a large class of gapless quantum spin-liquids, which possess exotic properties such as emergent fermions and photons, must be stable. In a similar vein, I will show that certain quantum transitions must lie beyond a simple Landau order parameter description. Finally, I will discuss a generalization of such arguments to disordered quantum systems in the context of many-body localization transition. Specifically, I will show that at a continuous many-body localization transition, the system is necessarily ergodic.

1:03PM M52.00004 Einstein’s Equations From Entanglement, BRIAN SWINGLE, Stanford — I will outline a path by which a semi-classical geometry obeying Einstein’s equations emerges holographically from entanglement in certain quantum many-body systems. Although some challenges remain, I will argue that the core concepts are in place. I will discuss in particular two crucial results, one establishing the existence of tensor networks for a wide class of quantum many-body systems, and one showing how the equivalence principle is encoded in the universality of entanglement. The first result establishing the existence of tensor networks has independent interest for the classical simulation of quantum many-body physics.

1:39PM M52.00005 Quantum Entanglement and the Topological Order of Fractional Hall States1, EDWARD REZAYI, Cal State Univ. Los Angeles — Fractional quantum Hall states or, more generally, topological phases of matter defy Landau classification based on order parameter and broken symmetry. Instead they have been characterized by their topological order. Quantum information concepts, such as quantum entanglement, appear to provide the most efficient method of detecting topological order solely from the knowledge of the ground state wave function. This talk will focus on real-space bi-partitioning of quantum Hall states and will present both exact diagonalization and quantum Monte Carlo studies of topological entanglement entropy in various geometries. Results on the torus for non-contractible cuts are quite rich and, through the use of minimum entropy methods, yield the modular S-matrix and hence uniquely determine the topological order, as shown in recent literature. Concrete examples of minimum entropy states from known quantum Hall wave functions and their corresponding quantum numbers, used in exact diagonalizations, will be given.

In collaboration with Clare Abreu and Raul Herrera. Supported by DOE grant DE-SC0002140


11:15AM M53.00001 Importance of anisotropic exchange interactions in honeycomb iridates. New phenomena due to Kitaev interactions.1, NATALIA PERKINS, Univ of Minnesota, Minneapolis — We investigate the microscopic nature of the magnetism in honeycomb iridium-based systems. We show that the minimal model describing the magnetism in A2IrO3 includes both isotropic and anisotropic Kitaev-type spin-exchange interactions between nearest and next-nearest neighbor Ir ions, and that the magnitude of the Kitaev interaction between next-nearest neighbor Ir magnetic moments is comparable with nearest neighbor interactions. We computed the low temperature phase diagram of the effective model with classical Monte Carlo simulations. Due to the presence of the anisotropic Kitaev interactions and the frustration introduced by the competition of the spin couplings between nearest and next-nearest neighbors, the resulting phase diagram is very rich. It contains both various commensurate states and incommensurate single-Q and multi-Q phases, whose regions of stability are controlled by the ratios between competing exchange constants. We showed that the second neighbor Kitaev term plays an important role in the stabilization of the commensurate antiferromagnetic zigzag phase which has been experimentally observed in Na2IrO3. In our simulations, we found this phase to be the ground state for parameters of the model of both the correct signs and magnitudes.

1 NSF grant DMR-1255544
11:51AM M53.00002 Magnetic and Orbital Excitations in α-A₂IrO₃ (A = Li, Na) Probed by Resonant Inelastic X-ray Scattering, JAMES CLANCY, University of Toronto — The honeycomb lattice iridates Na₂IrO₃ and Li₂IrO₃ are two of the most promising candidates for the experimental realization of Kitaev-like physics. Although the formation of long-range magnetic order (T_N ~ 15 K) excludes a pure Kitaev model, there are many extended Kitaev models (which include contributions such as isotropic Heisenberg exchange, further-neighbour interactions, symmetric off-diagonal exchange, and structural distortions) that may be relevant to these materials. We have performed high-resolution Ir L₃-edge resonant inelastic x-ray scattering (RIXS) measurements to investigate the excitation spectra of Na₂IrO₃ and Li₂IrO₃. In Na₂IrO₃, we observe a new branch of dispersive magnetic excitations, which reaches a maximum energy of ~35 meV at the Γ point [1]. This mode is distinct from the low energy (~6 meV) magnon mode observed in previous inelastic neutron scattering measurements [2], and implies the presence of a significant bond-dependent Kitaev interaction. The d-d excitations in Na₂IrO₃ and Li₂IrO₃ reveal important information about crystal electric field effects, and the potential impact of trigonal and monoclinic structural distortions [3]. New developments in high pressure RIXS allow us to study the evolution of these excitations up to 6 GPa, providing insight into future prospects for tuning Kitaev interactions via applied pressure.

Work performed in collaboration with H. Gretarsson, J.A. Sears, Y.-J. Kim (University of Toronto), M.H. Upton, J. Kim, Y. Ding, A.H. Said, D. Casa, T. Gog (Argonne National Laboratory), S. Desgreniers (University of Ottawa), Y. Singh (IISER Mohali), S. Manni, P. Gegenwart (University of Gottingen), X. Liu, J.P. Hill (Brookhaven National Laboratory), V.M. Katukuri, L. Hozoi, J. van den Brink (IFD Dresden).


12:27PM M53.00003 ABSTRACT WITHDRAWN

1:03PM M53.00004 Generic spin model for the honeycomb iridates with trigonal distortion, JEFFREY G. RAU, University of Waterloo — Recently, realizations of Kitaev physics have been sought in the A₂IrO₃ family of honeycomb iridates, originating from oxygen-mediated exchange through edge-shared octahedra. However, for the j = 1/2 Mott insulator in these materials exchange from direct d-orbital overlap is relevant, and it was proposed that a Heisenberg term should be added to the Kitaev model. Here we provide the generic nearest-neighbour spin Hamiltonian when both oxygen-mediated and direct overlap are present, containing a bond dependent off-diagonal exchanges in addition to Heisenberg and overlap is relevant, and it was proposed that a Heisenberg term should be added to the Kitaev model. Near the Kitaev limit, we find new magnetic phases, 120 degree and incommensurate spiral order, as well as extended regions of zigzag and stripy order. By including a small amount of trigonal distortion, as found in Na₂IrO₃ and Li₂IrO₃ reveal important information about crystal electric field effects, and the potential impact of trigonal and monoclinic structural distortions. For the latter material, very recent magnetic resonant X-ray diffraction experiments allowed a complete solution of the magnetic structure. Incommensurate magnetic order with non-coplanar and counter-rotating Ir moments are found, similar as also realized in another polytype, the “stripy/honeycomb” γ-Li₂IrO₃. Theoretically, such structure is stabilized by dominant Kitaev interactions. The similarities between the two materials which share similar local connectivity between the Ir neighbors suggest dominating Kitaev magnetic exchange in both materials. Work in collaboration with F. Freund, S. Manni, Y. Singh, S. Choi and R. Coldea.

11:00AM - 11:00AM
Session P1 APS DPOLY/DBIO GSNP/GSOFT: Poster Session II (11:00 am - 2:00 pm) Exhibit Hall C -

P1.00001 SOFT CONDENSED MATTER

P1.00002 Slow Relaxations of Supercooled Water Determined by Energy Landscape Sampling, NATHAN WALTER, YANG ZHANG, Univ of Illinois - Urbana — Molecular Dynamics simulations have been widely used to provide insight into atomistic scale materials behavior and to compare with neutron scattering experiments. However, such simulations are inhibited by temporal scale and spatial scale constraints. As a consequence, it is only possible to predict the dynamical behavior of materials at short times, while atomistic simulations beyond microsecond remain a challenge. The energy landscape sampling methods have been suggested to predict materials behavior at long times. Herein, we show that by efficiently sampling the activation barriers of the high-dimensional energy hypersurface we were able to study the slow dynamics of supercooled ST2 water down to deeply supercooled temperatures. Furthermore, the method allows us to quantify the statistics of the activation barriers, yielding insight into the slow and fast dynamics of ST2 water at low temperatures. The computed transport coefficients across a wide temporal range are useful to bridge the gap between neutron scattering experiments and other bulk measurements.

P1.00003 Single-stranded DNA induced chirality and helical twist in achiral liquid crystals, RAJRAJAT BASU, US Naval Academy — A small quantity of single-stranded DNA (Deoxyribonucleic acid—cellulose single-stranded from calf thymus DNA in lyophilized powder form) was doped in an achiral liquid crystal (LC), and the mixture was found to exhibit a weak degree of chirality. The induced chirality in the LC was probed by means of the electroclinic effect in the LC's smectic-A phase, which showed significant pretransitional behavior on approaching the smectic-A—smectic-C transition temperature from above. The same DNA was doped in an achiral nematic LC and the mixture was found to exhibit an average mechanical twist over macroscopic dimensions. The single-stranded DNA-induced chiral pitch length P was determined by measuring the radius of curvature of the LC mixture, the LC's benzene rings interact with the nucleobases of the DNA through π—π stacking, which induces a molecular conformational demerization in the LC.

P1.00004 Magnetic properties of hexagonal iridates, PHILIPP GEGENWART, Experimentalphysik VI, Augsburg University, Germany — Hexagonal iridates AᵢIrO₃ (A=Na, Li) are discussed in the context of realizing magnetic Kitaev exchange between j=½ moments. This talk reports experimental investigation of magnetic properties of Na₂IrO₃ and α-Li₂IrO₃, crystallizing in a layered honeycomb structure, as well as the related “hyper-honeycomb” β-Li₂IrO₃. For the latter material, very recent magnetic resonant X-ray diffraction experiments allowed a complete solution of the magnetic structure. Incommensurate magnetic order with non-coplanar and counter-rotating Ir moments are found, similar as also realized in another polytype, the “stripy/honeycomb” γ-Li₂IrO₃. Theoretically, such structure is stabilized by dominant Kitaev interactions. The similarities between the two materials which share similar local connectivity between the Ir neighbors suggest dominating Kitaev magnetic exchange in both materials. Work in collaboration with F. Freund, S. Manni, Y. Singh, S. Choi and R. Coldea.

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P1.00003 Single-stranded DNA induced chirality and helical twist in achiral liquid crystals, RAJRAJAT BASU, US Naval Academy — A small quantity of single-stranded DNA (Deoxyribonucleic acid—cellulose single-stranded from calf thymus DNA in lyophilized powder form) was doped in an achiral liquid crystal (LC), and the mixture was found to exhibit a weak degree of chirality. The induced chirality in the LC was probed by means of the electroclinic effect in the LC's smectic-A phase, which showed significant pretransitional behavior on approaching the smectic-A—smectic-C transition temperature from above. The same DNA was doped in an achiral nematic LC and the mixture was found to exhibit an average mechanical twist over macroscopic dimensions. The single-stranded DNA-induced chiral pitch length P was determined by measuring the radius of curvature of the LC mixture, the LC's benzene rings interact with the nucleobases of the DNA through π—π stacking, which induces a molecular conformational demerization in the LC.
P1.00004 Local environment of iron in garden soil Vs Plants

Sunil Dehipawala, Chaojung Dong, Stephen Smith, Patricia Schneider. Queensborough Community College of CUNY, Harry Gafney. Queens College of CUNY — Iron is an essential nutrient not only for humans, but also for all types of plants. Plants use iron for chlorophyll formation, RNA metabolism, and transpiration process regulation. Iron is one of the most abundant metals in the soil and occurs in a wide range of chemical forms. The correlation between the iron species presents in soil and in Petrostelium crispum (parsley) plants were investigated using the room temperature Mössbauer spectroscopy. Mössbauer spectrum of garden soil consists of two doublets. Based on the established isomer shift and quadrupole splitting values of iron, these doublets can be identified as due to octahedrally coordinated Fe$^{3+}$ and tetrahedrally coordinated Fe$^{2+}$. Most of the iron present in the parsley has the form Fe$^{3+}$ or electron density at the site of the iron nucleus similar to that of Fe$^{3+}$. These findings will help establish soil conditions necessary to increase Fe$^{3+}$ intake by plants similar to the form of iron present in most supplements.

1Sunil Dehipawala acknowledges financial support provided by PSC-CUNY.

P1.00005 Chemotaxing and haptotaxing random walkers having directional persistence

Tae Goo Kwon, Korea Univ, Kyoungjin Lee Team, TaeSeok Daniel Yang Team — Biological cell crawling is a rather complex process involving various bio-chemical and bio-mechanical processes, many of which are still not well understood. The difficulties in understanding the crawling are originating not just from cell-intrinsic factors but from their complex social interactions, cell-to-substrate interactions and nonlinear responses toward extrinsic factors. Here, in this report we investigate chemotactic behavior of mathematical model cells that naturally have directional persistence. A cell density is measured as a function of time and space, then the resulting steady state is compared with that of the well-known Keller-Segel model, which describes a population of chemotactic random walker. Then, we add a cell-to-cell interaction, mimicking a “haptotaxis” mediated interaction, to the model and access its role as for altering the steady-state cell density profile. This mathematical model system, which we have developed and considered in this work, can be quite relevant to the chemotactic responses of interacting immune cells, like microglia, moving toward and around a site of wound, as for an example. We conclude by discussing some relevant recent experimental findings.

P1.00006 Aqueous Foam Stabilized by Tricatonic Amphiphilic Surfactants

Seth Heerschap, John Marafino, Kristin Mckenna, Kevin Caran, Klebert Feitosa, James Madison University, Kevin Caran’s Research Group Collaboration — The unique surface properties of amphiphilic molecules have made them widely used in applications where foaming, emulsifying or coating processes are needed. The development of novel architectures with multi-cephalic/tailed molecules have enhanced their anti-bacterial activity in connection with tail length and the nature of the head group. Here we report on the foamability of two triple head double, tail cationic surfactants (M-1,14,14, M-P, 14, 14) and a triple head single tail cationic surfactant (M-1,14,14) and compare them with commercially available single headed, single tailed anionic and cationic surfactants (SDS, CTAB and DTAB). The results show that bubble rupture rate decrease with the length of the carbon chain irrespective of head structure. The growth rate of bubbles with short tailed surfactants (SDS) and longer, single tailed tricationic surfactants (M-1,14,14) was shown to be twice as high as those with longer tailed surfactants (CTAB, M-P,14,14, M-1,14,14). This fact was related to the size variation of bubbles, where the foams made with short surfactants exhibited higher polydispersivity than those with short tails. This suggests that foams with tricationic amphiphiles are closed linked to their tail length and generally insensitive to their head structure.

P1.00007 Reversible mechano-memory in sheared cross-linked actin networks

Sayantan Majumdar, Margaret L. GarDEL, MRSEC and the James Franck Institute, University of Chicago, IL 60637 — Is it possible to control the shear modulus of a material mechanically? We reconstitute a network of actin filaments cross-linked with Filamin A and show that the system has remarkable property to respond under shear in a deformation history dependent manner. When a large shear stress pulse is applied to the system, the system remembers the direction of deformation long after the stress pulse is removed. For the next loading cycle, shear response of the system becomes anisotropic; if the applied pulse direction is same as the previous one, the system behaves like a viscoelastic solid but a transient liquefaction is observed if the pulse direction is reversed. Imaging and normal force measurements under shear suggest that this anisotropic response comes from stretching and bending dominated deformation directions induced by the large shear deformation giving rise to a direction dependent mechano-memory. The long time scale over which the memory effect persists has relevance in various deformations in cellular and multicellular systems.

1S.M. acknowledges support from a Kadanoff-Rice Post Doctoral fellowship from MRSEC, University of Chicago.

P1.00008 Understanding hydrodynamics in the cell at the molecular level

Xiaoyu Bai, Peter WolyneS, Rice Univ — Cellular collective motion is a result of complex coupling of nonequilibrium mechano-chemical events in the cytoskeleton, of which the underlying physics is far from completely understood. In an attempt to study the cytoskeletal dynamics, we develop analytical theories based on a coarse-grained model, Cat’s Cradle. Our current work highlights how the activated events due to energy-consuming molecular motors are coupled by hydrodynamic interaction and therefore reveals the modified cytoskeletal dynamics. Within our framework, we were able to find the stability limit of the uniformly flowing phase, which is consistent with the predictions from the well-studied continuum models. In the model we accounted for the effect of shear-stretching forces on the extended structure of molecular motors. The resulting influenced stochastic properties of motor power strokes provide us with further insights into the nonequilibrium aspects of cellular dynamics.

P1.00009 Behavior of Caulobacter Crescentus Diagnosed Using a 3-Channel Microfluidic Device

Jay Tang, Michael Morse, Brown University, Remy Colin, Max Planck Institute-Marburg, Laurence Wilson, University of York — Many motile microorganisms are able to detect chemical gradients in their surroundings in order to bias their motion towards more favorable conditions. We study the biased motility of Caulobacter crescentus, a singly flagellated bacteria, which alternate between forward and backward swimming, driven by its flagella motor, which switches in rotation direction. We observe the swimming patterns of C. crescentus in an oxygen gradient, which is established by flowing atmospheric air and pure nitrogen through a 3 parallel channel microfluidic device. In this setup, oxygen diffuses through the PDMS device and the bacterial medium, creating a linear gradient. Using low magnification, dark field microscopy, individual cells are tracked over a large field of view, with particular interest in the cells’ motion relative to the oxygen gradient. Utilizing observable differences between backward and forward swimming motion, motor switching events can be identified. By analyzing these run time intervals between motor switches as a function of a cell’s local oxygen level, we demonstrate that C. crescentus displays aerotactic behavior by extending forward swimming run times while moving up an oxygen gradient, resulting in directed motility towards oxygen sources. Additionally, motor switching response is sensitive to both the steepness of the gradient experienced and background oxygen levels with cells exhibiting a logarithmic response to oxygen levels.

1Work funded by the United States National Science Foundation and by the Rowland Institute at Harvard University.

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1Work funded by the United States National Science Foundation and by the Rowland Institute at Harvard University.
P1.00010 Influence of Chirality in Ordered Block Copolymer Phases, ISHAN PRASAD, GREGORY GRASON, University of Massachusetts Amherst — Block copolymers are known to assemble into rich spectrum of ordered phases, with many complex phases driven by asymmetry in copolymer architecture. Despite decades of study, the influence of intrinsic chirality on equilibrium mesophase assembly of block copolymers is not well understood and largely unexplored. Self-consistent field theory has played a major role in prediction of physical properties of polymeric systems. Only recently, a polar orientational self-consistent field (oSCF) approach was adopted to model chiral BCP having a thermodynamic preference for cholesteric ordering in chiral segments. We implement oSCF theory for chiral nematoc polymers, where segment orientations are characterized by quadrupolar chiral interactions, and focus our study on the thermodynamic stability of bi-continuous network morphologies, and the transfer of molecular chirality to mesoscale chirality of networks. Unique photonic properties observed in butterfly wings have been attributed to presence of chiral single-gyroid networks, this has made it an attractive target for chiral metamaterial design.

P1.00011 Jamming, Self-Filtration and Cake Growth in Concentrated Particle Suspensions, YOUJING GUO, Chemical Engineering, Tongji University, Shanghai, SHOUBO LI, DONGLEI YANG, YONGLI MI, Department of Chemistry, Tongji University, Shanghai, XIAORONG WANG, Institute for Advanced Study, Tongji University, Shanghai, P. R. China — We study the flows of concentrated particle suspensions driven through a circular gap. Above a critical concentration, a jammed structure (i.e., quasi-solid sphere) often forms in the flow and at the entrance of the geometrical constriction. Once occurred this jammed structure grows fast as time t passes and produces a reduction in the solid concentration downstream. Our analysis shows that a combination of the particle jamming, the self-filtration, and the cake-formation with the flow passing through the pores of the jammed solid is responsible for the occurrence of such phenomena. Based on this mechanism, we establish a mathematical model to show how the jammed structure is propagated. Our results suggest that the size D of the jammed structure in this case is proportional to a 1/3 power of the time t. Experiments also support this conclusion.

P1.00012 Designing thermo-responsive nanocomposites with anti-fouling properties, YA LIU, GER-MALD MCFARLIN, University of Pittsburgh, XIN YONG, Binghamton University, OLGA KUKSENOK, ANNA BALAZS, University of Pittsburgh — Inspired by marine organisms that utilize active “defense” (such as active cilia) to prevent the biofouling of their surfaces, we use computational modeling to design synthetic gel-based composite films that provide dual “defense” for anti fouling applications. We design a nanocomposite gel film that can be harnessed to repel a variety of particles via either a temperature change or an imposed shear. Incorporation of stiff hydrophobic posts into a gel composed of cross-linked poly(N-isopropylacrylamide) chains allows us to drastically alter the film’s surface properties when gel undergoes temperature-induced volume phase transition. Depending on whether the system’s temperature is below or above the lower critical solution temperature (LCST) of the gel, the posts are hidden in the swollen gel or exposed to the external solution. We model our system using dissipative particle dynamics (DPD); we validate our model through comparisons with Flory-Rehner theory. We focus on the influence of shear and rotational motion on the position of the particles in the system and isolate the conditions under which adsorption of particles of different sizes to the substrate is effectively prevented.

P1.00013 Optically driven translational and rotational motions of micro-rod particles in a nematic liquid crystal, RALF STANNARIUS, ALEXEY EREMIN, HAJNALKA NADASI, HIDEO TAKEZOE, Otto von Guericke University, Magdeburg, PEMIKA HIRANKITTIWONG, NATTAPORN CHATTHAM, Kasetsart University, Bangkok, OSAMU HABA, KOICHIRO YONETAKE, Yamagata University, Yonexawa — Liquid crystals are self-organized mesomorphic materials with various symmetries and structures. Their unique features can be exploited for smart multi-functional materials. Cylindrical dispersions of micro- and nano-particles in LCs have been widely studied. We demonstrate controlled light-driven translational and rotational motions of micro-rods in a nematic liquid crystal. A small amount of azo-dendrimer molecules dissolved in a liquid crystal drives translation and rotation under non-polarized UV light irradiation. This is initiated by a light-induced trans-to-cis conformational change of the dendrimer adsorbed at the rod surface and the associated director reorientation. This system represents an optically driven molecular microactuator, which exploits molecular reorientation on a particle surface and transforms it into a mechanical torque.

P1.00014 Thermophoresis of micrometer-sized poly(N-isopropylacrylamide) microgel particles, KEVIN APTOWICZ, West Chester University, TIM STILL, ARJUN YODH, University of Pennsylvania — We investigate the diffusion and thermophoresis of micrometer sized poly(N-isopropylacrylamide) (PNIPAM) gel particles in a temperature gradient. Recently published results of the thermophoretic mobility of PNIPAM systems are puzzling. Cross-linked microgel particles show unusually large thermophoretic mobility whereas the mobility of micrometer-sized poly(N-isopropylacrylamide) chains allows us to drastically alter the film’s surface properties when gel undergoes temperature-induced volume phase transition. The adsorption behavior of CO2 under mesoporous confinement at room temperature is particularly relevant. Small Angle Scattering of X-ray (SAXS) and Neutron (SANS) were used to probe the adsorption process of CO2 under such mesoporous confinement MCM-41 and details of nucleation pathways were mapped out by fitting the scattering intensities with adsorption models. From both experiments, the nucleation of CO2 on the inner pore surface of MCM-41 is found to be a two-step process; high density liquid phase CO2 first forms uniform layers following the long range translational symmetry of the porous matrix, above one CO2 filling, determined by the pore size and capillary condensation initiates. The nucleation sites formed during capillary condensation start to separate the long range symmetry from the one at uniform layers. Finally, SAXS and SANS techniques are compared and they both showed their unique properties of probing the filling-dependent structures of adsorbed CO2 under such mesoporous system.

P1.00016 Divergence of the Long Wavelength Collective Diffusion Coefficient in Quasi-one and Quasi-two Dimensional Colloid Suspensions, BINHUA LIN, University of Chicago, BIANXIAO CUI, Stanford University, XINLIANG XU, MIT, RONEN ZANGI, Basque Foundation for Science, Spain, HAIM DIAMANT, Tel Aviv University, STEWART A. RICE, University of Chicago — We report the results of experimental study of the short-time long-wavelength collective diffusion behavior of particle displacements in q1D and q2D colloid suspensions. Our results are reported via the q>0 behavior of the hydrodynamic function H(q) that relates the effective collective diffusion coefficient, Dc(q), with the static structure factor S(q) and the self-diffusion coefficient of isolated particles Dc. H(q)Dc(q)S(q)/Dc. We find an apparent divergence of H(q) as q>0 with the form H(q)~(1−7q<1−9), for both q1D and q2D colloid suspensions. Given that S(q) does not diverge as we infer that Dc(q) does. This behavior is qualitatively different from that of the three-dimensional H(q) and Dc(q) as q>0, and the divergence is of a different functional form from that predicted for the diffusion coefficient in one component 1D and 2D fluids not subject to boundary conditions that define the dimensionality of the system.

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Predicting and measuring the effects of colloid polydispersity during spinodal decomposition. JOHN WILLIAMSON, Georgetown University, R. MIKE L. EVANS, University of Leeds — Polydispersity pervades soft matter physics, but remains so poorly understood that its effects are often guessed at or ignored entirely. Significant progress has been made on the phase equilibria of polydisperse colloids, but practical understanding of the kinetics that govern real systems lags behind. We employ Kinetic Monte Carlo simulation to study the gas-liquid spinodal decomposition of a size-polydisperse colloid, particularly focusing on fractionation (demixing) between the phases, an effect which causes the properties of the “daughter” phases to depart significantly from the overall “parent” particle distribution. We find that intricate fractionation takes place from the earliest times, so can play a role even in arrested, far-from-equilibrium states (e.g. gels). Novel techniques (in principle applicable to experiment) are developed to detect fractionation: a parameter-free method of systematically coarse-graining local volume fraction; and several spatial correlation functions. The qualitative features of fractionation, including a striking dependence on inter-particle potential, are correctly predicted by a theory requiring only a monodisperse reference free energy.


Cooperative dynamics in ultrastiff 2D crystals. JORIS SPRAKEL, Wageningen University, BEREND VAN DER MEER, MARJOLEIN DIJKSTRA, JASPER VAN DER GUCHT, Utrecht University — The creation, annihilation, and diffusion of defects in crystal lattices play an important role during crystal melting and deformation. Although it is well understood how defects form and react when crystals are subjected to external stresses, it remains unclear how crystals cope with internal stresses. We report a study in which we create a highly localized internal stress, by means of optical tweezing, in a crystal formed from micrometer-sized colloidal spheres and directly observe how the solid reacts using microscopy. We find that, even though the excitation is highly localized, a collective dance of colloidal particles results: these collective modes take the form of closed rings or open-ended strings, depending on the sequence of events which nucleate the rearrangements. Surprisingly, we find from Brownian Dynamics simulations that these cooperative dynamics are thermally-activated modes inherent to the crystal, and can even occur through a single, sufficiently large thermal fluctuation, resulting in the irreversible displacement of 100s of particles from their lattice sites.

Fabrication of Uniform Janus Microparticles by Photopolymerization-Driven Phase Separation and their Asymmetric Hybridization with Metal Nanoparticles. JANGWOO CHO, JEONG WON KIM, JIN WONG KIM, Hanyang Univ — In the field of colloid science, there is growing interest in synthesis of anisotropic particles, since they are desirable for controlling light scattering. These anisotropic particles have been developed by using sophisticated techniques, including clusternization, stamping, microfluidics, and controlled nucleation and precipitation. This study introduces a facile approach for fabrication of uniform Janus microparticles with anisotropic phases as well as selected surface chemistry. The technique we employed to synthesize these microparticles was the seeded swelling and polymerization method, in which complete compartmentalization of the particles into two distinct phases occurred upon polymerizing the monomer-swollen droplets. Then, we patched nanoparticles, such as gold nanoparticles and magnetic nanoparticles, onto one of the compartmentalized phases of the Janus microparticles. Finally we demonstrate that these asymmetrically hybridized Janus microparticles are of great importance and play a role in the designated colloidal 2D array.

Fabrication of Uniform Hydrogel Microparticles with Alternate Polyelectrolyte/Silica Shell Layers for Applications of Controlled Loading and Releasing. EUN SOOK JEONG, JIN WONG KIM, Hanyang Univ — Hydrogel particles, also known as microgels, consist of cross-linked three-dimensional water-soluble polymer networks. They play an essential role in loading and delivering active ingredients in medicine, cosmetics, and foods. Despite their excellent biocompatibility as well as structural diversity, much wider applications are limited due mainly to their intrinsically loose network nature. This study introduces a practical and straightforward method that enables fabrication of hydrogel microparticles layered with a mechanically robust hybrid thin shell. Basically highly monodisperse hydrogel microparticles were produced in microcapillary devices. Then, their surface was coated with alternate polyelectrolyte layers through the layer-by-layer deposition. Finally a thin silica layer was again formed by reduction of silicate on the amino-functionalized polyelectrolyte layer. We have figured out that these hybrid hydrogel microparticles showed controlled loading and releasing behaviors for water-soluble probe molecules. Moreover, we have demonstrated that they can be applied for immobilization of biomacromolecules, such as bacteria and living cells, and even for targeted releasing.

2D Colloidal Wigner crystals in confined geometries. RUBEN HIGLER, JORIS SPRAKEL, Wageningen University — Crystalization of bulk systems has been widely studied using colloids as a model system. However, study into colloidal crystallization in confined geometries has been sparse and little is known about the effects of confinement on the dynamics of colloidal crystal. In our research we prepare 2D crystals from charged colloids in an apolar solvent to study crystal dynamics, formation, and structure in circular confinements. These confining geometries are made using soft lithography techniques from SU-8. In order to broaden the parameter space we can reach in experiments we employ Brownian dynamics simulations to supplement our experimental results. Using single-particle tracking we have subpixel resolution positional information of every particle in the system. We study the vibrational modes of our confined crystals and find well defined modes unique to confined systems, such as a radially symmetric compression (or breathing) mode, a collective rotation mode, and distinct resonance modes. Furthermore, due to the circular nature of our confinements, defectless crystals are impossible, we find, for sufficiently high area fractions, that the defects order at well defined points at the edge. The effect of this “defect-localization” has a clear influence on the vibrational modes.

Shear-induced demixing of glassy suspension. TIES VAN DE LAAR, JORIS SPRAKEL, KARIN SCHROEN, Wageningen University — The ground state of a binary suspension composed of particles of incommensurate size is that of two demixed crystal phases. However this has never been experimentally observed, due to the prohibitively long time scales associated with diffusion in a glass. Here we show that enhancing particle mobility in a glass, by means of flow, can lead to this type of solid-solid demixing. We study this phenomenon at the scale of single particles by means of high speed confocal imaging of suspensions flowing through microfluidic concentrators and deformation of glasses.
for both systems will be presented and discussed in light of available experimental data. The POL FF showed a much stronger sensitivity to the details of biphenyl conformational properties and was able to predict $T_{NI}$ which is very close to the experimental $T_{NI}$. We derive the equations that couple the electric potential to the orientation of the NLC’s director field and use asymptotic and computational methods to address the question: Under what conditions is the uniform field assumption justified, and when is it inappropriate?

The electric field is generated by the applied voltage across the NLC cell, which consists of two plates with a liquid crystal mixture between them. One of the plates is a photosensitive plate, while the other has a coating of azo dye molecules.

P1.00025 Hyperuniformity of self-assembled soft colloidal spheres, COLINE BRETZ, University of Pennsylvania, YU XU, Complex Assemblies of Soft Matter, CNRS-Rhodia-UPenn; University of Pennsylvania, TIM STILL, University of Pennsylvania, JEAN BAUDRY, ESPCI ParisTech/CNRS, LAWRENCE A. HOUGH, Complex Assemblies of Soft Matter, CNRS-Rhodia-UPenn, ARJUN G. YODH, University of Pennsylvania, SALVATORE TORQUATO, Princeton University, REMI DREYFUSS, Complex Assemblies of Soft Matter, CNRS-Rhodia-UPenn, COMPLEX ASSEMBLIES OF SOFT MATTER TEAM3, DEPARTMENT OF PHYSICS AND ASTRONOMY TEAM2, LABORATOIRE DE COLLOIDES ET MATIERES DIVISES TEAM3 — Hyperuniformity characterizes a state of matter for which density fluctuations vanish on large scales. Hyperuniform materials are of technological importance as they exhibit interesting photonic properties. We have shown that such materials can be obtained by assembling spheres into a disordered 2D-packed. To this end, we use a binary mixture of large and small Poly(NIPAM) particles confined between two cover slips. These soft spheres have been chosen for their temperature-sensitive properties. We can locally increase or decrease the volume fraction occupied by the spheres by finely tuning the temperature.

By applying various temperature patterns, we are studying the spatial arrangements of the microgels and characterizing their hyperuniform properties through reconstruction and detection algorithms.

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P1.00026 Model colloidal system for interfacial adsorption kinetics, STEVEN HUDSON, PAUL SALIPANTE, NIST — An experimental colloidal model for sorption behavior may allow direct observation of the effects of particle shape and concentration on adsorption and desorption kinetics. Here we investigate spherical colloidal adsorption to a near solid surface. The attraction is induced by depletion interaction. The colloid-

P1.00027 ABSTRACT WITHDRAWN

P1.00028 Interfacial Behavior of Polymer Coated Nanoparticle, LUQING QI, HADI SHAMSIJAZEYI, JASON MANN, RAFAEL VERDUZCO, GEORGE HIRASAKI, Rice Univ, RICE UNIVERSITY TEAM — Oxidized carbon black (OCB) nanoparticle is functionalized with different coatings, i.e. alkyl group, polyvinyl alcohol (PVA) and partially sulfonated polyvinyl alcohol (spVA). In oil and water systems, the functionalized nanoparticle is found to have a versatile dispersion i.e. in lower aqueous phase, in upper oil phase, or in middle phase microemulsion. Oil substitute n-octane and commercial oil IOSPAR have been test as oil phase; series of commercially available surfactant, C12-4.5 orthoxylene sulfonate(OXS), i-C13-(PO)7 –SO4Na (S13B), surfactant blend of anionic Alfolterna with nonionic Tergitol have been test as additive to help with the OCB dispersion. It is found that the OCB with sulfonated polyvinyl alcohol attachment (spVA-OCB) stays in microemulsion; with the increase of salinity, it follows the microemulsion to go from lower phase, to middle phase, and to upper phase. The dispersion of spVA and alkyl functionalized OCB (Cn-OCB-spVA) is the balance of the length of alkyl and spVA and the degree of sulfonation of PVA, depending on which, it can either disperse into microemulsion or form a separate layer. The spVA-OCB also indicates a tolerance of high salinity; this is shown by the stable dispersion of it in blend surfactant solution of anionic Alfolterna and nonionic Tergitol at high salinity API brine (8% NaCl and 2% CaCl2). The study of different functionality on OCB dispersion can help design appropriate modified nanoparticle as additive for enhanced oil recovery either to reduce the interfacial tension between oil and water, or to stabilize microemulsion.

P1.00029 Nematic Liquid Crystal reorientation with a Photosensitive layer, ADRIAN REYES, LAURA PALOMARES, PATRICIA GUTIERREZ, Universidad Nacional Autonoma de Mexico — We assume a nematic cell in a planar configuration for which one of their confining plates, is submitted to a hard-anchoring boundary condition and the other plate has a coating monolayer of azo dye molecules, such that the change of the orientation of azo dye isomers, due to light, causes changes in the nematic director. We find an approximated expression for the density of isomers, written in terms of the director angle, which allows us to close the equation for the director’s angle on the boundary having a photosensitive plate. We have managed to decouple the director’s angle and the isomer densities by assuming extremely different temporal time scales between them. We show that switching times inversely depend on trans-cis transition rate of photo-excitation meanwhile relaxation times do not depend on it, for a given sample. On the other hand, switching and relaxation times linearly depend on surface viscosity values.

P1.00030 Electric field variation within a nematic liquid crystal layer1, LINDA CUMMINGS, ENSELA MEMA, CHENJING CAI, LOU KONDIC, New Jersey Institute of Technology — A thin layer of Nematic Liquid Crystal (NLC) across which an electric field is applied is a setup of great industrial importance in Liquid Crystal Display devices, and there is a wide associated literature. A common assumption is that an electric field generated by constant-potential electrodes at the two bounding surfaces of the layer will produce a field that is uniform: the presence of NLC does not affect the electric field. We derive the equations that couple the electric potential to the orientation of the NLC’s director field and use asymptotic and computational methods to address the question: Under what conditions is the uniform field assumption justified, and when is it inappropriate?

1 Supported by NSF Grant No. DMS-1211713.
P1.00032 Polarized Raman Spectroscopic and Conoscopic study of twist-bend nematic liquid crystal CB7CB

JINXIN FU, KARTHIK NAYANI, JUNG OK PARK, MOHAN SRINIVASARAO, Georgia Institute of Technology — The liquid crystal CB7CB, which exhibits a new twist bend nematic phase, has aroused lots of interests recently. We use polarized Raman Spectroscopy to measure the liquid crystal order parameters, which are crucial to know the molecular orientation distribution and to understand the phase transition. It is found that in the twist-bend phase, both $P<200$ and $P<400$ increase with temperature before the nematic transition takes place at 103°C, and then decrease in the nematic region until the LC becomes isotropic at 116°C. Conoscopy is a convenient tool to determine the structure and orientation of crystals. We develop a monochromatic conoscopy method to study the uniaxial and biaxial behavior of CB7CB in the different phases.

1This work was supported from the U.S. Office of Basic Energy Sciences, Department of Energy; Grant No. DE-SC0001412.

P1.00033 Ground states of lyotropic chromonic liquid crystals in cylindrical capillaries

RUI CHANG, School of Chemical and Biological Engineering, Georgia Institute of Technology, KARTHIK NAYANI, JINXIN FU, School of Material Science and Engineering, Georgia Institute of Technology, ELSA REICHMANIS, School of Chemical and Biological Engineering, Georgia Institute of Technology, JUNG OK PARK, MOHAN SRINIVASARAO, School of Material Science and Engineering, Georgia Institute of Technology — We investigate the ground states of nematic lyotropic chromonic liquid crystals (LCLCs) confined in cylindrical capillaries. Two line defects with double helical configuration is observed for Sunset Yellow FCF with the homeotropic anchoring being obtained by parylene-N coating. The striking features of nematic-isotropic phase transition is also studied, in which we find a coexistence of double helix configuration and escape radial configuration mediated with point defects in biphasic temperature range. However with Disodium Cromoglycate (DSCG) we observe that the anchoring is planar anchoring in both parylene-N coated and uncoated boro silicate capillaries.

1We acknowledge the support from the U.S. Office of Basic Energy Sciences, Department of Energy: grant DE-SC 0001412.

P1.00034 ABSTRACT WITHDRAWN —

P1.00035 Lipid Nanodiscs as potential carriers of enzymes: a light scattering study

KIRIL STRELETZKY, GAITH TAWALBEH, MEKKI BAYACHOU, Cleveland State University — The structure and dynamics of discoidal phospholipid protein complexes (nanodiscs) with and without endothelial nitric oxide synthase (eNOS) were studied with multilength polarized and depolarized light scattering. Nanodiscs present a mobile system that is similar to enzyme’s native microenvironment which allows to explore the potential effect of membrane phospholipids on the activity of eNOS. Light scattering revealed at least two different size distribution modes for empty nanodiscs, and nanodiscs loaded with eNOSs and eNOSs. In both cases, the first mode was diffusive (linear $Γ$ vs $q^2$ with a small intercept) with apparent Rh $= 4.5$ nm for empty nanodiscs and 4.9nm for loaded nanodiscs, sizes consistent with nanodisc dimensions. The second mode contributed only about 20% to the intensity and showed non-diffusive behavior which might correspond to coalesced nanodiscs present in solution. Studied concentration dependencies and depolarized scattering measurements on enzyme free and enzyme loaded nanodiscs corroborated these findings. Also, the specific activity of nanodiscs-bound eNOS was found to be significantly lower than the specific activity of free eNOS.

P1.00036 Active motion induced break-up of colloidal gels

MEGAN SZAKASITS, MICHAEL SOLOMON, University of Michigan — We found that fractal gel networks of polystyrene colloids can be broken up by active motion of Janus colloids that have been incorporated into them. Janus particles were synthesized by electron beam deposition of platinum onto one micron carboxylate modified polystyrene particles. Through addition of the divalent salt magnesium chloride, an initially stable suspension of Janus and polystyrene colloids, present in equal proportion, underwent aggregation to yield a fractal gel. The Janus colloids were activated by addition of 30% v/v hydrogen peroxide through a porous hydrogel membrane. Changes in structure and dynamics were visualized by two channel confocal laser scanning microscope (CLSM). By means of image analysis, we calculated the mean squared displacement (MSD) and radial distribution function (RDF) for gel samples before and after addition of hydrogen peroxide. The MSD confirmed the Janus particles we synthesized undergo active motion. The RDF and cluster size distribution of gel samples before and after addition of peroxide demonstrate how active motion broke apart the gel network into smaller clusters.

P1.00037 Direct visualization of photoinduced glassy dynamics on the amorphous silicon carbide surface by STM movies

DUC NGUYEN, LEA NIENHAUS, RICHARD T. HAASCH, JOSEPH LYDING, MARTIN GRUBELE, Univ of Illinois - Urbana — Glassy dynamics can be controlled by light irradiation. Sub- and above-bandgap irradiation cause numerous phenomena in glasses including photosynthesis, photodimerization, photoreduction and photoduced fluidity. We used scanning tunneling microscopy to study surface glassy dynamics of amorphous silicon carbide irradiated with above- bandgap 532 nm light. Surface clusters of $\sim 4$-5 glass forming unit in diameter hop mostly in a two-state fashion, both without and with irradiation. Upon irradiation, the average surface hopping activity increases by a factor of 3. A very long ($\sim 1$ day) movie of individual clusters with varying laser power density provides direct evidence for photoinduced enhanced hopping on the glass surfaces. We propose two mechanisms: heating and electronic for the photoenhanced surface dynamics.

P1.00038 A Simulation Study on Translation-Rotation Decoupling and its Dependence on Tracer Shape in Two Dimensional Colloids

JEONGMIN KIM, BONG JUNE SUNG, Department of Chemistry and Research Institute for Basic Science, Sogang University — Near the glass transition, translation is often faster than expected from the viscosity of liquids unlike rotation. We acknowledge the support from the U.S. Office of Basic Energy Sciences, Department of Energy: grant DE-SC 0001412.

P1.00039 Trimerization of Phenyl Cyanate Ester

MADHUSUDHAN REDDY PALLAKA, SINDEE L. SIMON, Texas Tech Univ — The kinetics of phenyl cyanate ester trimerization is studied in the bulk using differential scanning calorimetry. Dynamic experiments for different heating rates are analyzed for the activation energy using the model-free Kissinger-Akahira-Sunose(KAS) isocconversion method. The activation energy and other kinetic parameters are also obtained by fitting the dynamic data to a first order autocatalytic reaction model, which well describes the experimental data. The activation energy obtained from the KAS isocconversion method (70.1 kJ/mol) is in good agreement with that obtained from the kinetic model (73.2 kJ/mol) and is much lower than the more bulky cyanate esters studied in our laboratory, which have activation energies of approximately 95 kJ/mol. In addition, the rate constant for the phenyl cyanate ester is one to two orders higher than the bulkier cyanate esters in the temperature range of 200 to 300°C. Further elucidation of the dynamic experiments revealed a strong dependence of the reaction kinetics on the sample weight. Future work aims to understand this finding.
AT model is known to exhibit a fluctuation-driven first-order transition. An analytical renormalization group treatment by Cardy predicts that disorder rounds in the presence of quenched disorder. In this context, we numerically study the critical behavior of a three-color Ashkin Teller (AT) model in the presence of bond randomness. The clean phase transitions can be related to the eigenvalues of the transition matrix which governs the stochastic dynamics of the representative point in the FEL. We apply this formalism to various structures of the FEL which include the small world and the scale free network. We show that the TTT diagram is sensitive to the structure of the FEL, indicating the possibility of obtaining the structural information from the TTT diagram.

This work was supported in part by KAKENHI (25400429).

Critical adsorption and colloidal interaction in binary liquid mixtures. SHARMINE ALAM, RAMI OMARI, CHRISTOPHER GRABOWSKI, ASHIS MUKHOPADHYAY, Wayne State Univ — We studied critical adsorption on colloidal nanoparticles in binary liquid mixture of 2,6 lutidine + water by using fluorescence correlation spectroscopy (FCS). Our results indicated that the adsorbed film thickness is a decreasing function of temperature. The former behavior is believed to be controlled by the thermodynamics and the latter is governed by the slow dynamics. Exploiting the merit of the free energy landscape (FEL) approach which can handle both thermodynamic and dynamic processes in the same framework, we investigated the crystallization of super-cooled liquids as the first passage process of a representative point to the crystalline basin in the FEL. We first show that the crystallization time can be related to the eigenvalues of the transition matrix which governs the stochastic dynamics of the representative point in the FEL. We apply this formalism to various structures of the FEL which include the small world and the scale free network. We show that the TTT diagram is sensitive to the structure of the FEL, indicating the possibility of obtaining the structural information from the TTT diagram.

Acknowledgements are made to the Donors of the American Chemical Society Petroleum Research fund (PRF # 51694-ND10) for support of this research.

Control of nanoparticle formation using the constrained dewetting of polymer brushes. THOMAS LEE, School of Chemistry, The University of Sydney, Campdenown, NSW 2006, Australia, SHAUN C. HENDY, MacDiarmid Institute for Advanced Materials and Nanotechnology, Department of Physics, University of Auckland, Auckland 1142, New Zealand, CHIARA NETO, School of Chemistry, The University of Sydney, Campdenown, NSW 2006, Australia — We have used coarse-grained molecular dynamics simulations to investigate the use of pinned micelles formed by the constrained dewetting of polymer brushes to act as a template for nanoparticle formation. The evaporation of a thin film containing a dissolved solute from a polymer brush was modeled to study the effect of solubility, concentration, grafting density, and evaporation rate on the nucleation and growth of nanoparticles. Control over particle nucleation could be imposed when the solution was dilute enough such that particle nucleation occurred following the onset of constrained dewetting. We predict that nanoparticles with sizes on the order of 1 nm to 10 nm could be produced from a range of organic molecules under experimentally accessible conditions. This method could allow the functionality of organic materials to be imparted onto surfaces without the need for synthetic modification of the functional molecule, and with control over particle size and aggregation, allowing for the preparation of surfaces with useful optical, pharmaceutical, or electronic properties.

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Critical behavior of the disordered three-color Ashkin-Teller Model – A Monte Carlo study. QIONG ZHU, XIN WAN, Zhejiang University, RAJESH NARAYANAN, Indian Institute of Technology, Madras, JOSÉ A. HOYOS. Instituto de Física de São Carlos, Universidade de São Paulo, THOMAS VOJTA, Missouri University of Science and Technology — The impact of quenched disorder on systems undergoing first-order phase transitions has received less attention than its effects on critical points. A notable exception is the seminal work by Aizenmann and Wehr. Building on earlier work by Imry, Ma and others, they rigorously proved the vanishing of latent heat in dimensions \( d \leq 2 \) in the presence of quenched disorder. In this context, we numerically study the critical behavior of a three-color Ashkin Teller (AT) model in the presence of bond randomness. The clean AT model is known to exhibit a fluctuation-driven first-order transition. An analytical renormalization group treatment by Cardy, predicted that disorder rounds this transition and leads to a critical point in the clean Ising universality class. However, recent numerical work has questioned the veracity of these results. We therefore use Monte-Carlo techniques to re-examine the role of quenched disorder on the three-color AT model. We determine the order of the phase transition, and we perform a systematic finite-size scaling analysis of various thermodynamic quantities to extract the critical behavior.
P1.00046 Discontinuous phase transitions via cooperative contagion . FAKHTEH GHANBARNEJAD, Max-Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany, WEIRAN CAI, TU Dresden, Germany, LI CHEN, Robert Koch-Institute, 13353 Berlin, Germany, PETER GRASSBERGER, Forschungszentrum Juelich, 52425 Juelich, Germany — We study the spreading of two diseases that interact cooperatively (the presence of one helps the other one to spread) on different network topologies, and with two microscopic realizations, both of which are stochastic versions of an SIR type studied by us recently in mean field approximation. We had shown that cooperativity can lead to discontinuous transitions (DT). However, due to the rapid mixing implied by the mean field assumption, DTs were seen only when there were finite (non-zero) densities of sick individuals in the initial state. In this paper we find that the results on the stochastic model depend strongly on the underlying network. In particular, DTs are found when there are few short but many long loops: (i) No DTs exist on trees, due to the absence of loops; (ii) On 2-d lattices with local contacts there are no DTs either, but because of too many short loops; (iii) We do find DTs on Erdos-Renyi (ER) networks, on d-dimensional lattices with $d \geq 4$, and on 2-d lattices with sufficiently long-ranged contacts; (iv) On 3-d lattices with local contacts the results depend on the microscopic details of the implementation. All found discontinuous transitions are of “hybrid” type, i.e. they display also scaling features usually associated with continuous transitions.

P1.00047 ABSTRACT WITHDRAWN –

P1.00048 Origin of the $1/f^\alpha$-Spectral-Noise in Chaotic and Regular Quantum Systems . LEONARDO A. PACHON, Instituto de Fisica, Universidad de Antioquia. Department of Chemistry and Chemical Biology, Harvard University., ARMANDO RELAÑO, Departamento de Fisica Aplicada I and GISC, Universidad Complutense de Madrid, Spain., BORJA PEROPÁDRE, ALAN ASPURÚ-GUZIK, Department of Chemistry and Chemical Biology, Harvard University. — Based on the recent connection between the spectral form factor and the probability to return [Phys. Rev. Lett. 102, 150401 (2009)], the origin of the $1/f^\alpha$-noise in fully chaotic and fully integrable systems is tracked to the quantum interference between invariant manifolds of the classical dynamics and the dimensionality of those manifolds. This connection and the order-to-chaos transition are analyzed in terms of the statistics of Floquet’s quasienergies of a classically chaotic driving non-linear system. The direct connection established here allows for predicting that in the presence of decoherence, the statistics of the spectral correlations of both, chaotic and integrable, coincide.

P1.00049 Enhanced rare-region effects in the contact process with long-range correlated disorder . AHMED K. IBRAHIM, HATEM BARGHATHI, THOMAS VOJTA, Missouri Univ of Sci & Tech — We investigate the nonequilibrium phase transition in the disordered contact process in the presence of long-range spatial disorder correlations. These correlations greatly increase the probability for finding rare regions that are locally in the active phase while the bulk system is still in the inactive phase. Specifically, if the correlations decay as a power of the distance, the rare-region probability is a stretched exponential of the rare-region size rather than a simple exponential as is the case for uncorrelated disorder. As a result, the Griffiths singularity transforms into a non-power-law form. The critical point itself is of infinite-randomness type but with critical exponent values that differ from the uncorrelated case. We report large-scale Monte Carlo simulations that verify and illustrate our theory. We also discuss generalizations to higher dimensions and applications to other systems such as the random transverse-field Ising model, itinerant magnets, and the superconductor-metal transition.

P1.00050 Critical Initial Slip Scaling for Driven-dissipative Bose-Einstein Condensation1 . WEIGANG LIU, UWE TAUBER, Department of Physics, Virginia Tech — We investigate the universal non-equilibrium critical behavior at the driven- dissipative Bose-Einstein condensation phase transition by means of the perturbative field-theoretic renormalization group method. Such criticality may be realized experimentally in driven open systems on the interface of quantum optics and many-body physics, ranging from exciton-polariton condensates in optically pumped semiconductor wells to cold atomic gases. We describe the critical dynamics through a noisy and dissipative Gross- Pitaevski or time-dependent Ginzburg-Landau equation with complex coefficients. We focus on the universal critical behavior of this system in the early stages of the relaxation process following a quench from an initially (Gaussian distributed) disordered state that is characterized by broken time translation invariance and governed by the “initial slip” exponent $\theta$. We compute $\theta$ to first order in the dimensional $z = 4 - d$ expansion with respect to the upper critical dimension $d=4$, and find that its one-loop value is identical to that of the classical relaxational model $A$ for a two-component non-conserved order parameter.

1Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-09ER46613.

P1.00051 Energy flow between two hydrodynamically coupled particles kept at different effective temperatures1 . SERGIO CILIBERTO, ENSL-CNRS, ANTOINE BERUT, ENSL, ARTYOM PETROSYAN, ENSL-CNRS, EQ 2 TEAM — We measure the energy exchanged between two hydrodynamically coupled micron-sized Brownian particles trapped in water by two optical tweezers. The system is driven out of equilibrium by random forcing the position of one of the two particles. The forced particle behaves as it has an “effective temperature” higher than that of the other bead. This driving modifies the variance functions and cross-correlation functions of the bead positions: we measure an energy flow between the particles and an instantaneous cross-correlation, proportional to the effective temperature difference between the two particles. A model of the interaction which is based on classical hydrodynamic coupling tensors is proposed. The theoretical and experimental results are in excellent agreement.

1ERC-Outfelcoup

P1.00052 Effect of Graphene in Quenching Fluorescence from Strained Conjugated Polymer Doped Polystyrene Composite Films1 , XUAN LONG HO, YAN-HAO CHEN, JONATHON DAVID WHITE, NEN-WEN PU, Yuan Ze University, Taiwan, ARNOLD CHANG-MOU YANG, National Tsing Hua University, Taiwan — Introduction of graphene into films and solutions of conjugated polymers has been observed to dramatically quench photoluminescence (PL) of MEH-PPV. In other work, the PL of MEH-PPV well dispersed in an optically inert matrix was seen to be dramatically increased when the individual molecular strands were fully stretched. Strong polarization effects indicated that stretching individual polymer chains was responsible for the observed enhancement. We examine the combined effect of stress and the addition of reduced graphene oxide (rGO) on PL. We found that the addition of a small amount of rGO (0.3%) into polystyrene films lightly doped with 1% MEH-PPV quenched 40% of the PL. Stretching resulted in the creation of local deformation zones (LDZ) of high stress and strain. Within these zones, while the PL efficiency increased dramatically (rGO) on PL. We found that the addition of a small amount of rGO (0.3%) into polystyrene films lightly doped with 1% MEH-PPV quenched 40% of the PL.

1Supported by the Ministry of Science and Technology of the Republic of China

P1.00053 Mechanical Properties of Hydrogel Beads . KEELY CRIDDLE, THOMAS BENNS, DAN SHORTS, KLEBERT FEITOSA, James Madison University — Fragile solids made of dense disordered packing of bubbles, droplets and grains are able to withstand small stresses by virtue of system-wide force chains that lock the system into a jammed state. The nature of the jamming transition in such soft materials has been the subject of intense research, but despite much effort, a deep understanding remains elusive. In this experiment we study the mechanical properties of hydrogel beads to exploit them as force transducers in densely packed systems. The experiment consists of applying uniaxial planar compressions on the beads, and correlating the force to the bead’s strain and contact area. The results show that while the strain scales linearly with the diameter of the contact area, the force and strain are found to obey a power law relation with two distinct exponents at small and large strains. This result leads to a power law dependence of the force on the contact area diameter of the compressed bead.
P1.00054 The nature of long-ranged forces between pinned particles in a jammed system. JUAN-JOSE LIETOR-SANTOS, JUSTIN BURTON, Emory University — We explore the interaction between two fixed-position particles immersed in a binary, two-dimensional jammed system of disks at $T=0$. In our simulations, the two pinned particles develop an interaction along their alignment direction. At short distances, their interaction can be described by a mean-force potential derived from the particle-particle correlation function, $g(r)$, and thus have a repulsive and attractive nature which depends on separation. However, there is an additional repulsive force that dominates at large particle separation or when the ambient jammed disks are much smaller than the pinned particles. We will show that the nature of this repulsive force stems from fluctuations near the jamming transition, in analogy with other fluctuation-induced forces, such as the thermal Casimir effect. We expect these results will be relevant to other studies of pinned particles near the glass transition [1]. The dependence of the long-ranged force on packing fraction, particle separation, and the size ratio of pinned to free particles will be discussed.


P1.00055 “Anti-Equilibrium”: The limiting frozen state of kappa distributions. GEORGE LIVADIOTIS, Southwest Research Institute, USA — The kappa distribution of particle velocities provides an unambiguous replacement of the Maxwell distribution for systems out of thermal equilibrium. The kappa index is a measure of how far the system of particles is from thermal equilibrium. This “thermodynamic distance” is inversely proportional to the kappa index; it becomes zero at thermal equilibrium where the kappa index is infinite, while it obtains its maximum at the furthest state from thermal equilibrium, where the kappa index is zero, a state called “anti-equilibrium.” By keeping fixed the temperature and decreasing the kappa index, the particles approach this peculiar state of anti-equilibrium and are characterized by a power-law distribution density with spectral index $\sim 1.5$; this constitutes a universal behavior, independent of the system’s number of particles or degrees of freedom. As the kappa decreases and the system approaches the anti-equilibrium state, the particles lose their kinetic energy. This procedure of “kappa-freezing” by decreasing the kappa index at a fixed temperature is similar to the more familiar freezing procedure of decreasing temperature and approaching the “absolute zero” for a fixed kappa index.

P1.00056 The price of anarchy is maximized at the percolation threshold. BRIAN SKINNER, Argonne National Laboratory — When many independent users try to route traffic through a network, the flow can easily become suboptimal as a consequence of congestion, if the number of efficient paths is small. The degree of this suboptimality is quantified by the so-called “price of anarchy” (POA), but so far there are no general rules for when to expect a large POA in a random network. Here I address this question by introducing a simple model of flow through a network with randomly-placed “congestible” and “incongestible” links. I show that the POA is maximized precisely when the fraction of congestible links matches the percolation threshold of the lattice. Both the POA and the total cost demonstrate critical scaling near the percolation threshold.

P1.00057 Four Parameter Characterization of Network Reliability and Analysis of Critical Point Phenomenology. MADHURIMA NATH, STEPHEN EUBANK, MINA YOUSSEF, YASAMIN KHORRAMZADEH, SHAHIR MOWLAEI, Virginia Tech — A new characterization of network structure as represented by the reliability polynomial is introduced that requires only four parameters. Exact evaluation of the polynomial is not feasible for large graphs. Approximation to within a specified error is feasible, but a complete specification of the polynomial still requires many parameters. However, it turns out that a two-parameter family of functions fits the non-trivial part of the reliability polynomial to within approximation error. We demonstrate this by fitting the reliability polynomials of both random graphs with different sizes and synthetic social networks to the error function. The network reliability can be viewed as a partition function of a physical system, for example percolation on a network. This method produces a good analytical approximation to the partition function and suggests a way to explore critical point phenomenology.

P1.00058 Diffusion theory of Brownian particles moving at constant speed in $D$ dimensions. FRANCISCO J. SEVILLA, Instituto de Física, Universidad Nacional Autónoma de México — The propagation of Brownian-active particles that move at constant speed in the limit of short times, differs from wave-like propagation in that active particles propagate without leaving a wake trailing characteristic of wave propagation in even dimensions. In the long time regime, normal diffusion is expected due to random fluctuations that disperse the particle direction of motion. A phenomenological equation that describe the transition from the behavior free of effects of wake, to the normal diffusion of the particles is proposed. A comparison of the results predicted by such equation with those obtained from models using Langevin equations is presented in the spherically symmetric case.

1FJS acknowledges support from PAPIIT-UNAM through the grant IN113114.

P1.00059 ABSTRACT WITHDRAWN —

P1.00060 Nature of the Congested Traffic and Quasi-steady States of the General Motor Models. BO YANG, Institute of High Performance Computing, XIHUA XU, National University of Singapore, JOHN Z.F. PANG, CHRISTOPHER MONTEROLA, Institute of High Performance Computing — We look at the general motor (GM) class microscopic traffic models and analyze some of the universal features of the (multi-)cluster solutions, including the emergence of an intrinsic scale and the quasistationary dynamics in the real traffic dynamics, especially the phase transition from the free flow to the congested phase, from which the wide moving jams emerges (the F-S-J transition pioneered by B.S. Kerner). In particular, the congested phase can be associated with either the multi-cluster quasi-steady states, or their more homogeneous precursor states. In both cases the states can last for a long time, and the narrow clusters will eventually grow and merge, leading to the formation of the wide moving jams. We present a general method to fit the empirical parameters so that both quantitative and qualitative macroscopic features can be reproduced with a minimal GM model. We present numerical results for the traffic dynamics both with and without the bottleneck, including various types of spontaneous and induced “synchronized flow,” as well as the evolution of wide moving jams. We also discuss its implications to the nature of different phases in traffic dynamics.

P1.00061 New Analysis Techniques for Avalanches in a Conical Bead Pile with Cohesion. CATHERINE TIEMAN, SUSAN LEHMÁN, Department of Physics, College of Wooster, Wooster, OH — Avalanche statistics and pile geometry for 3 mm steel spheres dropped on a conical bead pile were studied at different drop heights and different cohesion strengths. The pile is initially built on a circular base and is subsequently slowly driven by adding one bead at a time to the apex of the pile. We investigate the dynamic response of the pile by recording avalanches off the pile over the course of tens of thousands of bead drops. The level of cohesion is tuned through use of an applied uniform magnetic field. Changes in the pile mass and geometry were investigated to determine the effect of cohesion and drop height on the angle of repose. The angle of repose increased with cohesion strength, and decreased somewhat for higher drop heights. The packing density of beads is expected to decrease as magnetic cohesion increases, but for our 20 000-bead pile, this effect has not been observed. The proportion of beads removed from the pile by different avalanche sizes was also calculated. Although larger avalanches are much rarer occurrences, they carry away a larger fraction of the total avalanching mass than small avalanches. As the pile cohesion increases, the number of small and medium avalanches decreases so that this mass loss distribution shifts more strongly to large sizes.
Use of a magnetic field to modify and detect avalanche behavior on a conical bead pile. NATHAN J. HAYNES, SUSAN LEHMAN. Department of Physics, College of Wooster, Wooster, OH — A conical bead pile subject to slow driving and an external magnetic field is used to test the effects of drop height and cohesion on avalanche statistics. Magnetically susceptible beads were dropped onto a pile from different heights and into different strengths of magnetic field. Avalanches were recorded by the change in mass as beads fall off the pile. For beads dropped from a low drop height with no cohesion, the avalanche size distribution follows a power law. As cohesion increases, we observe an increase in the probability of very large avalanches and decreases in the mid-size avalanches. The resulting bump in the avalanche distribution moves to larger avalanche size as the cohesion in the system is increased, matching the prediction by an analytic theory from a mean-field model of slip avalanches. The model also makes predictions for avalanche duration, which is not measurable with our current system. Since the steel beads are magnetized while in the applied magnetic field, their motion during an avalanche creates a change in magnetic field. To detect this motion, we have placed a large-diameter pick-up coil around the pile. Results of the testing and calibration of this coil to measure avalanche duration are presented.

Granular gas mediated attraction of intruders in a granular Casimir effect. GEORGE WILKES, BRIAN UTTER. James Madison University — When two objects are submerged in a granular gas, entropic effects due to inelastic collisions lead to attractions between the objects. This has been referred to as an analog to the Casimir effect, though arises via a different mechanism. In this experiment, we place two objects (such as vertical plates or spheres) in either a strongly driven granular gas or dense fluid. We find that when the plates are closely spaced, there is a net attractive force. By analyzing high-speed video, we track the distance between these plates and characterize the effective force versus distance with changes in the vibration parameters and initial separation. A 2D simulation is also used to further explore parameter space.

Fingerling in Confined Elastic Layers. JOHN BIGGINS, University of Cambridge, L. MAHADEVAN, Harvard, Z. WEI, Stanford, B. BAUDOUIN-SAINTEVES, Harvard, E. BOUCHAUD. Commissariat à l’énergie atomique et aux énergies alternatives — Fingerings has recently been observed in soft highly elastic layers that are confined between and bonded to two rigid bodies. In one case an injected fluid invades the layer in finger-like protrusions at the layer’s perimeter, a solid analogue of Saffman-Taylor viscous finger. In a second case, separation of the rigid bodies (with maintained adhesion to the layer) leads air to the formation of similar fingers at the layer’s perimeter. In both cases the finger formation is reversible: if the fluid is removed or the separation reduced, the fingers vanish. In this talk I will discuss a theoretical model for such elastic fingers that shows that the origin of the fingers is large-strain geometric non-linearity in the elasticity of soft solids. Our simplified elastic model unifies the two types of fingerling and accurately estimates the thresholds and wavelengths of the fingers.

Non-equilibrium relaxation between two quasi-stationary states in a stochastic lattice Lotka-Volterra model. SHENG CHEN, UWE C. TÄUBER. Department of Physics, Virginia Tech — Spatially extended stochastic models for predator-prey competition and coexistence display complex, correlated spatio-temporal structures and are governed by remarkably large fluctuations. Both populations are characterized by damped erratic oscillations whose properties are governed by the reaction rates. Here, we specifically study a stochastic lattice Lotka-Volterra model by means of Monte Carlo simulations that impose spatial restrictions on the number of occupants per site. The system tends to relax into a quasi-stationary state, independent of the imposed initial conditions. We investigate the non-equilibrium relaxation between two such quasi-stationary states, following an instantaneous change of the predation rate. The ensuing relaxation times are measured via the peak width of the population density Fourier transforms. As expected, we find that the initial state only influences the oscillations for the duration of this relaxation time, implying that the system quickly loses any memory of the initial configuration.

Implications of lack-of-ergodicity in 2D Potts model. SMITA OTA. None — Microcanonical Monte Carlo simulation is used to study two dimensional (2D) q state Potts model. We consider a 2D square lattice having N×N spins with periodic boundary condition and simulated the system with N=15 and q=10. The demon energy distribution is found to be exponential for high system energy and large system size. For smaller system size and above the first order transition the demon energy distribution is found to deviate from exp(-βE) and has the form exp(-βE + γD). Here β = 1/k_BT and k_B is the Boltzmann constant. It is found that γ is finite at higher temperatures. As the system energy is reduced γ becomes zero near the first order transition. It is found that during cooling γ changes sign from negative to positive and then to negative again near the 1st order transition. Therefore the demon energy distribution becomes exp(-βE^*P(x)) (or ergodic) at two properties of system energy near the 1st order transition. Further cooling or at still lower temperatures the system shows lack of ergodicity. However, difference in heating cooling curves are apparent in E vs γ. The system energies for which γ is zero during cooling can represent the ‘ergodic’ states. This can be related to the two-level systems observed in glasses at low temperatures.


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**P1.00069 Signatures of the Berezinskii-Kosterlitz-Thouless transition on the zeros of the canonical partition function for the 2D XY-model.** JULIO ROCHA, LUCAS MOL, BISMARCK COSTA, Universidade Federal de Minas Gerais — In this work we show that the canonical partition function zeros, the Fisher zeros, can be used to uniquely characterize a transition as being in the Berezinskii-Kosterlitz-Thouless (BKT) class of universality. By studying the zeros map for the 2D XY model we found that its internal border coalesces into the real positive axis in a finite region corresponding to temperatures smaller than the BKT transition temperature. This behavior is consistent with the predicted existence of a line of critical points below the transition temperature, allowing one to distinguish the BKT class of universality from other ones.

This work was partially supported by CNPq and Fapemig, Brazilian Agencies.

**P1.00070 Nonlinear dynamics of three gravitating rods.** ZIYI SANG, JOHN LINDNER, The College of Wooster — As a generalization of Newton’s three body problem, we explore the dynamics of three massive line segments interacting gravitationally. The extension of each line segment or slash (/) provides extra degrees of freedom that enable the 1/2/3/4 rotating small third massive line segment to resist implosion or explosion. In two-dimensional Euclidean space, we find an equilibrium configuration of a rotating ring of massive dust whose inward gravity is the centripetal force that spins it. We find similar solutions in three-dimensional Euclidean and hyperbolic spaces, but only in the limit of vanishing mass. Finally, in three-dimensional Euclidean space, we generalize the two-dimensional result by finding an equilibrium configuration of a spherical shell of massive dust that supports itself against gravitational collapse by spinning isoclinically in four dimensions so its three-dimensional acceleration is everywhere inward. These Newtonian “atoms” illuminate classical physics and geometry.

**P1.00071 Balancing Newtonian gravity and spin to create localized structures.** MICHAEL BUSH, JOHN LINDNER, The College of Wooster — Using geometry and Newtonian physics, we design localized structures that do not require electromagnetic or other forces to resist implosion or explosion. In two-dimensional Euclidean space, we find an equilibrium configuration of a rotating ring of massive dust whose inward gravity is the centripetal force that spins it. We find similar solutions in three-dimensional Euclidean and hyperbolic spaces, but only in the limit of vanishing mass. Finally, in three-dimensional Euclidean space, we generalize the two-dimensional result by finding an equilibrium configuration of a spherical shell of massive dust that supports itself against gravitational collapse by spinning isoclinically in four dimensions so its three-dimensional acceleration is everywhere inward. These Newtonian “atoms” illuminate classical physics and geometry.

**P1.00072 BIOLOGICAL PHYSICS —**

**P1.00073 Single-molecule optical study of cholesterol-mediated dimerization process of EGFRs in different cell lines.** CHIEN YU LIN, JUNG Y. HUANG, Department of Photonics, Chiao Tung University, LEU-WEI LO, Institute of Biomedical Engineering and Nanomedicine, National Health Research Institutes — A growing body of data reveals that the membrane cholesterol molecules can alter the signaling pathways of living cells. However, the understanding about how membrane cholesterol modulates receptor proteins remains lacking. In this study we apply single-molecule optical tracking on ligand-induced dimerization process of EGFRs in the plasma membranes of several cancer and normal cell lines. We tracked individual EGFR and dual correlated receptors in the plasma membranes of live cells. We developed an energetic model based on the generalized Langevin equation and the Cahn-Hilliard equation to help extracting information from single-molecule trajectories. From the study, we discovered that ligand-bound EGFRs move from non-raft areas into lipid raft domains. This ligand-induced motion is a common behavior for all cell lines under study. By manipulating the total amount of cholesterol with methyl-Î²-cyclodextrin and the local concentration of cholesterol with nystatin, we found that the amount of cholesterol can affect the stability of EGFR dimers. The EGFR dimers in the plasma membrane of normal cells are more sensitive to the local concentration changes of cholesterol than EGFR dimers in the cancer cells.

**P1.00074 Conformational transitions of plasmid ds-DNA on ultrathin films of alkylamines on graphite.** CAROLINE FALK, HUA LIANG, NIKOLAI SEVERIN, WEI ZHUANG, Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin, STEFAN ZAUSCHER, Mechanical Engineering and Materials Science, Duke University, JÜRGEN P. RABE, Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin — DNA replication is an important process in the human body. Replication of double-stranded (ds)-DNA requires its local melting into two single strands [1]. DNA, when stretched in solution, overwinds and melts [2]. This was argued to give insight onto the replication mechanism. It is difficult, however, to access the direct conformational changes during stretching in solution. Recent work demonstrated that this transition can be imaged with scanning force microscopy on a graphite surface that is coated with an alkylamine layer [3]. ds-DNA can be controlled by an amphiphilic layer, since the DNA conformation depends on the amphiphile concentration. In particular we analyzed different DNA lengths on the same surface, and we found that at a specific concentration of octadecylamine the ds-DNA pUC19 plasmid ring splits into two single strands at one position. We will discuss methods to mark the DNA to determine the exact location at which the plasmid ring splits.  


**P1.00075 Modification of protein structure and function using photoactivated porphyrin ligands.** GABRIEL MORENO, University of Texas at San Antonio — The tremendous advances in genomic research have sparked an interest in investigating the possibility to “manipulate” the structure of proteins that modify existing functionality. This study makes use of small molecules (e.g., porphyrins) to photo-sensitize proteins and modify the higher order structure of the polypeptide with the goal of engineering novel functions, or affecting/eliminating native functions. The irradiation of non-covalently bound ligands prompts charge transfer events that have the potential to locally modify the structure of the host protein. The characterization of photoinduced conformational changes in the protein/porphyrin complex is carried out using a combination of electronic spectroscopy and kinetics (e.g., fluorescence spectroscopy, fluorescence decay, circular dichroism). This study is focused primarily on human serum albumin (HSA) as a model. The structure of HSA is well established, the binding sites for an array of ligands are well characterized (including one for protoporphyrins), and HSA provides a series of functions (including some allosteric activity) that can be tested.

**P1.00076 Bacterial Chemotaxis with a Moving Target.** COREY DOMINICK, Univ of Pittsburgh — Most chemotaxis studies so far have been conducted in a quiescent fluid with a well-defined chemical gradient. Such experiments may be appropriate for studying enteric bacteria, such as Escherichia coli, but the environment it provides is very different from that typically encountered by marine bacteria. Herein we describe an experiment in which marine bacterium Vibrio alginolyticus subject to stimulation by a small moving target. A micropipette of the tip size <1 ?m is used to slowly release a chemoattractant, serine, at different concentrations. The pipette is made to move with different patterns and speeds, ranging from 0 to 100 ?m/s; the latter is about twice the bacterial swimming speed. We found that if the pipette is moved slowly, with 1/4 of bacterial swimming speed, cells accumulate near the tip region but when it is moved with speed greater than 1/2 the bacterial swimming speed, cells trail behind the pipette over a large distance. The behaviors observed in V. alginolyticus are significantly different from E. coli, suggesting that the former is a better chemotaxer in a changing environment.
P1.00077 Bacterial Growth in Weak Magnetic Field
SAMINA MASOOD, University of Houston Clear Lake — We study the growth of bacteria in a weak magnetic field. Computational analysis of experimental data shows that the growth rate of bacteria is affected by the magnetic field. The effect of magnetic field depends on the strength and type of magnetic field. It also depends on the type of bacteria. We mainly study gram positive and gram negative bacteria of rod type as well as spherical bacteria. Preliminary results show that the weak magnetic field enhances the growth of rod shape gram negative bacteria. Gram positive bacteria can be even killed in the inhomogeneous magnetic field.

P1.00078 Phase Transitions in the Nucleus: the functional implications of concentration-dependent assembly of a Liquid-like RNA/Protein Body
LIAN ZHU, STEPHANIE WEBER, JOEL BERRY, NILESH VAIDYA, MIKKO HAATAJA, CLIFFORD BRANGWYNNIE, Princeton University — The nucleus is a liquid-like membrane-less nuclear body which plays an important role in cell growth and size control. By modulating nucleolar component concentration through RNAi conditions that change C. elegans cell size, we find that nucleoli only assemble above a threshold concentration; moreover, the ripening dynamics of nucleated droplets are consistent with the hypothesis that the assembly of the nucleolus represents an intracellular liquid-liquid phase transition. A key question is how this phase-transition is linked to the primary function of the nucleolus, in transcribing and processing ribosomal RNA. To address this, we characterize the localization of RNA Polymerase I, a key transcriptional enzyme, into nucleolar foci as a function of nucleolar component concentration. Our results suggest that there are a small number of key disordered phosphoproteins that may serve as a link between transcription and assembly. Finally, we present preliminary results using a reduced model system consisting of purified nucleolar proteins to assess the ability of nucleolar proteins to drive liquid-liquid phase separation in vitro. These results lay the foundation for a quantitative understanding of intracellular phase transitions and their impact on biomedically-critical RNA-processing steps.

P1.00079 Kinesin-1 Translocation along Human Breast Cancer Cell Microtubules in Vitro
MITRA SHOJANIA FEIZABADI, Physics Department, Seton Hall University, YONGGUN JUN, Developmental and Cell Biology, School of Biological Sciences, University of California, Irvine, CA — A principle approach to better understand intra-cellular microtubule based transport is to study such it in vitro. Such in vitro examinations have predominantly used microtubules polymerized from bovine brain tubulin, but motor function can also in principle be affected by the specific tubulin isotypes present in different cells. The human breast cancer cells carry different beta tubulin isotype distribution. However, it is entirely unknown whether transport along the microtubules is different in these cells. In this work we have characterized, for the first time, the translocation specifications of kinesin-1 along human breast cancer cell microtubules polymerized in vitro. We found that as compared with the translocation along bovine brain microtubules, kinesin-1 shows a fifty percent shorter protractive run length and slightly lower velocity under similar experimental conditions. These first time results support the regulatory role of tubulin isotypes in regards to motor protein translocations, and quantify the translocation specifications of kinesin-1 along microtubules of human breast cancer cells.

P1.00080 Dissipative Dynamics of Enzymes
AMILA ARIYARATNE, University of California Los Angeles, CHENHAO WU, University of California San Diego, CHIAO-YU TSENG, GIOVANNI ZOCCHI, University of California Los Angeles, ZOCCHI LAB FOR MOLECULAR BIO-PHYSICS TEAM — We explore enzyme conformational dynamics at sub - A resolution, specifically temperature effects. The ensemble averaged mechanical response of the folded enzyme is viscoelastic in the whole temperature range between the warm and cold denaturation transitions. The dissipation parameter γ of the viscoelastic description decreases by a factor 2 as the temperature is raised from 10 C to 45 C; the elastic parameter K shows a similar decrease. Thus when probed dynamically, the enzyme softens for increasing temperature. Equilibrium mechanical experiments with the DNA spring (and a different enzyme) also show, qualitatively, a small softening for increasing temperature.

P1.00081 Effects of solvent (effective medium versus explicit) on the structure of a protein (H3.1)
RAS PANDAY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — Structure and dynamics of a histone (H3.1) are studied in the presence of effective medium and explicit solvent over a range of temperatures with coarse-grained Monte Carlo simulations. The protein is represented by a coarse-grained chain of residues whose interactions are described by knowledge-based residue-residue and hydrophathy-index-based residue-solvent interactions. Each empty lattice site acts as a solvent in effective medium while a fraction of sites are occupied by mobile solvent constituents in explicit solvent medium. The presence of fluctuations with explicit solvent may affect the structure and dynamics of protein differently than that in effective solvent medium. Large scale simulations are performed to analyze the structure of the protein for a range of residue-solvent interactions and temperature, and a number of local and global physical quantities are analyzed. Differences due to type of solvent on the response of some of these quantities as a function of temperature will be presented.

P1.00082 ABSTRACT WITHDRAWN

P1.00083 ABSTRACT WITHDRAWN

P1.00084 Effect of Nanodiamond Surfaces on tRNA Dynamics Studied by Neutron Scattering and MD Simulations
GURPREET DHINDSA, DEBSINDHU BHOWMIK, Wayne State University, PANCHAPAKESAN GANESH, MONOJOY GOSWAMI, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, VADYM N. MOCHALIN, Drexel University, HUGH O'NEILL, Biology and Soft Matter Division, Oak Ridge National Laboratory, USA, YURY GOGOTSI, Drexel University, EUGENE MAMONTOV, SNS OakRidge National Laboratory, USA, XIANG QIANG CHU, Wayne State University — Nanodiamond (ND) inherits most of the superior properties of bulk diamond and delivers them at the nanoscale. ND is non-toxic and possesses excellent mechanical and optical properties with large surface area and surface functionality. ND mixed with biomolecules can be a good platform for drug delivery. Here we demonstrate the adsorption of tRNA on the ND surface and investigate the change in the tRNA dynamics using neutron scattering technique and molecular dynamics (MD) Simulations. We compare the dynamics of hydrated tRNA on ND surfaces with that of freestanding hydrated tRNA molecules and dry tRNA on ND surfaces. Both experiments and simulations show that the relaxational dynamics of tRNA on ND surface is faster than that of the freestanding tRNA molecules and dry tRNA on ND surfaces. Our results suggest that the tRNA on the ND surfaces has fewer hydration water molecules on it due to the water adsorption on the ND hydrophilic surface. Therefore fewer hydrogen bonds formed on its surface results in the tRNA faster motion. The MD simulations also show a “caged” dynamics of the water molecules adsorbed on the ND surfaces.

P1.00085 Fast loop modeling for protein structures
JIONG ZHANG, SON NGUYEN, YI SHANG, DONG XU, IOAN KOSZTIN, University of Missouri — X-ray crystallography is the main method for determining 3D protein structures. In many cases, however, flexible loop regions of proteins cannot be resolved by this approach. This leads to incomplete structures in the protein data bank, preventing further computational study and analysis of these proteins. For instance, all-atom molecular dynamics (MD) simulation studies of structure-function relationship require complete protein structures. To address this shortcoming, we have developed and implemented an efficient computational method for building missing protein loops. The method is database driven and uses deep learning and multi-dimensional scaling algorithms. We have implemented the method as a simple stand-alone program, which can also be used as a plugin in existing molecular modeling software, e.g., VMD. The quality and stability of the generated structures are assessed and tested via energy scoring functions and by equilibrium MD simulations. The proposed method can also be used in template-based protein structure prediction.
P1.00086 Bio-inspired metal-coordination dynamics: A unique tool for engineering novel properties in soft matter systems. SCOTT GRINDY, QIAOCHU LI, ABIGAIL HALIM, ROBERT LEARSCH, NIELS HOLTE-N-ANDERSEN, Massachusetts Inst of Tech-MIT — In soft matter systems, materials properties are generally governed by transient, dynamic interactions of many types over many hierarchical length- and time-scales. However, explicit control over these dynamics is not always possible, leaving open questions into how transient interactions can be exploited to design soft materials with unique and exceptional properties. Inspired by the adhesive chemistry and tough character of mussel byssal threads, we present several studies on both the mechanical properties of soft materials and templated crystallization kinetics to show the diverse array of materials properties that can be generated using bio-inspired metal-coordination. By studying our model systems, we can determine the explicit effects of metal-coordination dynamics on various bulk properties, further adding to the set of tools we can use to design soft material systems.

P1.00087 Examining the role of finite reaction times in swarming models. KATHERINE COPENHAGEN, University of California Merced, DAVID QUINT, Stanford University, AJAY GOPINATHAN, University of California Merced — Modeling collective behavior in biological and artificial systems has had much success in recent years at predicting and mimicking real systems by utilizing techniques borrowed from modeling many particle systems interacting with physical forces. However, unlike inert particles interacting with instantaneous forces, living organisms have finite reaction times, and behaviors that vary from individual to individual. What constraints do these physiological effects place on the interactions between individuals in order to sustain a robust ordered state? We use a self-propelled agent based model in continuous space based on previous models by Vicsek and Couzin including alignment and separation maintaining interactions to examine the behavior of a single cohesive group of organisms. We found that for very short reaction times the system is able to form an ordered state even in the presence of heterogeneities. However for larger more physiological reaction times organisms need a buffer zone with no cohesive interactions in order to maintain an ordered state. Finally swarms with finite reaction times and behavioral heterogeneities are able to dynamically sort out individuals with impaired function and sustain order.

P1.00088 High Intensity Pressure Noise Transmission in Human Ear: A Three Dimensional Simulation Study1, TAKUMI HAWA, RONG GAN, KEGER LECKNESS, The University of Oklahoma — High intensity pressure noise generated by explosions and jet engines causes auditory damage and hearing loss of the military service personal, which are the most common disabilities in the veterans. Authors have investigated the high intensity pressure noise transmission from the ear canal to middle ear cavity. A fluid-structure interaction with a viscoelastic model for the tympanic membrane (TM) as well as the ossicular chain has been considered in the study. For the high intensity pressure simulation the geometry of the ear was based on a 3D finite element (FE) model of the human ear reported by Gan et al. (Ann Biomed Eng 2004). The model consists of the ear canal, TM, ossicular chain, and the middle ear cavity. The numerical approach includes two steps: 1) FE based finite-volume method simulation to compute pressure distributions in the ear canal and the middle ear cavity using CFX; and 2) FE modeling of TM and middle ear ossicles in response to high intensity sound using multi-physics analysis in ANSYS. The simulations provide the displacement of the TM/ossicular chain and the pressure fields in the ear canal and the middle ear cavity. These results are compared with human temporal bone experimental data obtained in our group.

P1.00089 Computational Characterization of Type I collagen-based Extra-cellular Matrix1, LONG LIANG, Department of Physics, Arizona State University, CHRISTOPHER ALLEN RUCKSACK JONES, DANIEL LIN, Department of Physics, Oregon State University, YANG JIAO, Department of Materials Science and Engineering, Arizona State University, BO SUN, Department of Physics, Oregon State University — A model of extracellular matrix (ECM) of collagen fibers has been built, in which cells could communicate with distant partners via fiber-mediated long-range-transmitted stress states. The ECM is modeled as a spring-like fiber network derived from skeletonized confocal microscopy data. Different local and global perturbations have been performed on the network, each followed by an optimized global Monte-Carlo (MC) energy minimization leading to the deformed network in response to the perturbations. In the optimization, a highly efficient local energy update procedure is employed and force-directed MC moves are used, which results in a convergence to the energy minimum state 20 times faster than the commonly used random displacement trial moves in MC. Further analysis and visualization of the distribution and correlation of the resulting force network reveal that local perturbations can give rise to global impacts: the force chains formed with a linear extent much further than the characteristic length scale associated with the perturbation sites and average fiber length. This behavior provides a strong evidence for our hypothesis of fiber-mediated long-range force transmission in ECM networks and the resulting long-range cell-cell mechanical signaling.

1 This work was supported by DOD W81XWH-14-1-0228

P1.00090 Hidden Markov models for the analysis of single particle trajectories containing multiple mobile states. DYLAN YOUNG, JAN SCRIMGEOUR, Clarkson Univ — Single particle tracking offers significant insight into the molecular mechanics that govern the behavior of living cells. The analysis of trajectories that transition between different motive states, such as diffusive, driven and tethered modes, is of considerable importance, with even single trajectories containing significant amounts of information about a molecule’s environment and its interactions with structures such as the cell cytoskeleton, membrane or extracellular matrix. Traditional analysis of particle trajectories has relied heavily on evaluation of the mean squared displacement, but often struggles to extract information reliably from small quantities of data or when multiple mobile states are present. Here, we present hidden Markov models for the analysis of complex multi-mobility tracks, focusing on transitions between states exhibiting free diffusion and either driven or tethered motion. The models were tested using simulated trajectories and practical limitations on the track length and state switching probabilities needed for accurate extraction of the physical parameters in the model are identified. These results provide critical information for the design of particle tracking experiments where trajectories containing multiple mobile states are expected.

P1.00091 A theoretical analysis of inferring molecular interactions from single particle trajectories1. ZIYA KALAY, Kyoto University — Single molecule/particle tracking has become a valuable tool in microscopy that allows for recording trajectories of probes such as individual biological molecules with high temporal and spatial resolution. With the trajectory of a particle, mesoscale transport properties such as diffusion coefficients and first-passage times can be calculated. With the trajectories of two particles that interact, we can investigate the kinetics of reactions by analyzing the statistics of overlap between trajectories. This approach is useful for single molecule biophysics in exploring the kinetics of reversible binding among molecules in biological membranes and on the DNA. Nevertheless, extracting information from noisy trajectories, where the noise stems from a combination of thermal fluctuations and uncertainty introduced by measuring apparatus, is a challenging task. In this work, we consider an exactly solvable model of diffusion and reversible binding in a 1-D structure, such as the DNA, and present a mathematical analysis of how much information about the binding kinetics can be reliably extracted from experimental data. With insight gained from this low-dimensional model, we discuss the analysis of trajectory pairs in two-dimensional systems such as biological membranes.

1 This research was supported by JSPS Grant-in-Aid for Young Scientists (B) (26730150)
**P1.00092** Stochastic Movement of Multiple Motor Transported Cargo , DAVID ANDO, AJAY GOPINATHAN, JING XU, UC Merced — Experimental observations of cargo position during transport by multiple motors are determined by several coupled stochastic processes. During collective transport, each motor can transition between multiple kinetic states, with the state of each motor influencing the states of the others via mechanical coupling through a common cargo. We measured the motion of a micron sized bead as it is transported by two kinesins along a single microtubule track, focusing on cargo displacements which are both axial and transverse to the microtubule. We model the effects of inter-motor interference and the state of each motor throughout time, and back out motor properties using a systematic comparison of experimental observations with simulated model traces over a wide parameter space. Our model captures a surface-associated mode of kinesin, which is only accessible via inter-motor interference in groups, in which kinesin diffuses along the microtubule surface and rapidly “hops” between protofilaments without dissociating from the microtubule. This enhances local exploration of the microtubule surface, possibly enabling cellular cargos to overcome macromolecular crowding and to navigate obstacles along microtubule tracks without sacrificing overall travel distance.

**P1.00093** Light, Imaging, Vision: An interdisciplinary undergraduate course1, PHILIP NELSON, Univ Pennsylvania — The vertebrate eye is fantastically sensitive instrument, capable of registering the absorption of a single photon, and yet generating very low noise. Using eyes as a common thread helps motivate undergraduates to learn a lot of physics, both fundamental and applied to scientific imaging and neuroscience. I’ll describe an undergraduate course, for students in several science and engineering majors, that takes students from the rudiments of probability and statistical inference to the quantum character of light, including modern experimental methods like fluorescence imaging and Förster resonance energy transfer. After a digression into color vision, we then see how the Feynman principle explains the apparently wavelike phenomena associated to light, including applications like diffraction, subdiffraction imaging, total internal reflection and TIRF microscopy. Then we see how scientists documented the single-quantum sensitivity of the eye seven decades earlier than “ought” to have been possible, and finally close with the remarkable signaling cascade that delivers such outstanding performance. Parts of this story are now embodied in a new textbook (WH Freeman and Co, 1/2015); additional course materials are available upon request.

1Work supported by NSF grants EF–0928048 and DMR–0832802.

**P1.00094** A new course and textbook on Physical Models of Living Systems, for science and engineering undergraduates1, PHILIP NELSON, Univ Pennsylvania — I’ll describe an intermediate-level course on “Physical Models of Living Systems.” The only prerequisite is first-year university physics and calculus. The course is a response to rapidly growing interest among undergraduates in a broad range of science and engineering majors. Students acquire several research skills that are often not addressed in traditional courses:

- Basic modeling skills
- Probabilistic modeling skills
- Data analysis methods
- Computer programming using a general-purpose platform like MATLAB or Python
- Dynamical systems, particularly feedback control.

These basic skills, which are relevant to nearly any field of science or engineering, are presented in the context of case studies from living systems, including:

- Virus dynamics
- Bacterial genetics and evolution of drug resistance
- Statistical inference
- Superresolution microscopy
- Synthetic biology
- Naturally evolved cellular circuits.

1Work supported by NSF grants EF–0928048 and DMR–0832802.

**P1.00095** Analytical framework for modeling of long-range transport of fungal plant epidemics, OLEG KOGAN, KEVIN O’KEEFFE, DAVID SCHNEIDER, CHRISTOPHER MYERS, Cornell University, ANALYTICAL FRAMEWORKS FOR INFECTIOUS DISEASES DYNAMICS TEAM — A new framework for the study of long-range transport of fungal plant epidemics is proposed. The null nonlinear model includes advective transport through the free atmosphere, spore production on the ground, and transfer of spores between the ground and the advective atmospheric layer. The competition between the growth wave on the ground and the effect of the wind is most strongly reflected in upwind fronts, which can propagate into the wind for exponential initial conditions. If the rate of spore transfer into the advective layer is below critical, this happens for initial conditions with arbitrary steepness. Upwind fronts from localized initial conditions will propagate in the direction of the wind above this critical parameter, and will not propagate below it. On the other hand, the speed of the downwind front does not have a strong dependence on the rate of spore transfer between the advective layer and the ground. Thus, even vanishingly small, but finite transfer rates result in a substantial epidemic wave in the direction of the wind. We also consider the effect of an additional, random-walk like mechanism of transport through the near-ground atmospheric boundary layer, and attempt to understand which route dominates the transport over long distances.

**P1.00096** Interstitial flows promote an amoeboid cell phenotype and motility of breast cancer cells1, CHIH-KUAN TUNG, YU LING HUANG, ANGELA ZHENG, MINGMING WU, Department of Biological and Environmental Engineering, Cornell University — Lymph nodes, the drainage systems for interstitial flows, are clinically known to be the first metastatic sites of many cancer types including breast and prostate cancers. Here, we demonstrate that breast cancer cell morphology and motility is modulated by interstitial flows in a cell-ECM adhesion dependent manner. The average aspect ratios of the cells are significantly lower (or are more amoeboid like) in the presence of the flow in comparison to the case when the flow is absent. The addition of exogenous adhesion molecules within the extracellular matrix (type I collagen) enhances the overall aspect ratio (or are more mesenchymal like) of the cell population. Using measured cell trajectories, we find that the persistence of the amoeboid cells (aspect ratio less than 2.0) is shorter than that of mesenchymal cells. However, the maximum speed of the amoeboid cells is larger than that of mesenchymal cells. Together these findings provide the novel insight that interstitial flows promote amoeboid cell morphology and motility and highlight the plasticity of tumor cell motility in response to its biophysical environment.

1Supported by NIH grant R21CA138366
P1.00097 Robust Nonlinear Neural Codes\textsuperscript{1}. QIAINU LIANG, Rice Univ, XAQ PITKOW, Rice Univ. Baylor College of Medicine — Most interesting natural sensory stimuli are encoded in the brain in a form that can only be decoded nonlinearly. But despite being a core function of the brain, nonlinear population codes are rarely studied and poorly understood. Interestingly, the few existing models of nonlinear codes are inconsistent with known architectural features of the brain. In particular, these codes have information content that scales with the size of the cortical population, even if that violates the data processing inequality by exceeding the amount of information entering the sensory system. Here we provide a valid theory of nonlinear population codes by generalizing recent work on information-limiting correlations in linear population codes. Although these generalized, nonlinear information-limiting correlations bound the performance of any decoder, they also make decoding more robust to suboptimal computation, allowing many suboptimal decoders to achieve nearly the same efficiency as an optimal decoder. Although these correlations are extremely difficult to measure directly, particularly for nonlinear codes, we provide a simple, practical test by which one can use choice-related activity in small populations of neurons to determine whether decoding is suboptimal or optimal and limited by correlated noise. We conclude by describing an example computation in the vestibular system where this theory applies.
\textsuperscript{1}QY and XP was supported by a grant from the McNair foundation.

P1.00098 Spatiotemporal discrimination in neural networks with short-term synaptic plasticity. BENJAMIN SHLAER, PAUL MILLER, Brandeis Univ. — Cells in recurrently connected neural networks exhibit bistability, which allows for stimulus information to persist in a circuit even after stimulus offset, i.e. short-term memory. However, such a system does not have enough hysteresis to encode temporal information about the stimuli. The biophysically described phenomenon of synaptic depression decreases synaptic transmission strengths due to increased presynaptic activity. This short-term reduction in synaptic strengths can destabilize attractor states in excitory recurrent neural networks, causing the network to move along stimulus dependent dynamical trajectories. Such a network can successfully separate amplitudes and durations of stimuli from the number of successive stimuli\textsuperscript{1} and so provides a strong candidate network for the encoding of spatiotemporal information. Here we explicitly demonstrate the capability of a recurrent neural network with short-term synaptic depression to discriminate between the temporal sequences in which spatial stimuli are presented.


P1.00099 The Brain Physics: Multi Laser Beam Interaction with the Brain Topions (the Brain Neurocenters)\textsuperscript{1}. V. ALEXANDER STEFAN, Institute for Advanced Physics Studies, Stefan University, La Jolla, California 92037 — A novel method for the treatment of the neurological diseases is proposed. The multi-energy laser photons\textsuperscript{2} (the blue scanning photons and ultraviolet focusing photons) interact with the specific DNA molecules within the topion (such as Parkinson’s and Alzheimer’s brain topion) via the matching of laser frequency with the oscillation eigen-frequency of a particular molecule\textsuperscript{3} within the DNA\textsuperscript{4} . In this way, the corrupt molecules (the structure of molecules) can be manipulated so as to treat (eliminate) the neurological disease.

\textsuperscript{1}Supported by Nikola Tesla Labs, Stefan University.
\textsuperscript{2}V. Alexander Stefan, NEUROPHYSICS, STEM CELL PHYSICS, and GENOMIC PHYSICS: Beat-Wave-Driven-Free Electron Laser Beam Interactions with the Living Matter (S-U-Press, La Jolla, CA, 2012)
\textsuperscript{3} V. Stefan, B. I. Cohen, C. Joshi, Science, 243, 4890, (Jan.27, 1989); Stefan et al., Bull. APS, No.9, 1713, (1987); Stefan APS-March-2012, # K1.00177.
\textsuperscript{4} V. Alexander Stefan, APS-March-2013, #.H1.00208; APS-March-2014, #. P1.00063.

P1.00100 Network oscillations of inferior olive neurons: entrainment and phase-locking of locally-coupled oscillators. THOMAS CHARTRAND, MARK S. GOLDMAN, TIMOTHY J. LEWIS, University of California, Davis — Although the inferior olive is known to contribute to the generation of timing and error signals for motor control, the specific role of its distinctive spatiotemporal activity patterns is still controversial. Olfactory neurons display regular, sometimes synchronized oscillations of subthreshold membrane potential, driven in part by the highest density of electrical coupling of any brain region. We show that a reduced model of coupled phase oscillators is sufficient to reproduce and study experimental observations previously only demonstrated in more complex models. These include stable phase differences, variability of entrainment frequency, wave propagation, and cluster formation. Using the phase-response curve (PRC) of a conductance-based model of olivary neurons, we derive our phase model according to the theory of weakly-coupled oscillators. We retain the heterogeneity of intrinsic frequencies and heterogeneous, spatially constrained coupling as weak perturbations to the limit-cycle dynamics. Generalizing this model to an ensemble of coupled oscillator lattices with frequency and coupling disorder, we study the onset of entrainment and phase-locking as coupling is strengthened, including the scaling of cluster sizes with coupling strength near each phase transition.

P1.00101 Temporal Evolution Of Information In Neural Networks With Feedback\textsuperscript{1}. ARAM GIAHI SARAVANI, Baylor College of Medicine, XAQ PITKOW, Baylor College of Medicine/Rice University — Recurrent neural networks are pivotal for information processing in the brain. Here we analyze how the information content of a neural network is altered by dynamic feedback of a stimulus estimated from the network activity. We find that the temporal evolution of the Fisher information in the model with feedback is bounded by the Fisher information in a network of pure integrators. The available information in the feedback model saturates with a time constant and to a final level both determined by the match between the estimator weights and the feedback weights. This network then encodes signals specifically from either the beginning or the end of the stimulus presentation, depending on this match. These results are relevant to recent experimental measurements of psychophysical kernels indicating that earlier stimuli have a stronger influence on perceptual discriminations than more recent stimuli. We discuss consequences of this description for choice correlations, a measure of how individual neuronal responses relate to perceptual estimates.

\textsuperscript{1}McNair Foundation, Baylor College of Medicine, Rice University

P1.00102 ABSTRACT WITHDRAWN

P1.00103 The Deterministic Information Bottleneck. D.J. STROUSE, Princeton University, DAVID SCHWAB, Northwestern University — A fundamental and ubiquitous task that all organisms face is prediction of the future based on past sensory experience. Since an individual’s memory resources are limited and costly, however, there is a tradeoff between memory cost and predictive payoff. The information bottleneck (IB) method (Tishby, Pereira, & Bialek 2000) formulates this tradeoff as a mathematical optimization problem using an information theoretic cost function. IB encourages storing as few bits of past sensory input as possible while selectively preserving the bits that are most predictive of the future. Here we introduce an alternative formulation of the IB method, which we call the deterministic information bottleneck (DIB). First, we argue for an alternative cost function, which better represents the biologically-motivated goal of minimizing required memory resources. Then, we show that this seemingly minor change has the dramatic effect of converting the optimal memory encoder from stochastic to deterministic. Next, we propose an iterative algorithm for solving the DIB problem. Additionally, we compare the IB and DIB methods on a variety of synthetic datasets, and examine the performance of retinal ganglion cell populations relative to the optimal encoding strategy for each problem.
P1.00104 Modeling the Kinetics of a Memory-Associated Immediate Early Gene's Compartmental Expression After Sensory Experience1, ADAM WILLATS, Georgia Institute of Technology and Emory University; Dept. of Biomedical Engineering, TAMARA IVANOVA, ASTRID PRINZ, ROBERT LUU, Emory University; Dept. of Biology — Immediate Early Genes (IEGs) are rapidly and transiently transcribed in neurons after a sensory experience. Some of these genes act as effector IEGs, which mediate specific effects on cellular function. Arc is one such effector IEG that is essential for synaptic plasticity and memory consolidation in hippocampus and cortex. The expression of Arc in neurons has previously been examined using an imaging method known as Compartamental Analysis of Temporal Fluorescent In-Situ Hybridization. Previous work found that the time course of Arc expression within the nuclear and perinuclear cytoplasmic compartments of a neuron is altered by prior sensory experience. We explore a simple model of the kinetics of IEG transcription and nuclear export, with the aim of eventually uncovering possible mechanisms for how experience alters expression kinetics. Thus far, we characterize our compartmental model using phase-plane analysis and validate it against several IEG expression data sets, including one where prior experience with vocalizing mice alters the time course of call-induced Arc expression in the auditory cortex of a listening mouse. Our model provides a framework to explore why Arc expression may change depending on a receiver’s past sound experience and internal state.

1Adam Willats was supported by NIH Training grant 5T90DA032466. This research was also supported by NIDCD R01 DC8343

P1.00105 The brain as a complex system: plasticity at multiple scales and criticality, TONY NG, PAUL MILLER, Brandeis University — As a complex system, a successful organism is one that can react effectively to environmental fluctuations. Not only should its response repertoire be commensurate with the number of independent conditions that it encounters, behavioral and environmental variations need to be matched at the appropriate scales. In the cortex, neuronal clusters, not individual cells, operate at the proper scale that is necessary to generate appropriate responses to external states of the world. Single neurons, however, serve on a finer scale to mediate interactions between neuronal assemblies. The distinction of scales is significant, as plasticity mechanisms can operate on various spatial and temporal scales. The brain has apparently evolved complex-system strategies to calibrate its own dynamics at multiple scales. This makes the joint study of local balance and global homeostasis fundamentally important, where criticality emerges as a signature of a computationally powerful system. We show via simulations how plasticity mechanisms at multiple scales are inextricably tied to spike-based neuronal avalanches, which are microscopic in origin and poorly predictive of animal behavior, and cluster-based avalanches, which are manifest macroscopically and are relevant to cognition and behavior.

P1.00106 Marginalization in Random Nonlinear Neural Networks, RAJKUMAR VASUDEVA RAJU, Rice University, XAQ PITKOW, Rice University, Baylor College of Medicine — Computations involved in tasks like causal reasoning in the brain require a type of probabilistic inference known as marginalization. Marginalization corresponds to averaging over irrelevant variables to obtain the probability of the variables of interest. This is a fundamental operation that arises whenever input stimuli depend on several variables, but only some are task-relevant. Animals often exhibit behavior consistent with marginalizing over some variables, but the neural substrate of this computation is unknown. It has been previously shown (Beck et al. 2011) that marginalization can be performed optimally by a deterministic nonlinear network that implements a quadratic interaction of neural activity with divisive normalization. We show that a simpler network can perform essentially the same computation. These Random Nonlinear Networks (RNN) are feedforward networks with one hidden layer, sigmoidal activation functions, and normally-distributed weights connecting the input and hidden layers. We train the output weights connecting the hidden units to the output population, such that the output model accurately represents a desired marginal probability distribution without significant information loss compared to optimal marginalization. Simulations for the case of linear coordinate transformations show that the RNN model has good marginalization performance, except for highly uncertain inputs that have low amplitude population responses. Behavioral experiments, based on these results, could then be used to identify if this model does indeed explain how the brain performs marginalization.

P1.00107 Investigating structural details of lipid-cholesterol-A\(\beta\) interactions, DURGESH RAI, DIVINA ANUNCIADO, WILLIAM HELLER, HUGH O’NEILL, VOLKER URBAN, SHUO QIAN, Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — Alzheimer’s disease (AD) is the most common form of dementia and is predicted to affect 1 in 85 people around the world by 2050. Amyloid beta (A\(\beta\))-peptide, a peptide composed of 40-42 amino acids that is the product of cleavage from the amyloid precursor protein (APP), is regarded to play a major role in the development of AD. In addition, accumulating evidence points to a positive association between cholesterol and AD. Here, we present results from our studies about A\(\beta\)-peptide and cholesterol in bilayer by small-angle neutron scattering (SANS) using a combination of dimyristol, phosphocholine (DMPC) and partially deuterated cholesterol (cholesterol-d7) with and without A\(\beta\). We compare the results using gracing incidence and transmission SANS on lipid bilayer films and unilamellar vesicles respectively. The structural details on vesicles and bilayers work in conjunction with the circular dichroism on peptide in solution and oriented circular dichroism in bilayer films. The studies confirm a positive association of A\(\beta\) with the membrane layers. The results from different studies will be compared and contrasted in presentation.

P1.00108 Using Small Angle Neutron Scattering on Glucose Oxidase immobilized on Single Layer Graphene, DURGESH RAI, Oak Ridge National Lab, M. GURUSARAN, IISc Bangalore, S. QIAN, K. WEISS, V. URBAN, Oak Ridge National Lab, P. LI, Harvard Medical School, L. MA, P. AJAYAN, Rice University, T. NARAYANAN, TIFR Hyderabad, K. SEKAR, IISc Bangalore, S. VISWANATHAN, Newton Wellesley Hospital, V. RENUGOPALAKRISHANAN, Harvard Medical School — Reliable blood glucose monitoring using biosensors is valuable for health evaluations and medication in wake of chronic diabetic issues accompanying deviations from evolutionary human lifestyle. Glucose oxidase (GOx) is an ideal enyme because of its specificity and the ability to electrochemically transduce from the enzymatic reaction. We use graphene-based electrode with GOx sensor matrix so that the emitted electrons from sensor matrix can flow across graphene nearly without scattering; crucial for constructing ultrasensitive-sensors. Thereafter, establishing a structure-property based relationships to tune the sensor topology with electrochemically output forms the main focus of the device development process. We have developed a methodology to obtain low-resolution hierarchical models of the aggregate matrix using Small Angle Neutron Scattering (SANS) technique. A Unified Fit model is used in tandem with GNOM, DAMMIN and DAMAVER to construct low-resolution models for the device development process. We have developed a methodology to obtain low-resolution hierarchical models of the aggregate matrix using Small Angle Neutron Scattering (SANS) technique. A Unified Fit model is used in tandem with GNOM, DAMMIN and DAMAVER to construct low-resolution models for the device development process. We have developed a methodology to obtain low-resolution hierarchical models of the aggregate matrix using Small Angle Neutron Scattering (SANS) technique. A Unified Fit model is used in tandem with GNOM, DAMMIN and DAMAVER to construct low-resolution models for the device development process.

P1.00109 Interatomic Coulombic Decay Effects in Theoretical DNA Recombination Systems Involving Protein Interaction Sites1, E.L. VARGAS, D.A. RIVAS, A.C. DUOT, R.T. HOVEY, V.M. ANDRIANARIAJONA, Department of Physics, Pacific Union College, Angwin, CA 94508 — DNA replication is the basis for all biological reproduction. A strand of DNA will “unzip” and bind with another complementary strand to produce two identical molecules. In this study, we are considering how this process is affected by interactions for Homocysteine (Hcy) Decoyny (ICD), specifically how ICD affects the individual coding proteins’ ability to hold together. ICD mainly deals with how the electron returns to its original state after excitation and how this affects its immediate atomic environment, sometimes affecting the connectivity between interaction sites on proteins involved in the DNA coding process. Biological heredity is fundamentally controlled by DNA and its replication therefore it affects every living thing. The small nature of the proteins (within the range of nanometers) makes it a good candidate for research of this scale. Understanding how ICD affects DNA molecules can give us invaluable insight into the human genetic code and the processes behind cell mutations that can lead to cancer.

1Authors wish to give special thanks to Pacific Union College Student Senate in Angwin, California, for their financial support.
P1.00110 Gramicidin Induce Local Non-Uniform Distribution of Lipids in Multi-Component Membrane Domains, YU MAO, FAZLE HUSSAIN, JUYANG HUANG, Texas Tech University — In lipid membranes, gramicidin form transmembrane channels that are specific for monovalent cations. We performed Molecular Dynamics simulations of gramicidin in coexisting liquid-ordered (Lo) and liquid disordered (Ld) domains using GROMACS. The lipid compositions of Lo and Ld domains are DOPC/DSPC/Cholesterol = 6.5/52.6/40.9 and 74.4/10.6/15, respectively. In the Ld domain, the membrane thickness matches the hydrophobic length of gramicidin quite well, and water molecules can diffuse through the gramicidin channels. However, in the Lo lipid domain, the bilayer thickness is far greater than the hydrophobic length of gramicidin and majority of gramicidin do not form conducting channel. The simulation result explained our experimental finding that gramicidin partition favorably into the Ld domains. The calculated radial distribution functions of lipids indicate that gramicidin recruit a layer of short DOPC surrounding each protein and keep cholesterol and taller DSPC away from the protein-bilayer interface. Our result indicates that membrane proteins are capable of inducing non-uniform distributions of lipids and creating a local bilayer environment, which favors protein function.

P1.00111 Directly mapping the surface charge density of lipid bilayers under physiological conditions, THOMAS FUHS, LASSE HYLDGAARD KLAUSEN, FLEMMING BESENBAKER, MINGDONG DONG, Interdisciplinary Nanoscience Center, Aarhus University, Denmark — The surface charge density of lipid bilayers governs the cellular uptake of charged particles and guides cell-cell and cell-surface interactions. Direct probing of the potential requires sub nanometer distances as the electrostatic potential is screened by high physiological salt concentrations. This prevented direct measurement of the SCD under physiological conditions. In this study we investigate supported bilayers of lipid mixtures that form domains of distinct surface charges, submerged in 150mM NaCl. We use a scanning ion-conductance microscope (SCM) setup to measure the ionic current through a nanopipette as the pipette is scanned several nanometers above the sample. The charged headgroups of the lipids attract counter ions leading to a charge dependent enhancement of the ion concentration near the surface. This creates a measurable change of conductivity in the vicinity of the surface. As the dependency of the current on the SCD and pipette potential is non-trivial we characterized it using numerical solutions to Poisson and Nernst-Planck equations. Based on the simulation results we propose an imaging method. We confirm feasibility of the proposed method by experimentally mapping the local surface charge density of phase separated lipid bilayers.

P1.00112 Lipid mobility in supported lipid bilayers by single molecule tracking, MARYM KOHRAM, University of Akron, Department of Physics, XIAOJUN SHI, ADAM SMITH, University of Akron, Department of Chemistry — Phospholipid bilayers are the main component of cell membranes and their interaction with biomolecules in their immediate environment is critical for cellular functions. These interactions include the binding of polycationic polymers to lipid bilayers which affects many cell membrane events. As an alternative method of studying live cell membranes, we assembled a supported lipid bilayer and investigate its binding with polycationic polymers in vitro by fluorescently labeling the molecules of the supported lipid bilayer. We use single molecule tracking total internal reflection fluorescence microscopy (TIRF) to study phosphatidylinositol phosphate (PIP) lipids with and without an adsorbed polycationic polymer, quaternized polyvinylpyridine (QPVP). Individual molecular trajectories are obtained from the experiment, and a Brownian diffusion model is used to determine diffusion coefficients through mean square displacements. Our results indicate a smaller diffusion coefficient for the supported lipid bilayers in the presence of QPVP in comparison to its absence, revealing that their binding causes a decrease in lateral mobility.

P1.00113 Nanoparticle size and shape characterization with Solid State Nanopores, SANTOSHI NANDIVADA, MOURAD BENAMARA, JIALI LI, University of Arkansas — Solid State Nanopores are widely used in a variety of single molecule studies including DNA and biomolecule detection based on the principle of Resistive Pulse technique. This technique is based on electrophoretically driving charged particles through 35-60 nm solid state nanochannels. The translocation of these particles produces current blockage events that provide an insight to the properties of the translocation of nanoparticles and the nanopore. In this work we study the current blockage events produced by ~ 30nm negatively charged PS nanoparticles through Silicon Nitride solid state nanochannels. We show how the current blockage amplitudes and durations are related to the ratio of the volume of the particle to the volume of the pore, the shape of the particle, charge of the particle and the nanopore surface, salt concentration, solution pH, and applied voltage. The solid-state nanopores are fabricated by a combination of Focus Ion Beam and low energy Ion beams in silicon nitride membranes. High resolution TEM is used to measure the 3D geometry of the nanopores and a finite element analysis program (COMSOL) is used to simulate the experimental results.

P1.00114 ABSTRACT WITHDRAWN

P1.00115 Characterizing detergent mediated reconstitution of viral protein M2 in large unilamellar vesicles, MARIEL FREYRE, CARL GROSSMAN, CATHERINE CROUCH, KATHLEEN HOWARD, Swarthmore College — Influenza M2 is a model membrane protein whose function is to induce curvature and vesicle formation in the process of viral infection. To study embedded M2 in synthetic phospholipid vesicles (large unilamellar vesicles or LUVs), a concentration of detergent and buffer is optimized to balance protein solubility, proteolipid concentration, and LUV stability. Adding detergent also causes the LUVs to partially disassemble and form micelles, which warrants detergent removal to restore LUV integrity. We explore methods of measuring the coexistence of detergent micelles and LUVs to track the different phases of the system as detergent is removed. A combination of Fluorescence Correlation Spectroscopy, Dynamic Light Scattering, and chemical analysis are used to measure the properties of this system. With detergent/LUV number densities as high as 5 we find coexistence of micelles and LUVs at 50% to 60%. As the detergent is removed, the micelle concentration drops to lower than 30% while detergent levels drop to nearly zero. These results may indicate a polydispersed LUV size distribution after detergent mediated reconstitution.

1Supported by HHMI and Swarthmore College

P1.00116 Preventing drug resistance in severe influenza, HANA DOBOROVNY, Texas Christian Univ, LUCAS DEECKE, University of Cologne — Severe, long-lasting influenza infections are often caused by new strains of influenza. The long duration of these infections leads to an increased opportunity for the emergence of drug resistant mutants. This is particularly problematic for new strains of influenza since there is often no vaccine, so drug treatment is the first line of defense. One strategy for trying to minimize drug resistance is to apply periodic treatment. During treatment the wild-type virus decreases, but resistant virus might increase; when there is no treatment, wild-type virus will hopefully out-compete the resistant virus, driving down the number of resistant virus. We combine a mathematical model of severe influenza with a model of drug resistance to study emergence of drug resistance during a long-lasting infection. We apply periodic treatment with two types of antivirals: neuraminidase inhibitors, which block release of virions; and adamantanes, which block replication of virions. We compare the efficacy of the two drugs in reducing emergence of drug resistant mutants and examine the effect of treatment frequency on the emergence of drug resistant mutants.

P1.00117 Simultaneous influenza and respiratory syncytial virus infection in human respiratory tract, LUBNA JAHAN RASHID PINKY, HANA DOBOROVNY, Texas Christian University — Studies have shown that simultaneous infection of the respiratory tract with at least two viruses is not uncommon in hospitalized patients, although it is not clear whether these infections are more or less severe than single infections. We use mathematical models to study the dynamics of simultaneous influenza (flu) and respiratory syncytial virus (RSV) infection, two of the more common respiratory viruses, in an effort to understand simultaneous infections. We examine the roles of initial viral inoculum, relative starting time, and cell regeneration on the severity of the infection. We also study the effect of antiviral treatment on the course of the infection. This study shows that, unless treated with antivirals, flu always takes over the infection no matter how small the initial dose and how delayed it starts with respect to RSV.
P1.00118 Determining Mechanism of Action of Antivirals for Respiratory Illness. Irma Rodriguez, Hana Dobrovolny, Texas Christian University — Viral infections in the respiratory tract are common in humans and can cause serious illness and death. Drug treatment is the principal line of protection against many of these illnesses and many compounds are tested as antivirals. Often the efficacy of these antivirals is determined before a mechanism of action is understood. We use mathematical models to represent the evolution of these diseases and establish which experiments can help determine the mechanism of action of antivirals.

P1.00119 Object-adapted trapping and shape-tracking to probe a bacterial protein chain motor. Julian Roth, Matthias Koch, Alexander Rohrbach, University of Freiburg — The helical bacterium Spiroplasma is a motile plant and anthropod pathogen which swims by propagating pairs of kinks along its cell body. As a well suited model system for bacterial locomotion, understanding the cell's molecular motor is of vital interest also regarding the combat of bacterial diseases. The extensive deformations related to these kinks are caused by a contractile cytoskeletal protein ribbon representing a linear motor in contrast to common rotary motors as, e.g., flagella. We present new insights into the working of this motor through experiments with object-adapted optical traps and shape-tracking techniques. We use the given laser irradiation from the optical trap to hinder bacterial energy (ATP) production through the production of O₂ radicals. The results are compared with experiments performed under the influence of an O₂ Scavenger and ATP inhibitors, respectively. Our results show clear dependences of the kinking properties on the ATP concentration inside the bacteria. The experiments are supported by a theoretical model which we developed to describe the switching of the ribbon's protein subunits.

P1.00120 Modeling the Lymphocytic Choriomeningitis Virus: Insights into understanding its epidemiology in the wild. Christy Contreras, College of Liberal Arts and Sciences – Physics Department, Arizona State University, John Mckay, Applied Mathematics for the Life and Social Sciences, Arizona State University, Joseph Blattman, Susan Holecheck, The Biodesign Institute, Arizona State University — The lymphocytic choriomeningitis virus (LCMV) is a rodent-spread virus commonly recognized as causing neurological disease that exhibits asymptomatic pathology. The virus is a pathogen normally among rodents that can be transmitted to humans by direct or indirect contact with the virus in excretions and secretions from rodents and can cause aseptic meningitis and other conditions in humans. We consider an epidemiological system within rodent populations modeled by a system of ordinary differential equations that captures the dynamics of the diseases transmission and present our findings. The asymptotic nature of the pathogen plays a large role in its spread within a given population, which has motivated us to expand upon an existing SIRC model (Holechek et al in preparation) that accounts for susceptible-, infected-, recovered-, and carrier-mice on the basis of their gender. We are interested in observing and determining the conditions under which the carrier population will reach a disease-free equilibrium, and we focus our investigation on the sensitivity of our model to gender, pregnancy related infection, and reproduction rate conditions.

P1.00121 ABSTRACT WITHDRAWN —

P1.00122 Feeding strategies as revealed by the section moduli of the humerus bones in bipedal theropod dinosaurs. Scott Lee, Zachary Richards, University of Toledo — The section modulus of a bone is a measure of its ability to resist bending torques. Carnivorous dinosaurs presumably had strong arm bones to hold struggling prey during hunting. Some theropods are believed to have become herbivorous and such animals would not have needed such strong arms. In this work, the section moduli of the humerus bones of bipedal theropod dinosaurs (from Microvenator celer to Tyrannosaurus rex) are studied to determine the maximum bending loads their arms could withstand. The results show that bending strength is not of uniform importance to these magnificent animals. The predatory theropods had strong arms for use in hunting. In contrast, the herbivorous dinosaurs had weaker arms.

P1.00123 Microrheology of single microtubule filaments and synthesized cytoskeletal networks. Matthias Koch, Alexander Rohrbach, Lab for Bio- and Nano-Photonics, University of Freiburg — The ability to sense and respond to external mechanical forces is crucial for cells in many processes such as cell growth and division. Common models on mechanotransduction rely on the conversion of mechanical stimuli to chemical signals in the cell periphery and their translocation by diffusion (passive) or molecular motors (active). These processes are rather slow (~ seconds) and it has been argued that the cytoskeleton itself might be able to transport a mechanical signal within microseconds via stress waves. Microtubules are the stiffest component of the cytoskeleton and thus ideal candidates for this purpose. We study the frequency dependent response of single microtubule filaments and small networks thereof in a bottom-up approach using several (N=2-10) time-multiplexed optical tweezers together with back focal plane interferometry. Small synthesized networks with a defined geometry are constructed using trapped Neutravidin beads as anchor points for biotinylated filaments. The network is then probed by a defined oscillation of one anchor (actor). The frequency dependent response of the remaining beads (sensors) is analyzed experimentally and modeled theoretically over a wide frequency range.

P1.00124 Biviscous blood flow and a new method for velocity profile adjustment. Carlos Velazquez, Adrian Reyes, Universidad Nacional Autonoma de Mexico — In this paper we describe our proposal of a new numerical procedure for the adjusting of the velocity profile of body fluids with two viscosities. We have focused on the relevant case of the human blood and we have selected a particular model, the biviscous blood model, with the purpose of proving the convenience of our method. We start by describing the convenience of the biviscous stress equation as a model for the blood constitutive equation, then we solve it in the particular case of a stationary flow and use this solutions as the basis of our numerical procedure, which is described afterwards. Then, we present its implementation for analyzing in vivo measurements and exhibit its pertinence. Finally, we explain the design of a programmatic code of an automatic routine which is capable of applying our method and therefore could be used as the basis of an automated implementation in new diagnosis software within a measurement device.

P1.00125 Femoral bone strength in large theropod dinosaurs: A study by genus. Scott Lee, University of Toledo — The locomotion of bipedal theropod dinosaurs is controlled by the strength of the femur to resist bending torques (caused by the foot striking the ground and the action of muscles on the femur). The section modulus at the narrowest part measures the ability of the femur to resist such torques. We present the results of our study of the femoral section moduli for six genus of large theropods: Tyrannosaurus, Nanotyrannus, Gorgosaurus, and Albertosaurus of the Late Cretaceous, Acrocanthosaurus of the Early Cretaceous, and Allosaurus of the Late Jurassic. These animals had femora of lengths between 65 and 134 cm. The corresponding section moduli varied between 23 and 570 cm². Some species of Tyrannosaurus, Gorgosaurus, Allosaurus, and Albertosaurus had femora with lengths in the same 75 to 90 cm range. The section moduli of these animals are all in the same range, showing that the animals had the same abilities of locomotion. That is, Allosaurus of the Late Jurassic could locomote just as well as the Late Cretaceous Tyrannosaurus, Gorgosaurus, and Albertosaurus. There is no evidence that these later theropods had evolved to be any faster than similarly-sized theropods living about 80 million years earlier.
P1.00126 Alloometry in dinosaurs and mammals . SCOTT LEE, University of Toledo — The proportions of the leg bones change as the size of an animal becomes larger since the mass of the animal increases at a faster rate than the cross-sectional area of its leg bones. For the case of elastic similarity (in which the longitudinal stress in the legs remains constant in animals of all sizes), the diameter d and length L of the femur should be related as d = A L^{3/2}. For geometric similarity (in which all dimensions are scaled by the same factor), d = A L. For animals with femora longer than 20 cm, we find the power law relationship to be d = A L^3 with b = 1.13 ± 0.06 for extant mammals (the largest mammal being Loxodonta africana with a 1.00-m-long femur) and b = 1.18 ± 0.02 for dinosaurs (the largest dinosaur being Brachiosaurus brancai with a 2.03-m-long femur). These data show that extinct dinosaurs and extant animals scale in the same basic manner. The large sauropods (with femora twice as long as found in elephants) scale in a manner consistent with extrapolation of the scaling shown by extant mammals. These results argue that extinct dinosaurs moved in a manner very similar to extant mammals.

P1.00127 Direct Osmolyte-Macromolecule Interactions Confer Entropic Stability to Folded States1 . FRANCISCO RODRIGUEZ-ROPERO, NICO F. A. VAN DER VEGT, Tech Univ Darmstadt — Protective osmolytes are chemical compounds that shift the (bio)macromolecule folding/unfolding equilibrium toward the folded state under osmotic stresses. Traditionally it has been considered that osmolytes are depleted from the macromolecule first solution shell, leading to entropic stabilization of the folded state. Recent theoretical and experimental studies suggest that protective osmolytes may directly interact with the macromolecule. As an exemplary and experimentally well-characterized system, we herein discuss poly(N-isopropylacrylamide) (PNIPAM) in water whose folding/unfolding equilibrium shifts toward the folded state in the presence of urea. Based on Molecular Dynamics simulations we show that urea preferentially accumulates in the first solvation shell of PNIPAM driven by attractive van der Waals dispersion forces leading to the formation of urea clouds around the polymer. Solvation thermodynamics analysis of the folded and unfolded states discards direct urea/macromolecule interactions as driving force of the folding mechanism. Our data shows that entropic penalization of unfolded polymer chains upon increasing urea concentration drives the collapse of the polymer chain.

1 German Research Foundation (DFG), Cluster of Excellence 259 “Smart Interfaces - Understanding and Designing Fluid Boundaries.”

P1.00128 Quantifying macromolecular conformational transition pathways , SEAN SEYLER, AVISHEK KUMAR, MICHAEL THORPE, OLIVER BECKSTEIN, Arizona State University — Diverse classes of proteins function through large-scale conformational changes that are challenging for computer simulations. We introduce a comprehensive method (pathway similarity analysis, PSA) for quantitatively characterizing and comparing macromolecular pathways. The Hausdorff and Fréchet metrics (known from computational geometry) are used to identify the degree of similarity between polygonal curves in configuration space. A strength of PSA is its use of the full information available from the 3N-dimensional configuration space trajectory without requiring additional specific knowledge about the system. We compare a sample of eleven different methods for the closed-to-open transitions of the apo enzyme adenylate kinase (AdK) and also apply PSA to an ensemble of 400 AdK trajectories produced by dynamic importance sampling MD and the Geometrical Pathways algorithm. We discuss the method’s potential to enhance our understanding of transition path sampling methods, validate them, and help guide future research toward deeper physical insights into conformational transitions.

P1.00129 Interaction of Human Serum Albumin with Metal Protoporphyrins , JIEHU, URTSA, LORENZO BRANCACLEON, Physics Dept. UTSA — Fluorescence spectroscopy is widely used in biotechnology, nanotechnology, and molecular biophysics, since it can provide information on protein conformations, interactions etc. In this study, we present the photophysical properties of the interaction of human serum albumin (HSA) with a series of metal compound of Protoporphyrin IX (PPIX), including ZnPPIX, FePPIX, MgPPIX, MnPPIX and SnPPIX respectively, as well as the free base PPIX. Binding constants were retrieved independently using the Benesi-Hildebrand analysis of the porphyrin emission or absorption spectra and the fluorescence quenching (i.e. Stern-Volmer analysis) and reveal that the two methods yield a difference of approximately one order or magnitude between the two. Fluorescence lifetimes was used to probe whether binding of the porphyrin changes the conformation of the protein or if the interaction places the porphyrin at a location that can prompt resonance energy transfer with the lone Tryptophan residue. In recent years it has been discovered that HSA provides a specific binding site for metal-chelated protoporphyrins in subdomain IA. This has opened a novel field of study over the importance of this site for biomedical applications but it has also created the necessity to search for novel universality-breaking experimental perturbations.

P1.00130 Replica-exchange Wang-Landau simulations of the H0P model of protein folding, GUANGJIE SHI, DAVID P. LANDAU, Center for Simulational Physics, The University of Georgia, THOMAS WÜST, Scientific IT Services, ETH Zurich — The hydrophobic-polar (HP) model has served as a coarse-grained lattice protein folding model attracting scientists from various disciplines. However, simplification into H and P monomers may yield high ground state degeneracies which stands in contrast to the generally unique native states of natural proteins. We propose a simple modification, by introducing a new type of “neutral” monomer, 0, i.e. neither hydrophobic nor polar, rendering the model more realistic without increasing the difficulties of sampling significantly. With the newly developed parallel Wang-Landau (replica exchange Wang-Landau) scheme and an innovative method of estimating the ground state degeneracies1,2 we investigated some widely studied HP proteins and their H0P counterparts. Dramatic differences in ground state and thermodynamic properties have been observed, e.g. the estimation of ground state degeneracy for the 46mer is 460,000 for the HP version and only 20 for the H0P mapping. Similarly, the specific heat and structural properties: radius of gyration and etc. show more pronounced signals associated with folding.

1 Supported by NSF.
3 G. Shi, T. Vogel, T. Wüst, Y. W. Li, and D. P. Landau, Phys. Rev. E 90, 033307

P1.00131 Ergodic protein dynamics underlie the universal shape of protein distribution in populations , NAAMA BRENNER, EREZ BRAUN, Technion-Israel Institute of Technology, JAMES ROTELLA, HANNA SALMAN, University of Pittsburgh, NAAMA BRENNER COLLABORATION, EREZ COLLABORATION, JAMES ROTELLA AND HANNA SALMAN COLLABORATION — We have previously shown that protein fluctuations in cell populations exhibit a universal distribution shape under a broad range of biological realizations. Here we report new results based on continuous measurement in individual bacteria for over ~ 70 generations, which show that single-cell protein trajectories sample the available states with the same distribution shape as the population, i.e. protein fluctuations are ergodic. Analysis of temporal trajectories reveals that one effective random variable, sampled once each cell cycle, suffices to reconstruct the distribution from the trajectory. This in turn implies that cellular microscopic processes are strongly buffered and population-level protein distributions are insensitive to details of the intracellular dynamics. Probing them thus requires searching for novel universality-breaking experimental perturbations.
P1.00132 Two-Dimensional Graphene Optoelectronic Probes for DNA Detection. TU HONG, Department of Electrical Engineering and Computer Science, Vanderbilt University, RUI WANG, XUANYANG GE, Department of Physics and Astronomy, Vanderbilt University, YAQIONG XU, Department of Electrical Engineering and Computer Science, Vanderbilt University — With high charge-carrier mobility and large surface-area-to-volume ratio, graphene has become one of the most promising materials for biological and biomedical applications. Here, we demonstrate that graphene field-effect transistors combined with scanning photocurrent microscopy are ideal platforms for detecting DNA molecules. When negatively-charged DNA molecules are attached to graphene surface, significant photocurrent signals can be detected due to the local conductivity change in graphene. Our experimental results show that DNA-induced photocurrent response of graphene can be modulated by adjusting the electrochemical potential through an electrolyte gate. This study indicates that two-dimensional graphene optoelectronic probes can be used to explore the local electrostatic environment change with high electrical sensitivity.

P1.00133 FLUIDS —

P1.00134 Effect of Confinement on the Bubble Points of Hydrocarbons in Controlled-Pore Glasses. SHENG LUO, Harold Vance Department of Petroleum Engineering, Texas A&M University, JODIE LUTKENHAUS, Artie McFerrin Department of Chemical Engineering, Texas A&M University, HADI NASRABADI, Harold Vance Department of Petroleum Engineering, Texas A&M University, HADI NASRABADI TEAM — Phase behavior in shale remains a challenging problem in the petroleum industry due to many complexities. One complexity is the strong surface-fluid interactions in shale nano-scale pores. These interactions can lead to a heterogeneous distribution of molecules, which conventional bulk-phase thermodynamics fails to describe. Herein, we report a study on the bubble points of various hydrocarbons confined in nanoporous controlled-pore glasses of 4.3 to 38.1 nm pore diameter. Differential scanning calorimetry is used to measure the temperature at which the gas phase begins to form (i.e. bubble point). Besides pore diameter, the relative hydrocarbon loading in the controlled-pore glass is evaluated. The findings suggest that the bubble point is dramatically affected by pore diameter.

P1.00135 Liquid Crystals under Photo-patterned Spatially Varying Boundary Conditions1. MIAO JIANG, YU-BING GUO, QI-HOU WEI, Liquid Crystal Institute, Kent State Univ, Kent, OH — Liquid crystals under geometric confines are of not only fundamental interest but also practical importance to applications such as chemical sensing and smart windows. Orientations of liquid crystal molecules in most geometric confines are uniform at the boundaries and not highly controllable. In this paper, we will present a novel photoalignment technique to pattern spatially varying complex orientation fields, and discuss experimental studies on nematic liquid crystals under confines of two parallel plates with various well designed molecular orientation fields.

P1.00136 Two-dimensional Yukawa fluids. MINERVA GONZALEZ-MELCHOR, Instituto de Fisica “Luis Rivera Terrazas,” Benemerita Universidad Autonoma de Puebla, Apdo. Postal J-48, Puebla, 72570, Puebla, Mexico, ARLETTE MENDEZ, JOSE ALEJANDRE, Departamento de Quimica, Universidad Autonoma Metropolitana-Iztapalapa, Av. San Rafael Atlicoc 186, Col. Vicentina, 09340 Mexico Distrito Federal, Mex — When the movement of particles is performed predominantly in two dimensions, the systems can be considered at a good extent as two-dimensional. For instance the lipids in a bilayer, micrometric particles in a quasi-two-dimensional colloidal suspension, colloids in a monolayer deposited on the air-water interface, and DNA complexes trapped at the water surface can be described at a first approach as bidimensional fluids. These systems are important for many applications in surface and colloidal science. In simulations where the explicit interface between liquid and vapor is present, the line tension can be directly computed. In this work we present molecular dynamics results obtained for the liquid/vapor coexistence curve of 2D Yukawa fluids and for the line tension. A comparison with the three-dimensional case is also presented.

P1.00137 Heat Transfer Enhancement in Forced Convective Boiling in Microchannels by Periodic Electrospray Nanofiber Coatings. ALEXANDER YARIN, University of Illinois at Chicago, MARTIN FREYSTEIN, FELIX KOLBERG, Technische Universität Darmstadt, SUMIT SINHA-RAY, RAKESH SAHU, University of Illinois at Chicago, LUCAS SPIEGEL, TATIANA GAMBARYAN-ROISMAN, PETER STEPHAN, Technische Universität Darmstadt — To enhance heat transfer in forced convective boiling the microchannel bottom was amended by a nano-texture - periodic rectangular mats of electrospray polymer nanofibers. The fibers were ~300-500 nm in diameter and the mat thicknesses were about 6-15 µm. The test fluid was FC-72 and the flow in microchannels contained trains of Taylor bubbles. The role of the nanofibers was to retain the warm microchannel bottom wet, to prevent dry-out and thus to enhance the heat removal rate. In the present experiments the time-average heat flux and heat transfer coefficient at the nanofiber-covered domains were found to be 1.5-2 times higher than those at the uncoated ones. Accordingly, a significant decrease (by 5-8%) in the superheat was observed at the same Re of 387 and power supply of 36.1 kW/m². At a higher Re of 432 and lower power supply of 28.1 kW/m² similar trends in the heat removal rate and surface superheat were found. The significant enhancement of the heat transfer results from the fact that nanofiber mats facilitate wetting of surface under passing Taylor bubbles, thus delaying formation of vapor flow at the channel bottom. The interstices of the nanofiber mat act as the nucleation sites facilitating formation of tiny bubbles, which eventually results in a higher heat removal rate from the surface at a reduced superheat.

P1.00138 A simulation study of flow dynamics of erythrocytes through diverging and converging bifurcations1. TONG WANG, Nanjing University of Aeronautics and Astronautics, ZHONGWEN XING, Nanjing University — A numerical model has been developed to predict the cells deformation and motion in a symmetric diverging and converging bifurcation of a microchannel. Fluid dynamics and membrane mechanics are incorporated. The model was utilized to evaluate the effect of different biophysical parameters, such as: initial cell position, membrane stiffness and shape of the cells on deformation and motion of the erythrocytes in the bifurcating curved microchannel. The numerical results demonstrate that erythrocytes in microvessels blunt velocity profiles in both straight section and daughter branches, and the transit velocity of erythrocytes is strongly influenced by cell deformability, shape of the cells, and the vessel geometry. These results may provide fundamental knowledge for a better understanding of hemodynamic behavior of microscale blood flow.

P1.00139 Fluid flow calculations of Graphene Composites. AMRHESSAM TAHMASSEBI, ALPER BULDUM, University of Akron, Department of Physics — The flow of fluids through carbon nanotubes was investigated in order to get a better understanding of the unique properties and phenomena of nano-fluidics. The previous modeling and simulation efforts were based on diffusion of atoms or molecules that were thrown to the nanotubes with initial velocities. This talk has shed some light on the flow of fluids using molecular dynamic simulations of different types of carbon nanotubes that were embedded in liquid argon using a moving wall piston of graphene. We focused on analyzing pressure difference, velocities, and momentum conservation in different regions.

1Work supported by NSF CMMI-1436565
P1.00140 The effects of surface roughness on the contact line friction coefficients of water droplets on micro/nano-patterned surfaces, JIANGTAO CHENG, University of North Texas — We report the effects of surface roughness on contact line friction coefficient (CLFC) of water droplets on micro- and nano-patterned surfaces. Both advancing and receding CLFCs have been measured on smooth, one-tier (with micropillars), and two-tier (with CNTs grown on micropillars) surfaces. In comparison with smooth surface, superhydrophobic surfaces can decrease both the advancing and receding CLFCs by more than 10 times. However, droplets on one-tier surfaces exhibit different dynamic behaviors in advancing and receding movements. We investigated the Wenzel-Cassie state transition on micropillar structures and found that the receding motion of a droplet on micropillars is dominated by the Wenzel model with significant receding contact line pinning, which leads to higher receding CLFC. However, rolling mechanism of liquid particles near the advancing contact line controls the advancing motion of a droplet on micropillars. There is a high tendency for an advancing droplet to exhibit Cassie-type behavior on one-tier surfaces and hence advancing CLFC is considerably mitigated. On two-tier superhydrophobic surfaces, it is the Cassie-Baxter behavior that dominates both the advancing and receding contact line motions giving rise to less friction coefficients.

P1.00141 Patterns, Instabilities, Colors, and Flows in Vertical Foam Films, SUBINUER YILXIATI, EWELINA WOJCICK, YIRAN ZHANG, COLLIN PEARSSALL, VIVEK SHARMA, Chemical Engineering, University of Illinois Chicago — Foams find use in many applications in daily life, industry and biology. Examples include beverages, firefighting foam, cosmetics, foams for oil recovery and foams formed by pollutants. Foams are collection of bubbles separated by thin liquid films that are stabilized against drainage by the presence of surfactant molecules. Drainage kinetics and stability of the foam are strongly influenced by surfactant type, addition of particles, proteins and polymers. In this study, we utilize the thin film interference colors as markers for identifying patterns, instabilities and flows within vertical foam films. We experimentally study the emergence of thickness fluctuations near the borders and within thinning films, and study how buoyancy, capillarity and gravity driven instabilities and flows, are affected by variation in bulk and interfacial physicochemical properties dependent on the choice of constituents.

P1.00142 Diving dynamics of seabirds, SUNGHWAN JUNG, BRIAN CHANG, MATT CROSON, Virginia Tech, LORIAN STRAKER, CARLA DOVE, Smithsonian Museum — Diving is the activity of falling from air into water, which is somewhat dangerous due to the impact. Humans dive for entertainments less than 20 meters high, however seabirds dive as a hunting mechanism from more than 20 meters high. Moreover, most birds including seabirds have a slender and long neck compared to many other animals, which can potentially be the weakest part of the body upon axial impact compression. Motivated by the diving dynamics, we investigate the effect of surface and geometric configurations on structures consisting of a beak-like cone and a neck-like elastic beam. A transition from non-buckling to buckling is characterized and understood through physical experiments and an analytical model.

P1.00143 POLYMER PHYSICS —

P1.00144 Orthogonal gradient networks via post polymerization reaction, PANDYARAJAN CHINNAYAN KANNAN, JAN GENZER, North Carolina State University — We report a novel synthetic route to generate orthogonal gradient networks through post polymerization reaction using pentafluorophenylmethacrylate (PFPMac) active ester chemistry. These chemoselective monomers were successfully copolymerized with 5 mole% of the photo (methacryloyloxybenzophenone) and thermal (styrerensulfonylazide) crosslinkers. Subsequently, the copolymers were modified by a seris of amines having various alkyl chain lengths. The conversion of post polymerization reaction was monitored using Fourier Transform Infrared Spectroscopy (FT-IR) and noticed that almost all pentafluorophenyl moieties are substituted by amines within an hour without affecting the crosslinkers. In addition, the incorporation of photo and thermal crosslinkers in the polymer enabled us to achieve stable and covalently surface-bound polymer gradient networks (PGN) in an orthogonal manner, i.e complete control over the crosslink density of the network in two opposite directions (i.e. heat vs photo). The network properties such as wettability, swelling and tensile modulus of the gradient coatings are studied and revealed in the paper.

P1.00145 Enthalpy Relaxation of a DGEBA Epoxy as a function of Time, Temperature, and Cooling Rate, CAITLYN M. CLARKSON, JOHN D. MCCOY, New Mexico Tech, JAMIE M. KROPKA, Sandia National Laboratories — Enthalpy relaxation resulting from physical aging of a DGEBA epoxy, Epon 828, cross-linked with an amine curative, Jeffamine T-403, was studied for two isothermal aging temperatures at sequential aging times up to two weeks. Results were analyzed using the peak shift method to obtain the relaxation parameters \(\beta\), \(\delta\) (\(\delta^H\)), and \(\chi\). The individual effects of cooling rate from the equilibrated state, aging time, and aging temperature were isolated to understand the initial state of the glassy epoxy and its evolution during physical aging. [Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000]

P1.00146 Frank-Kasper and other superlattice formations in a set of giant molecules having ABn type of Janus particles, XUEYAN FENG, YIWEN LI, MINGJUN HUANG, CHI-HAO HSU, STEPHEN Z.D. CHENG, University of Akron — A novel series of precisely defined giant molecules having ABn type of Janus particles has been designed and synthesized. They are consisted of one functionalized hydrophilic polyhedral oligomeric silsesquioxane (POSS) (A) connected with different number of hydrophobic POSS cages (B, \(n=2-6\)). With variation of the interaction functional groups on A and the number of the coordinated hydrophobic POSS B, different superlattice structures could be formed at a sub-10-\(nm\) scale. For example, the superlattice structure of DPOSS-BPOSS2 (DPOSS represents seven hydroxyl group functionalized POSS and BPOSS represents isobutyl POSS) could change from a double-dyroids phase to a hexagonally packed cylinder phase with increasing temperature, due to an order-order transition in the weak segregation region. For DPOSS-BPOSS3 and DPOSS-BPOSS4, both of these giant molecules could form A15 phase, which is a Frank-Kasper phase. With deep understanding of this set of ABn type giant molecules based on the POSS nano atoms, it may be promising to construct new generations of giant molecules for further development of functional materials with desired structures and macroscopic properties.

P1.00147 Strain Rate Dependence of Compressive Yield and Relatization in DGEBA Epoxies, GABRIEL K. ARECHEDDERRA, RILEY C. RÉPROGLE, CAITLYN M. CLARKSON, JOHN D. MCCOY, New Mexico Tech, JAMIE M. KROPKA, KEVIN N. LONG, ROBERT S. CHAMBERS, Sandia National Laboratories — The mechanical response in uniaxial compression of two diglycidyl ether of bisphenol-A epoxies were studied. These were 828DEA (Epon 828 cured with diethanolamine (DEA)) and 828T403 (Epon 828 cured with Jeffamine T-403). Two types of uniaxial compression tests were performed: A) constant strain rate compression and B) constant strain rate compression followed by a constant strain relaxation. The peak (yield) stress was analyzed as a function of strain rate from Eyring theory for activation volume. Runs at different temperatures permitted the construction of a mastercurve, and the resulting shift factors resulted in an activation energy. Strain and hold tests were performed for a low strain rate where a peak stress was lacking and for a higher strain rate where the peak stress was apparent. Relaxation from strains at different places along the stress-strain curve was tracked and compared. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
P1.00148 Template-directed synthesis of structurally-defined branched polymer architectures, AMANDA MARCIEL, UIUC — In this work, we describe a hybrid synthetic strategy to produce structurally-defined branched polymer architectures based on chemically-modified DNA. Overall, this approach enables precise control over branch placement, grafting density, and chemical identity of side branches. We utilize a two-step scheme based on polymerase chain reaction (PCR) for site-specific incorporation of non-natural nucleotides, followed by copper-free click chemistry for grafting side branches at specific locations along the main polymer backbone. Linear DNA backbones are first synthesized via PCR utilizing the promiscuity of a high yield thermostable DNA polymerase to incorporate nucleotides containing bioorthogonal dibenzocyclooctyne functional groups at precise locations along one strand of a double stranded DNA backbone. Following PCR, copper-free click chemistry is used to attach synthetic polymer branches or oligonucleotide branches to the DNA backbone, thereby allowing for the design and synthesis of a variety of precise polymer architectures, including three-armed stars, H-polymers, and graft block copolymers.

P1.00149 Light scattering measurement of sodium polyacrylate products, NISHA LAMA, DAVID NORWOOD, Southeastern Louisiana Univ, STEVEN BOONE, VALERIE MASSIE-BOYER, Bercen Inc. — In the presentation, we will describe the use of a multi-detector HPLC incorporating the DAWN EOS multi-angle laser light scattering (MALLS) detector to measure the properties such as molecular weight, RMS radius, contour and persistence length and polydispersity of sodium polyacrylate products. The samples of sodium polyacrylate are used in various industries as thickening agents, coating dispersants, artificial snow, laundry detergent and disposable diapers. Data and results obtained from the experiment will be presented.

P1.00150 Kinetics of the coil-to-globule transition in aqueous solution of poly (N-isopropoylacrylamide). REZA FARASAT, University of Alabama at Birmingham — In an aqueous solution, poly (N-isopropoylacrylamide) (PNIPAM) undergoes a reversible coil-to-globule phase transition that occurs above the lower critical solution temperature (LCST). The transition is driven by temperature-dependent molecular interactions that include hydrogen bonding and hydrophobic association. By increasing the temperature above LCST, the PNIPAM-water bonds break, and the polymer coils collapse to globules. The process is accompanied by an endothermic thermal effect which is detectable by Differential Scanning Calorimetry (DSC). A 10 wt. % solution of PNIPAM in water was prepared and subjected to DSC experiments under different heating rates (from 0.5 to 16°C min⁻¹). With increasing the heating rate, the transition temperature as well as the DSC peak shift to higher temperature. The DSC data have been analyzed by an isocorrectional method to evaluate the temperature dependence of the effective activation energy of the process. The resulting dependencies have been interpreted in terms of a nucleation kinetics model. The process has also been studied under nanoconfinement by introducing the PNIPAM solution into the silica nanorods. The results obtained under nanoconfinement are compared to those obtained for the bulk solution.¹

¹Partial financial support of this work by the National Science Foundation under grant CHE 1052828 is gratefully acknowledged.

P1.00151 SEMI CRYSTALLINE POLYMERS

P1.00152 Effect of Crystallinity on Melt Memory of Random Ethylene Copolymers, XUEJIAN CHEN, AL MAMUN, ALAMO G. RUFINA, FAMU-FSU College of Engineering, Department of Chemical and Biomedical Engineering, Tallahassee, Fl 32310 — A strong melt memory effect of crystallization has been observed in random ethylene copolymers even above the equilibrium melting temperature. Melt memory is associated with seeds that increase the crystallization rate of copolymers in a range of comonomer content between 0.5 and 4.5 mol%. The seeds are taken as molten ethylene sequences that remain in close proximity and are unable to diffuse fast to the randomized melt state. Fast diffusion is restricted by topological chain constraints (loops, knots, and other entanglements) that build in the intercrystalline region during crystallization. The molten nature of the self-seeds is supported by a linear variation of Tᵢ with Tₘₐₓ n NMR experiments in a range from 180 °C to 100 °C, covering both the homogeneous and heterogeneous melt regions. The effect of topological constraints on melt memory, or on number of seeds that remain in the melt, was analyzed studying copolymers with different levels of crystallinity. There is a threshold level of crystallinity, which depends on type and concentration of comonomer, below which copolymers do not display strong melt memory. Increasing 1-hexene content from 0.5 to 3.5 mol%, the crystallinity threshold decreases from 39 to 4%, while decreasing branch length from hexyl to ethyl, the threshold crystallinity decreases from 18% to 5% in agreement with stronger melt memory in copolymers with increasing comonomer content and with shorter branches.

P1.00153 Structural Analysis of Semiconducting Polymers Exposed to High Energy Radiation, SAEED AHMADI VASELABADI, University of Pittsburgh, NIHKLIA MAHADEVAPURAM, Intel Corporation, DAVID SHAKARISAZ, University of Houston, JOSEPH STRZALKA, Argonne National Laboratory, PAUL RUCHHOEFT, GILA STEIN, University of Houston — Semicrystalline polymers are used in low-cost electronics such as solar cells, thin film transistors, and light-emitting diodes. Their optoelectronic performance in these devices is partly dictated by molecular ordering and nanoscale structure, which the latter is particularly difficult to control. We used atom-beam radiation to crosslink the polymer poly(3-hexylthiophene) into nanoscale and microscale patterns. Ionizing radiation sources generate intermolecular cross-links that render the polymer insoluble in organic solvents. Grazing-incidence Wide-angle X-ray Scattering (GIWAXS) was used to investigate the effects of irradiation on molecular ordering of poly(3-hexylthiophene). We found that crosslinking will disrupt intermolecular ordering (reduce crystallinity and crystalline grain sizes). We also found that X-ray exposure during the WAXS measurements can induce the crosslinking through a similar mechanism, and we propose a simple method to test for the damage caused by these measurements. As an example, we find that poly (3-hexylthiophene) has measurable cross-links after 20 sec exposure to 7.35 keV radiation with flux of 1 × 10¹¹ photons/sec at an incident angle of 0.5°.

P1.00154 Mechanical properties of syndiotactic polypropylene (sPP) gels: the effects of temperature and solute concentration, RYUSUKE OKOSHI, ATSUISHI HOTTIGA, Department of Mechanical Engineering, Keio University — The effects of the solute concentration on the microstructures and the mechanical properties of quenched syndiotactic polypropylene (sPP) gels were investigated. Our group has previously reported a highly resilient sPP gel quenched using liquid nitrogen (Gel LN). In this research, sPP/decahydronaphtalene gels were prepared varying the sPP concentrations from 5 to 20 wt%. Compression test was carried out to evaluate the mechanical properties. Scanning electron microscopy (SEM) was conducted to analyze the microstructures. Gel LN with the sPP concentration of 20 wt% presented a high fracture stress of 2400 kPa. A high fracture strain of 70% was also observed for all Gel LN samples. By contrast, sPP gels with the sPP concentration of 25 wt% cooled at 25 degrees C showed lower fracture stress of 480 kPa. The fracture strain of Gel 25 ranged from 21 to 37% depending on the sPP concentrations. The SEM results revealed that the Gel LN samples had homogeneous networks regardless of the sPP concentrations. The Gel 25, however, possessed inhomogeneous networks with spherulites. It was therefore concluded that the strengthening of the sPP gels could be effectively achieved by Gel LN regardless of the sPP concentrations.
P1.00155 Structural Characterization of Layered Morphologies in Precise Copolymers . EDWARD B. TRIGG, L. ROBERT MIDDLETON, Univ of Pennsylvania, TAYLOR W. GAINES, KENNETH B. WAGENER, Univ of Florida, KAREN J. WINEY, Univ of Pennsylvania — Layered morphologies have been observed in precise polyethylene-based copolymers that contain acid, charged, or polar functional groups precisely spaced along a linear alkane chain. Sufficiently long alkane segments form structures resembling orthorhombic polyethylene crystals, while the functional groups form 2-D layers that disrupt the alkane crystal structure to varying degrees. Here, layered morphologies in precise copolymers containing acrylic acid, phosphonic acid, imidazolium bromide, and sulfone groups are studied via X-ray scattering. Specifically, the composition profiles of the layered structures are obtained by Fourier synthesis, and the coherence length is investigated using peak width analysis. This analysis indicates that the layers of functional groups are frequently bordered by two crystallites, which suggests different dynamics relative to layers bordered by one crystalline and one amorphous microdomain. Detailed understanding of the structure of the layered morphologies will allow for a systematic investigation of proton and ion conductivity mechanisms, which are expected to occur through the high-dielectric layers.

P1.00156 Polymer Crystals Formed at Liquid-Liquid Interface Show Broken Symmetry . WENDA WANG, HAO QI, ZIYIN HUANG, CHRISTOPHER Y. LI, Drexel University, SOFT MATTER RESEARCH GROUP TEAM — Curved space is incommensurate with typical ordered structures with three-dimensional translational symmetry. However, upon assembly, soft matter, including colloids, amphiphiles, and block copolymers, often form structures depicting curved surface/interface. On the other hand, twisted and curved crystals are often observed in crystalline polymers. Various mechanisms have been proposed for these non-flat crystalline morphologies. In this presentation, we will discuss the recent development of crystallization at flat and curved liquid/liquid (L/L) interface. We show that structure, morphology and chain folding behaviors are strongly affected by L/L interfacial energy and polymer chain ends. Both polyethylene and poly-L-lactic acid single crystal shells have been obtained using curved L/L interface. Polymer crystallization behavior at L/L interface will be compared with solution and bulk crystallization.

P1.00157 POLYMERIC ELASTOMERS AND GELS —

P1.00158 Correlating solubility parameters and solvatochromic parameters with the self-assembly of poly(3-hexylthiophene) in mixtures of organic solvents , MADELEINE GORDON, DAVID BOUCHER, College of Charleston — We have studied the assembly and crystallinity of poly(3-hexylthiophene) (P3HT) (M_w ≈ 28.2 kDa, regioregularity > 96%, PDI ≈ 1.3) in >100 binary solvent mixtures using UV-Vis absorption spectroscopy, and it is clear that the identity of the poor solvent used to drive aggregation has a significant impact on the structural order and crystallinity of the P3HT aggregates in solution. Here we report our findings using Hansen solubility parameters (HSPs), specifically the solubility distance vector, R_1, and the Kamlet-Taft solvatochromic parameters of the solvent mixtures to better understand the dominant solvent forces driving the self assembly of P3HT. We find that the directionality of the R_1 vector provides a better measure of the crystallinity of the P3HT assemblies formed in the solvent mixtures than does the magnitude of the R_1 vector. Our analysis of the Kamlet-Taft (α, β, π*) and E(30) solvatochromatic parameters reveals that the β parameter correlates best with the crystallinity of P3HT and that, in general, assemblies having higher structural order are formed in solvent mixtures with lower values of β.

P1.00159 Demixing transition and molecular interactions in Poly(N-isopropyl acrylamide) solutions compared to its monomer , MORITZ FUTSCHER, MARTINE PHILIPP, PETER MUELLER-BUSCHBAUM, Technical University Munich, ALFONS SCHULTE, University of Central Florida — Temperature-sensitive hydrogels such as poly(N-isopropyl acrylamide) (PNIPAM) exhibit a coil to globule transition of the polymer chains with a lower critical solution temperature (LCST) near 305 K. The cooperative dehydration of bound water molecules upon heating plays a significant role. The hydrogen bonding with the amide groups in the side chains has to be contrasted with the hydration interaction of the hydrophobic main chain hydro-carbons. Employing FTIR spectroscopy we probe molecular changes in the various chemical groups. PNIPAM and its monomer NIPAM are investigated at a concentration of 20% in aqueous solution. We observe a nearly discontinuous shift of the peak frequencies and the intensities of vibrational bands (amides, CH) in PNIPAM, whereas in NIPAM there is a continuous linear shift with temperature. The results are discussed with respect to hydration changes in the amide group and cooperative interactions with bound water along the backbone chain.

P1.00160 Pressure and temperature response of Poly(N-isopropyl acrylamide) in aqueous solution probed with Raman microscopy , COLEMAN CARIKER, ALFONS SCHULTE, University of Central Florida — Poly(N-isopropylacrylamide) (PNIPAM) is a thermo-responsive hydrogel that exists in a hydrated state beneath its lower critical solution temperature (LCST) near 305 K. Above this temperature water is expelled by the polymer as it undergoes a coil to globule collapse. High pressure is an important variable as it influences the strength of hydrogen bonding and can destabilize hydrophobic contacts. We present results from optical imaging on a micron scale and Raman spectroscopic measurements as a function of temperature (295 - 315 K) and hydrostatic pressure (0.1 - 400 MPa). Samples consisted of 25% PNIPAM in aqueous solution in micro-capillaries with 100 micron cross section. Our experiments reveal differences in the spatial evolution of the phase change across the temperature and pressure transitions. These are corroborated by bond specific and hydration changes observed in the Raman spectra.

P1.00161 POLYMER MELTS AND SOLUTIONS —

P1.00162 ABSTRACT WITHDRAWN

P1.00163 Systematic Investigation of the Mechanical and Surface Properties of Poly(dimethylsiloxane) Networks , MATTHEW MELILLO, ZOE KLEIN, EDWIN WALKER, JAN GENZER, North Carolina State Univ — Poly(dimethylsiloxane) (PDMS) is one of the most common elastomers. Its applications range broadly from medical devices to absorbents for water treatment, and recently it has seen rapid growth in the use of microfluidic devices. Despite extensive research and characterization of PDMS networks, the static water contact angles of these elastomers reported in the literature range broadly from a low near 90 degrees upwards to greater than 120 degrees. To investigate this large gap in reported surface properties, we have systematically studied the effects of polymer molecular weight, degree of tetra-functional crosslinker loading, end-group chemical functionality, and the extent of dilution of the curing mixture on the mechanical and surface properties of end-linked PDMS networks. The gel and sol fractions, mechanical properties, and water contact angles have been shown to vary greatly based on the aforementioned variables. This study provides insight to the factors that contribute to such a wide range of surface properties reported in the literature. Furthermore, these results demonstrate the need to fully and carefully consider the manner and environment in which PDMS networks are formed when preparing them for specific applications.
P1.00164 Effect of system compliance and indenter geometry on puncture mechanics of soft materials, SHRUTI RATTAN, SAMI FAKHOURI, ALFRED CROSBY, Univ of Mass - Amherst — Puncture mechanics in soft materials is critical for the development of new surgical instruments as well as new materials used in personal protective equipment. However, fundamental knowledge of how geometry and material properties control the nucleation of a crack, i.e., puncture, at large deformations in a soft material is currently limited. We describe a simple experimental method to study the resistive forces and failure of a soft gel being indented and punctured with a small needle. We show that puncture stresses can reach two orders of magnitude greater than the material modulus and that the force-deformation response is insensitive to the geometry of indenter at large indentation depths. We determine a transition between stress-limited and energy-limited failure modes, which is governed by the indenter size and the balance between fracture energy and cohesive stress. In addition, we examine the influence of system compliance on puncture of soft gels. It is well-known that system compliance influences the peak force in adhesion and traditional fracture experiments; however, its effect on crack nucleation is unresolved. We find that as the system becomes more compliant lower peak puncture forces were measured, which is associated with increased energy available for fracture.

P1.00165 Rheology of Poly(V-isopropylacrylamide)-Clay Nanocomposite Hydrogels, JACK LOM-BARDI, DI XU, DIVYA BHATNAGAR, DILIP GERSAPPE, JONATHAN SOKOLOV, MIRIAM RAFAILOVICH, Materials Science and Engineering Department, Stony Brook University, Stony Brook, NY 11790, USA — The stiffness of PNIPA Gels has been reported could be significant improved by gelation with clay fillers. Here we conducted systematic rheology study of synthesized PNIPA-Clay Composites at different clay concentration, in a range from fluid to strong gel, where G”’ dominant changed to G’ dominant. Molecular dynamics simulation was employed to analyze the structure of composites and corresponding mechanical changes with increased clays. Where we found viscoelastic behavior become significant only 1.5 times above percolation threshold. The yield stress extrapolated from our rheology results shows good fitting to modified Mooney’s theory of suspension viscosity.

P1.00166 Self-Assembly and Relaxation Behavior of Graphene Containing Acrylic Triblock Copolymer Gels, MAHLA ZABEL, SEYEDMEYSAM HASEMNEJAD, SANTANU KUNDU, Dave C. Swalm School of Chemical Engineering, Mississippi State University, MS State, MS — Investigation of gel mechanical properties as a function of their structure is a significant research interest. This study presents the effect of graphene (or few-layer graphene) on the self-assembly and the relaxation behavior of a thermoreversible gel consists of a physically cross-linked poly (methyl methacrylate)-poly (n-buty lacrylate)-poly (methyl methacrylate) [PMMA-PnBA-PMMA] triblock copolymer in 2-ethyl-1-hexanol, a midblock selective solvent. Graphene was obtained by sonicating exfoliated graphite in 2-ethyl-1-hexanol at various concentrations. Filtration technique and spectrophotometry were utilized to measure the graphene concentration in the dispersions. The dispersed graphene was then incorporated in a series of gels and the effect of graphene on mechanical properties, including the relaxation behavior were studied. Small angle X-ray scattering (SAXS) was used to investigate the microstructure of these gels at room temperature. SAXS data were analyzed to estimate the number of end blocks per junction zone, the average spacing between the junctions, and the change of these properties as a function of graphene concentration. The results indicate that the presence of graphene affects the self-assembly process.

P1.00167 POLYMER BLENDS —

P1.00168 Bottlebrush additives drive formation of vesicle chains in polymer blends, HUI ZHEN MAH, PANTEA AZFALI, Univ of Houston, RAFAEL VERDÚZCO, Rice University, GILA STEIN, Univ of Houston — The effects of bottlebrush polymer additives with polystyrene (PS) and poly (methyl methacrylate) (PMMA) blends were studied. Results were compared to PS/PMMA blends with diblock copolymer PS-b-PMMA compatibilizer and without any additive. Thin films were spin casted from toluene onto a “neutral” silicon surface and then annealed at a fixed temperature of 150°C for a range of times (up to 85 mins). The morphology of the films was characterized using optical microscopy and atomic force microscopy. In the absence of any additive, the PS/PMMA blend rapidly de-mixes to form macroscale domains, while high loadings of the PS-b-PMMA additive can compatibilize the blend and suppress phase separation. However, the bottlebrush polymer additive drives the formation of well-organized vesicle chains in the PS/PMMA blend films. This morphology is favored by entropic considerations as the bottlebrush polymers are more stable than linear chains at the PS/PMMA interface and the brush like surface attracts.

P1.00169 Phase Equilibria in Ternary Blends of Two Linear Homopolymers and A Ring Gradient Copolymer, DACHUAN SUN, JUNHAN CHO, Dankook Univ — Phase equilibria in a ternary blend of linear A/B homopolymers of equal sizes and a symmetric A-co-B ring gradient copolymer as an amphiphile with α as the ratio of their chain sizes are investigated in the mean-field picture. The monomer sequence on the copolymer chain is taken as either a step gradient or a fully linear gradient, to which a gradient number λ = 0 or 1 is assigned, respectively. Along the isopleth of equal homopolymer amounts, the resultant phase diagrams for the blends are to be built from multicritical points such as Lifshitz or bulk tricritical point depending on α and λ. The stabilization of lamellar mesophase or its equilibrium with A and B-rich bulk phases is accordingly controllable by the pair of α and λ.

This work was supported by the Basic Science Research Program (No. 2014023297) from National Research Foundation of Korea. The authors also acknowledge the support from the Center for Photofunctional Energy Materials, which is funded by Gyeonggi Regional Research Center Program (GRRCDankook2011-B01).

P1.00170 ABSTRACT WITHDRAWN —

P1.00171 COPOLYMERS —

P1.00172 Characteristic Phase Behaviors for Symmetric PS-b-PAMAs (n= 176) and Their Pressure Dependence, YONGHOON LEE, HOYEON LEE, Yonsei University, DONG HYUN LEE, Dankook University, DU YEOL RYU, Yonsei University, YONSEI UNIVERSITY COLLABORATION, DANKOOK UNIVERSITY COLLABORATION — A series of polystyrene-b-poly(alkyl methacrylates) (PS-b-PAMAs) that pertain to the weakly interacting BCP homologues exhibited a variety of phase behaviors by varying alkyl chain length (n) in methacrylate unit. The enthalpic and volumetric changes at phase transitions were measured by the differential scanning calorimetry (DSC) and in-situ spectroscopic ellipsometry with increasing pressure. Together with the overview on the characteristic phase behaviors for symmetric PS-b-PAMAs (n = 1 ? 6), the pressure coefficient (dT/dP) of transition temperatures was calculated on the basis of the Clauseius-Clapeyron equation and compared with the reference values. The strong baroplastic character of the closed-loop transitions could be attributed to the significant negative volume changes on mixing at both phase transitions.
P1.00173 Orienting Nanostructured Block Copolymer Thin Films via Entropy, TING-YA LO, Department of Chemical Engineering, National Tsing Hua University, ASHKAN DEHGHAH, Department of Physics and Astronomy, McMaster University, PROKOPIOS GEORGOPANOS, APOSTOLOS AVGEROPoulos, Department of Materials Science & Engineering, University of Ioannina, AN-CHANG SHI, Department of Physics and Astronomy, McMaster University, RONG-MING HO, Department of Chemical Engineering, National Tsing Hua University — Controlling the orientation of nanostructured thin films of block copolymers (BCPs) is essential for next generation lithography using BCPs. According to conventional wisdom, the orientation of BCPs is mainly determined by molecular interactions (enthalpy-driven orientation). Here, we demonstrate that entropic effect can also control the orientation of BCP thin films. Specifically, the architecture of star-block copolymers consisting polystyrene (PS) and poly(dimethylsiloxane) (PDMS) blocks is used to regulate the entropic contribution to the self-assembled nanostructures. Our experimental and theoretical results unequivocally demonstrate that entropy-driven perpendicular orientation of BCP nanostructures can be induced by increasing the arm number of the star-block copolymers with the same volume fractions of PS and PDMS.

P1.00174 A Facile Method to Fabricate Double Gyroid as A Polymer Template for Nanohybrids, HISIAO-FANG WANG, RONG-MING HO, Department of Chemical Engineering, National Tsing Hua University — Here, we suggest a facile method to acquire double gyroid (DG) phase from the self-assembly of chiral block copolymers (BCPs*), polystyrene-b-poly(L-lactide) (PS-PDLLA). A wide region for the formation of DG can be found in the phase diagram of the BCPs*, suggesting that helical phase (H*) from the self-assembly of BCPs* can serve as a stepping stone for the formation of the DG due to an easy path for order-order transition from two-dimensional to three-dimensional (network) structure. Moreover, the order-order transition from metastable H* to stable DG can be expedited by blending the PS-PDLLA with compatible entity. Moreover, PS-PDLLA blends are prepared by using styrene oligomer (S) to fine-tune the morphologies of the blends at which the molecular weight ratio of the S and compatible PS block (r) is less than 0.1. Owing to the use of the low-molecular-weight oligomer, the increase of BCP chain mobility in the blends significantly reduces the transformation time for the order-order transition from H* to DG. Consequently, nanoporous gyroid SiO2 can be fabricated using hydrolyzed PS-PDLLA blends as a template for sol-gel reaction followed by removal of the PS matrix.

P1.00175 Selective Permeating Properties of Butanol and Water through Polystyrene-b-polydimethylsiloxilane-b-polystyrene Pervaporation Membranes, CHAEYOUNG SHIN, ZACHARY BAER, X. CHELSEA CHEN, A. EVREN OZCAM, DOUGLAS CLARK, NITASH BALSARA, University of California, Berkeley — Polystyrene-b-polydimethylsiloxane-b-polystyrene (SDS) membranes have been studied in butanol-water binary pervaporation experiments and pervaporation experiments integrated with viable fermentation broth. Polydimethylsiloxane has been widely known to be a particular material for separating organic chemicals from aqueous solutions, and it thus provides a continuous matrix phase in SDS membranes for permeation of small molecules. The polystyrene block provides mechanical stability to maintain the membrane structure in the pervaporation membranes. We take advantage of these features to fabricate a thin and butanol-selective SDS membrane for in situ product removal in fermentation.

P1.00176 Effect of Asymmetric Confinement on the Microdomain Morphology of Block Copolymers, YOUNGKEOL KIM, Seoul Natl Univ, GUIDUK YU, Samsung Electro-Mechanics, KOOKHEON CHAR, Seoul Natl Univ — Nanometer scale confinement could impose constraints to change the bulk equilibrium behavior of block copolymers (BCPs). The self-assembly of BCPs confined by two parallel surfaces (one-dimensional confinement) has been both theoretically and experimentally studied. More recently, cylindrical pores where the diameter of the pores are only several repeat periods of the copolymers have been employed to investigate the influence of two-dimensional confinement on the behavior of BCPs. However, the analysis on confinement by asymmetric geometry has not been thoroughly studied yet. Given the size of confining channels, singularity arising from the asymmetric geometry such as triangles and squares, could have a significant effect on the structure and symmetry of BCP morphologies self-assembled within such confinement. We prepared AAOs with triangular pores based on aluminum substrates with inverse-hexagonal packing pattern. Based on the detailed observation of BCP self-assembly within porous triangular columns, we analyzed the structural transition of BCPs induced by asymmetric confinement. Furthermore, we found that the packing frustration imposed by such confinement could be released by adding homopolymers into the BCP system.

P1.00177 Synthesis of zwitterionic polymer-based amphiphilic triblock copolymers by atom transfer radical polymerization for production of extremely stable nanoemulsions, JIN YONG LEE, JI EUN KIM, JIN WOONG KIM, Hanyang Univ — In fields of soft matter, there have been growing interests in utilizing amphiphilic block copolymers due to their intriguing properties, such as surface activity as well as self-assembly. In this work, we synthesize a series of poly (2-(methacryloyloxy)ethyl phosphorylcholine)-b-poly (ε-caprolactone)-b-poly (2-(methacyryloyloxy)ethyl phosphorylcholine) (PMPC-b-PCL-b-PMPC) triblock copolymers by using atom transfer radical polymerization (ATRP). A particular interest is in using poly (2-(methacryloyloxy)ethyl phosphorylcholine) (PMPC) as a hydrophilic block, since it can have both electrostatic repulsion and steric repulsion in complex fluid systems. Assembling them at the oil-water interface by using the phase inversion method enables production of highly stable nanoemulsions. From the analyses of the crystallography and self-assembly behavior, we have found that the triblock copolymers assemble to form a flexible but tough molecular thin film at the interface, which is essential for the remarkable improvement in the emulsion stability.

P1.00178 Ab initio molecular dynamics simulations of the thermal degradation of model compounds of industrially-relevant copolyesters, EROL YILDIRIM, Fiber and Polymer Science Program, North Carolina State University, ANDREW T. DETWILER, CURT CLEVEN, Eastman Chemical Company, AHMED EL-SHAFEI, MELISSA A. PASQUINELLI, Fiber and Polymer Science Program, North Carolina State University — The thermal degradation of copolyesters can be impacted by a variety of factors beyond the chemical composition of the polymer, including the solvent and processing conditions, as well as the presence of oxygen, moisture, additives, and dyes. Thus, we investigated the role that these factors play for a series of model compounds of industrially relevant copolyesters using ab initio molecular dynamics simulations. Some recent development of in-situ soft x-ray scattering with in-vacuum sample environment will be discussed. In order to study sciences in naturally occurring conditions, we need to overcome the sample limitations by using low penetration depth of soft x-rays and requirement of high vacuum. Adapting to the evolving environmental cell designs utilized increasingly in the Electron Microscopy community, customized designed liquid/gas environmental cells will enable soft x-ray scattering experiments on biological, electro-chemical, self-assembly, and hierarchical functional systems in both static and dynamic fashion. Recent RSoXS results on organic electronics, block copolymer thin films, and membrane structure will be presented.

P1.00180 CHARGED AND ION-CONTAINING POLYMERS —
we found distinctly dissimilar domain sizes at the same molecular weight and composition. A range of ionic liquids (ILs) were incorporated into the PSP-
and hexagonally packed cylindrical phases, were observed with PL. Remarkably, upon comparing the morphology of PSP-
owing to their self-dissociation ability. In this study, we have synthesized a set of phosphonated block copolymers, poly(styrenephosphonate-methylbutylene)
temperature operation has discouraged their practical uses in fuel cells. In this respect, phosphonated polymers have drawn intensive attention in recent years
device efficiency. While the sulfonic acid group guarantees high proton conductivity of membranes under humidified conditions, the growing need for high
transition when assembled in the presence of sodium chloride. The question remains as to how multivalent cations affect the nature of the transition. Here,
hydrates LbL assemblies made of model polyelectrolytes, poly(diallyldimethylammonium chloride) (PDAC) and poly(styrene sulfonate) (PSS), exhibit a thermal transition with features of a glass transition and a lower critical solution temperature transition when assembled in the presence of sodium chloride. The question remains as to how multivalent cations affect the nature of the transition. Here,
we present results on the thermal transition of PDAC/PSS LbL assemblies exposed to various multivalent salts. Quartz crystal microbalance (QCM-D) and
modulated differential scanning calorimetry (MDSC) is used to assess the transition.

The effect of multivalent ions on the thermal transition of hydrated polyelectrolyte multilayers, DARIYA REID, JODIE LUTKENHAUS, Texas A&M University, Department of Chemical Engineering — Layer-by-layer (LbL) assembly is a commonly studied technique in the production of uniform thin films. Hydrate LbL assemblies made of model polyelectrolytes, poly(diallyldimethylammonium chloride) (PDAC) and poly(styrenephosphonate-methylbutylene) (PSP−-PMB), by varying phosphorylation level (PL). A wide variety of self-assembled morphologies, i.e., disordered, lamellar, hexagonally perforated lamellae and hexagonally packed cylindrical phases, were observed with PL. Remarkably, upon comparing the morphology of PSP−-PMB and that of sulfonated analog, we found distinctly disimilar domain sizes at the same molecular weight and composition. A range of ionic liquids (ILs) were incorporated into the PSP−-PMB block copolymers and their ion transport properties were examined. It has been revealed that the degree of confinement of ionic phases (domain size) impacts the ion mobility and proton dissociation efficiency of IL-containing polymers.

Molecular Dynamics of Coarse-grained Ionomers Containing Ionic Liquids , HA YOUNG JUNG, SUNG YEON KIM, MOON JEONG PARK, Pohang Univ of Sci & Tech — As the focus on proton exchange fuel cells continues to escalate in the era of alternative energy systems, the rational design of sulfonated polymers has emerged as a key technique for enhancing device efficiency. While the sulfonic acid group guarantees high proton conductivity of membranes under humidified conditions, the growing need for high

Effect of multivalent ions on the thermal transition of hydrated polyelectrolyte multilayers, DARIYA REID, JODIE LUTKENHAUS, Texas A&M University, Department of Chemical Engineering — Layer-by-layer (LbL) assembly is a commonly studied technique in the production of uniform thin films. Hydrate LbL assemblies made of model polyelectrolytes, poly(diallyldimethylammonium chloride) (PDAC) and poly(styrenephosphonate-methylbutylene) (PSP−-PMB), by varying phosphorylation level (PL). A wide variety of self-assembled morphologies, i.e., disordered, lamellar, hexagonally perforated lamellae and hexagonally packed cylindrical phases, were observed with PL. Remarkably, upon comparing the morphology of PSP−-PMB and that of sulfonated analog, we found distinctly disimilar domain sizes at the same molecular weight and composition. A range of ionic liquids (ILs) were incorporated into the PSP−-PMB block copolymers and their ion transport properties were examined. It has been revealed that the degree of confinement of ionic phases (domain size) impacts the ion mobility and proton dissociation efficiency of IL-containing polymers.

Effects of Acid and Ionic Aggregation on the Polymer Dynamics in Precise Ionomers1, LURI ROBERT MIDDLETON, University of Pennsylvania, JACOB TARVER, National Institute of Standards and Technology, JASON AZOULAY, DUSTIN MURTAGH, Sandia National Laboratory, KEN WAGENER, University of Florida, CHRISTOPHER SOLES, National Institute of Standards and Technology, KAREN WINERY, University of Pennsylvania — Interest in acid- and ion-containing polymers arises from applications as single-ion conductors for selectively transporting a counter ion of the opposite charge for energy applications. The relatively low dielectric constant of the organic polymer and strong ionic interactions leads to ionic aggregation. Ion aggregation anchors the polymer chain, decreasing the mobility of the ion and the polymer. In precise poly(ethylene-acrylic acid) copolymers and ionomers (pAAC-%IL) we report on the effect of carbon spacer length (x=9, 15, 21) between the acid groups and the effect of the percent of acid groups neutralized with Li on backbone dynamics. The polymer backbone motion is investigated through quasi-elastic neutron scattering measurements. At nano-second timescales a single relaxation fits the data. Systematic changes in dynamics were observed with increasing neutralization percent where polymer dynamics are confined due to anchoring effects. Intriguingly, systematic changes in the spacer lengths did not result in similar behavior. At pico-second timescales multiple overlapping relaxations are observed but even at these short timescales systematic changes in atomic motion are observed with ion content.

Structure and Proton Conductivity in Mixtures of Poly(acrylic acid) and Imidazole, HAN-CHANG YANG, PHILIP J. GRIFFIN, KAREN I. WINERY, University of Pennsylvania, UNIVERSITY OF PENNSYLVANIA TEAM — Proton conductivity in polymer electrolyte membranes (PEMs) typically involves water, which requires that during operation the humidity of the PEM be carefully controlled. In contrast, anhydrous protic polymer membranes promote proton transport by incorporating heterocyclic molecules, such as imidazole and its derivatives, into acid-containing polymers. In this work, we explore the interplay between nanoscale-structure and proton conduction of poly(acrylic acid) (PAA) blended at varying compositions with 2-ethyl-4-methylimidazole (EMI). We present the glass transition temperature from differential scanning calorimetry, morphology characterization from X-ray scattering, and proton conduction from electrical impedance spectroscopy.

pH-Responsive Behavior of Poly(acrylic acid) Brushes of Varying Thickness, VIVEK YADAV, MEGAN ROBERTSON, JACINTA CONRAD, Univ of Houston — We have investigated the pH-dependent response of polyelectrolyte brushes of varying thickness. Our model system consists of poly(acrylic acid) brushes, which change from hydrophobic and neutral at low pH to hydrophilic and negatively charged at high pH, by varying phosphorylation level (PL). A wide variety of self-assembled morphologies, i.e., disordered, lamellar, hexagonally perforated lamellae and hexagonally packed cylindrical phases, were observed with PL. Remarkably, upon comparing the morphology of PSP−-PMB and that of sulfonated analog, we found distinctly disimilar domain sizes at the same molecular weight and composition. A range of ionic liquids (ILs) were incorporated into the PSP−-PMB block copolymers and their ion transport properties were examined. It has been revealed that the degree of confinement of ionic phases (domain size) impacts the ion mobility and proton dissociation efficiency of IL-containing polymers.
P1.00188 Influence of Hydration Level on Polymer and Water Dynamics in Alkaline Anion Exchange Fuel Cell Membranes. JACOB TARVER, JENNY KIM, MADHU TYAGI, CHRISTOPHER SOLES, National Institute of Standards and Technology, TSUNG-HAN TSAI, BRYAN COUGHLIN, University of Massachusetts - Amherst — Triblock copolymers based on poly(chloromethylstyrene)-b-poly(ethylene)-b-poly(chloromethylstyrene) can be quaternized to different extents to yield anion exchange membranes for alkaline fuel cells. In the absence of moisture, these membranes demonstrate bilayer lamellar morphology. Upon high levels of hydration, however, in-situ small angle neutron scattering reveals the emergence of higher-order diffraction peaks. This phenomena has previously been observed in analogous diblock copolymer-based membranes and has been attributed to the induction of a multilamellar lamellar morphology in which selective striping of water occurs in the center of the ion-rich domain. By conducting humidity-resolved quasielastic neutron scattering (QENS) measurements using deuterated water, we are able to isolate differences in the pico- to nanosecond timescale dynamics of the hydrogenated membrane upon hydration. QENS measurements in the presence of a hydrogenated water source subsequently permit deconvolution and isolation of the translational and rotational dynamics of water as a function of relative humidity, revealing spatial and temporal changes in polymer and water motion at high levels of hydration.

P1.00189 Understanding the impact of nanoscale aggregation on charge transport and structural dynamics in room temperature ionic liquids. PHILIP GRIFFIN, University of Pennsylvania, ADAM HOLT, University of Tennessee, YANGYANG WANG, Oak Ridge National Lab, ALEXEI SOKOLOV, University of Tennessee — Amphiphilic room temperature ionic liquids (ILs) segregate on the nanoscale, forming intricate networks of charge-rich ionic domains intercalated with charge-poor aliphatic domains. While this structural phenomenon has been well established through x-ray diffraction studies and atomistic MD simulations, the precise effects of nanophase segregation on ion transport and structural dynamics in ILs remains poorly understood. Using a combination of broadband dielectric spectroscopy, light scattering spectroscopy, and rheology, we have characterized the ionic conductivity, structural dynamics, and shear viscosity of a homologous series of quaternary ammonium ionic liquids over a wide temperature range. Upon increasing the length and volume fraction of the alkyl side chains of these quaternary ammonium ILs, ionic conductivity decreases precipitously, although no corresponding slowing of the structural dynamics is observed. Instead, we identify the dynamical signature of supramolecular aggregates. Our results directly demonstrate the role that chemical structure and ionic aggregation plays in determining the charge transport properties of amphiphilic ILs.

P1.00190 Spray-assisted layer-by-Layer (Lbl) assembly of anisotropic materials. SOUVIK DE, PILAR SUAREZ MARTINEZ, AVANTI KAVARTHAPU, JODIE LUTKENHAUS, Department of Chemical Engineering at Texas A&M University — Layer-by-Layer (Lbl) assembly has gained tremendous interest as it allows one to incorporate a large variety of molecules with nano-scale precision and very good reproducibility. In addition to charged polymers, the technique has become extremely popular to fabricate tailor-made thin films containing anisotropic nanomaterials (e.g., graphene oxide sheets). The challenge is that a standard protocol to fabricate “all-polyelectrolyte” Lbl films may not necessarily give rise to satisfactory film growth when applied to Lbl assembly where one of the adsorbing components is an anisotropic nanomaterial. Therefore, in this contribution, we combine polymers and anisotropic nanomaterials via dip- and spray-assisted Lbl assembly and investigate the effect of charge density, exfoliation, concentration etc. of the components on the growth behavior and the film quality. The end result is a conformal, pin-hole free coating on model substrates (glass, silicon, metal) over a large area.

P1.00191 Morphology and charge transport in ammonium based polymerized ionic liquids. MAXIMILIAN HERES, JOSÉPH MINUTOLO, JACOB SHAMBLIN, MAIK LONG, Univ of Tennessee, Knoxville, STEFAN BERDZINSKI, VERONIKA STREML, Department of Chemistry and Institute for Coatings and Surface Chemistry, Hochschule Niederrhein University of Applied Sciences, Krefeld, Germany, JOSHUA SANGORO, Univ of Tennessee, Knoxville — Ionic conduction, structural dynamics and morphology in a series of ammonium based polymers and anisotropics are investigated using broadband dielectric spectroscopy, temperature-modulated differential scanning calorimetry, and neutron as well as x-ray scattering techniques. The dielectric spectra are dominated on the low frequency regime by electrode polarization while hopping conduction is the underlying mechanism at higher frequencies. At their respective calorimetric glass transition temperatures, a strong correlation between the morphology and ionic conductivity is found. These results are discussed within the recent approaches proposed to explain the decoupling of charge transport from structural dynamics.

P1.00192 Effect of Supercharging on Coacervation Between Proteins and Polyelectrolytes. BRADLEY OLSEN, ALLIE OBERMEYER, CAROLYN MILLS, XUEHUI DONG, MIT — Complex coacervates have attracted a great deal of attention as a method to encapsulate biological molecules including DNA and proteins. However, a large fraction of proteins will not form coacervates with oppositely charged polymers unless their surface charge density is increased through a process known as supercharging. Using mass spectrometry, we are able to quantify the formal charge distribution of proteins after supercharging, and with this knowledge of the chemical state of the protein measure coacervate formation for a panel of proteins as a function of charge. While many of the proteins studied do not form coacervates or coacervate over only a narrow range of composition in their native form, all proteins form coacervates above a critical charge level with increasing range of composition as charge density increases. The resulting data is consistent with a strong induced charging effect in the coacervate state, as the largest coacervates form near a charge ratio corresponding to proteins at their maximum charge. These observations in bulk coacervation are translated to the design of coacervate core micelles, providing an increased quantitative description.
Spray Deposition of Multilayer Gas Barrier Thin Films, TARA GIVENS, FANGMING XIANG, JAIME GRUNILAN, Texas A&M Univ — Dip-assisted assembly is the norm for making multilayer thin films (also known as layer-by-layer [LbL] assembly). Spray-based deposition possesses several advantages over dipping, but has not been studied in great detail, especially for gas barrier layers. In this study, polyethyleneimine [PEI]/poly(acrylic acid) [PAA] bilayers were deposited with varying spray parameters. Spraying time was found to be the most influential parameter to control the roughness, thickness, and gas barrier of the PEI/PAA assembly. A spray-coated sample was prepared using optimized parameters and compared to a dip-coated sample using the same deposition time (5s). The sprayed sample was better in terms of thickness, roughness, and gas barrier. This study is the first report showing that a sprayed multilayer assembly has better properties than its dipped counterpart. These findings could revolutionize the multilayer deposition process, making it more commercially-friendly.

Inexpensive Fabrication of Metallic Interconnects on Flexible Substrates, ADITI NAIK, ROHIT KOTHARI, JAMES WATKINS, University of Massachusetts - Amherst — Sub-micron metallic interconnects on flexible substrates are important to produce inexpensive bendable devices and electronics. The key component hindering high-performance flexible electronics is the lack of high transistor integration density. Previous researchers have created solution-processable semiconductor and dielectric layers; however, sub-micron solution-processable copper electrodes have yet to be developed. Using cost-effective processing techniques, including soft nanolithography and photonic sintering, with a commercial copper oxide ink, we have demonstrated the fabrication of sub-micron copper interconnects on glass and plastic substrates. This inexpensive, solution-processable method is amenable to high-speed printing over large areas by roll-to-roll processing and will lead to the development of low-cost flexible electronics.

A Molecular Perspective of Inter-filament Bonding in Fused Deposition Modeling 3-D Printing, EDWARD DURANTY, BRANDON SPRADLIN, MARK DADMUN, University of Tennessee — Fused deposition 3D printing is an important tool for low-cost and rapid prototyping of objects with complex geometries. 3D printed materials are composed of many filaments deposited on a heated substrate, requiring the bonding of neighboring filaments during the deposition process. Filament deposition often creates voids between filaments, which requires necking between them to create a robust sample. Therefore the amount of interfacial contact and interdiffusion between filaments become important parameters that control the macroscopic physical properties of the printed prototype. Our research focuses on quantifying the interfacial adhesion between ABS filaments and its impact on structural properties. The time evolution of the temperature profile near the heated substrate demonstrates that the deposited filaments are repeatedly heated above the Tg of ABS allowing interpenetration of the polymer chains between adjacent filaments. Results of DMA experiments on samples of different geometries have been correlated to microphotography that monitors the degree of necking between filaments and the thermal history. Results indicate that interfacial contact area between filaments and increased thermal energy are crucial to their mechanical properties.

THEORY AND SIMULATION OF MACROMOLECULES

Contrasting Polymer Behavior Under Nanoconfinement using Thermomechanically Consistent Coarse-Grained Models, SINAN KETEN, WENJIE XIA, DAVID HSU, Northwestern University — We present a systematic, two-bead per monomer coarse graining strategy that simulates the thermomechanical behavior of polymers several hundred times faster than all-atom MD (Hsu et al. JCTC, 2014). The predictive capability of the technique is illustrated here for 5 different methacrylate monomers and polystyrene stereoisomers. The approach involves optimization of analytical bonded potentials from atomistic bonded distributions to emulate local structure, as validated by chain end-to-end length and the radius of gyration comparisons with experiments and random coil theory. Nonbonded Lennard-Jones potentials are tuned to reproduce the elastic modulus (E) and glass transition temperature (Tg) at a single thermodynamic state. Density-corrected parameters capture temperature-modulus dependence in the 150-600 K range. Flory-Fox constants of the CG models are commensurate with all atomistic and experimental results, even though all calibrations are done at a single molecular weight. Finally, we further demonstrate the predictive capabilities of the models by examining thin film nanoconfinement effects for different polymers, film thicknesses, interfacial energies, and molecular weights. Our technique, called thermomechanically consistent coarse graining (TCCG), is demonstrated, using polystyrene and poly(methylmethacrylate) as universal benchmarks, to be a robust and effective technique to understand the thermomechanical behavior of polymers thin films and nanocomposites.

ABSTRACT WITHDRAWN

Coarse-Graining in Simulations of Multicomponent Polymer Systems, SETHURAMAN VAIYANATHAN, VENKAT GANESAN, Department of Chemical Engineering, University of Texas at Austin, Austin, Texas 78712, USA — We investigate the mapping required between the interaction parameters of two different coarse-grained simulation models to ensure a match of the long-range structural characteristics of multicomponent polymeric system. We investigate the extensibility of mapping functions deduced in the context of symmetric block copolymers by Morse and coworkers to other polymeric systems by studying a variety of systems, including, asymmetric diblock copolymers, symmetric triblock copolymers and diblock copolymer-solvent mixtures. We observe excellent agreement for peak in the inverse structure between two popular coarse grained models for all polymer concentrations investigated, thus showing that the mapping function proposed for diblock copolymer melts is transferable to other polymer melts irrespective of the blockiness or overall composition. We use our findings to propose a methodology to create ordered morphologies in simulations involving hard repulsive potentials in a computationally efficient manner.

Structural analysis of liquid crystalline order in polymer melts and blends, KIRAN KHANAL, JUTTA LUETTMEER-STRATHMANN, The University of Akron — Blends of liquid crystalline and flexible polymers have interesting physical behaviors and important applications in organic electronics. We investigate the liquid crystalline transition in melts and blends of semiflexible polymers with Monte Carlo simulations of a bond fluctuation lattice model. For polymer melts we study the influence of attractive interactions on the isotropic to nematic phase transition for different polymer concentrations. We observe that the structure of the ordered phase is different for melts with and without attractive interactions. We construct the phase diagram and find the transition temperature increases with increasing strength of the attractive interaction. To analyze the structure of ordered and disordered regions in polymer melts and blends, we calculate a set of pair distribution functions. We also investigate the effect of an ordering field on the liquid crystalline order in polymer melts and blends.

Size and Shape Descriptors of Two Dimensional Polymer Sheets in Solution near the Crossover Concentration, SALOMON TURGMAN COHEN, JACOBI TANNER, Kettering Univ — We investigate the size and shape of two dimensional polymer sheets near the crossover concentration as a function of sheet size and concentration. Specifically, fully flexible sheets with local square connectivity in implicit, atheletic solvent are investigated by molecular dynamics simulations in the NVT ensemble with a Langevin thermostat. Sheet sizes of $N = 100, 400$, and $1600$ are explored. We monitor the average radius of gyration ($R_g$) tensor and the relative shape anisotropy around the cross-over concentration. Opposite to linear, one dimensional polymers, preliminary results show that the size of the sheets as measured by the average radius of gyration increases as the cross-over concentration is approached. The trends in the relative shape anisotropy suggest that the increasing overlap between the sheets at high concentrations leads to the sheets favoring flatter conformations, explaining the larger values of $R_g$ observed.
P1.00205 The effect of copolymers on the interfaces in incompatible homopolymers blend: Molecular dynamics study

JIHO RYU, WON BO LEE, Sogang Univ — Using molecular dynamics simulations the effect of copolymers as compatibilizer for reducing interfacial tension and enhancement of interfacial adhesion at the interface of thermodynamic unfavorable homopolymers blend is studied with block- and graft-copolymers. We have calculated local pressure tensor of system along the axis perpendicular to interface, varying bending potential energy of one part, which consist of just one kind of beads, of copolymer chain to examine the effect of stiffness of surfactin molecules. Here we consider symmetric diblock copolymer (f=1/2) having 1/2 N make of beads of type A and the other part made of beads of type B, and graft copolymer having backbone linear chain consist of 1/2 N beads of type A and branched with two side-chain consist of 1/4 N beads of type B. All simulations were performed under the constant NPT ensemble at T*. Also we studied changes of effect of copolymers with increasing pairwise repulsive interaction potential between two beads of types A and B while homopolymers chain length are fixed, N=30.

\[ P = \frac{\Delta F}{\Delta V} \]

\[ \Delta G = \Delta H - T \Delta S \]

\[ \Delta H = \sum \Delta H_i \]

\[ \Delta S = \sum \Delta S_i \]

\[ V = \sum V_i \]

\[ P = \frac{\Delta F}{\Delta V} = \frac{\Delta G}{\Delta V} = \frac{\Delta H}{\Delta V} - T \frac{\Delta S}{\Delta V} \]

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P1.00206 Monte Carlo Simulations on Phase Transitions and Conformational Properties of Catenated Double-ring Copolymers

DACHUAN SUN, JUNHAN CHO, Dankook Univ — The thermodynamic and conformational properties of catenated double-ring A/B copolymer melts are investigated through lattice Monte Carlo simulations. The topological constraint on the catenated copolymers is shown to suppress demixing of A and B monomers. This action results in their order-to-disorder transition (ODT) at an increased segregation level and the lamellae below ODT with reduced order, when compared to diblock copolymers of linear or single-ring topology. The A and B rings are pulled closer by catenation in the copolymer, which leads to its smaller gyration radius, lamellar domain spacing, and distance between mass centers of the two rings than for the diblock copolymers. With increasing segregation tendencies, the gyration radii of the A rings of the catenated copolymers stretch along the direction normal to lamellae, while the A-block conformations of the single-ring copolymers change their shapes from ellipsoid to sphere.

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P1.00207 Using graphs to interrogate the atomic structure of polymer blends

OLGA WODO, State Univ of NY - Buffalo, BASKAR GANAPATHYSUBRAMANIAN, Iowa State University — The nanomorphology of polymer blend thin films critically affects performance especially in electronic devices. However, many aspects of the underlying physics linking morphology to performance are still poorly understood. Furthermore, there is increasing evidence that atomic organization can hold the key to efficient charge transport within organic electronic devices. In this work, we take advantage of recent advances in molecular dynamics simulations and quantify atomic-scale morphological aspects of the thin films. Specifically, we present a graph-based technique that allows quantifying the point-cloud data. In our approach, we first convert the point cloud data from atomic simulation into a labelled, weighted, undirected graph and then use standard graph-based algorithms to calculate and quantify morphology features. The conversion of the CGMD-data into a graph preserves all the topological and geometric information about the internal structure, and local connectivity between individual atoms/atoms/bonds (along and across the polymer chains). Our method provides hierarchical information about the charge paths that a hole/elecbeads needs to take to reach the electrode (path length, fraction of intra-molecular hops, path balance). We showcase capabilities of our approach by analyzing coarse grained molecular simulations, and quantifying effect of various thermal treatment as well as electrode materials on the P3HT:PCBM blend.

P1.00208 An atomistic model for cross-linked HNBR elastomers used in seals

NICOLA MOLINARI, ADRIAN SUTTON, Imperial College London, Department of Physics, London SW7 2AZ, UK, JOHN STEVENS, Baker Hughes, Materials Centre of Excellence, Houston, Texas 77019-2118, USA, ARASH MOSTOFI, Imperial College London, Departments of Materials and Physics, London SW7 2AZ and the Thomas Young Centre for Theory and Simulation of Materials, UK — Hydrogenated nitrile butadiene rubber (HNBR) is one of the most common elastomeric materials used for seals in the oil and gas industry. These seals sometimes suffer “explosive decompression,” a costly problem in which gases permeate a seal at the elevated temperatures and pressures pertaining in oil and gas wells, leading to rupture when the seal is brought back to the surface. The experimental evidence that HNBR and its unsaturated parent, NBR, have markedly different swelling properties suggests that cross-linking may occur during hydrogenation of NBR to produce HNBR. We have developed a code compatible with the LAMMPS molecular dynamics package to generate fully atomistic HNBR configurations by hydrogenating initial NBR structures. This can be done with any desired degree of cross-linking. The code uses a model of atomic interactions based on the OPLS-AA force-field. We present calculations of the dependence of a number of bulk properties on the degree of cross-linking. Using our atomistic representations of HNBR and NBR, we hope to develop a better molecular understanding of the mechanisms that result in explosive decomposition.

P1.00209 Pattern Recognition of Adsorbing HP Lattice Proteins

MARTIN P. LANDAU, Center for Simulational Physics, University of Georgia, THOMAS WUST, Scientific IT Services, ETH Zurich, DAVID P. LANDAU, Center for Simulational Physics, University of Georgia, FRIEDERIKE SCHMID, Institute of Physics, Johannes Gutenberg University — Protein adsorption is relevant in fields ranging from medicine to industry, and the qualitative behavior exhibited by course-grained models could shed insight for further research in such fields. Our study on the selective adsorption of lattice proteins utilizes the Wang-Landau algorithm to simulate the Hydrophobic-Polar (H-P) model with an efficient set of Monte Carlo moves. Each substrate is modeled as a square pattern of 9 lattice sites which attract either H or P monomers, and are located on an otherwise neutral surface. The fully enumerated set of 102 unique surfaces is simulated with each protein sequence. A collection of 27-monomer sequences is used—each of which is non-degenerate and protein-like. Thermodynamic quantities such as the specific heat and free energy are calculated from the density of states, and are used to investigate the adsorption of lattice proteins on patterned substrates.

1 Research supported by NSF.

P1.00210 Calculating Pressure and Surface Tension of Lattice Polymers

QIANG WANG, PENGFEI ZHANG, Department of Chemical and Biological Engineering, Colorado State University — Calculating pressure and related surface tension of polymeric systems in lattice Monte Carlo simulations is an important but nontrivial subject. Here we propose several novel, efficient, and accurate methods. In the first method, we combine chain insertion/deletion with the Wang-Landau — Optimized Ensemble (WL-OE) simulation, which is very efficient at low to intermediate polymer volume fractions . In the second method, we introduce a repulsive wall with bridging bonds, which is similar to the repulsive wall method but eliminates its confinement effects. This method works especially well at high , where all the methods using chain insertion/deletion fail. Finally, we combine the above two methods, which gives complete thermodynamics over the entire range of continuous and exact -values with negligible finite-size effects. To demonstrate our methods, we apply them to calculate the bulk pressure and surface tension of nano-confined homopolymers.
P1.00211 Protein-like folding and other phase transitions of a single polymer chain, MARK TAYLOR, Dept. of Physics, Hiram College, WOLFGANG PAUL, Martin-Luther-Universitat, Halle, Germany, KURT BINDER, Johannes-Gutenberg-Universitat, Mainz, Germany — A single polymer chain can undergo a series of conformational transitions analogous to the phase transitions exhibited by bulk materials. We have recently studied the conformational transitions of a flexible square-well polymer chain using a Wang-Landau simulation approach in which we directly compute the single-chain partition function. For the case of a tangent-sphere chain, the temperature-interaction range phase diagram includes both a coil-globule and globule-crystal transition as well as an “all-or-none” coil-crystal transition. Despite the non-unique homopolymer ground state, the thermodynamics of this direct freezing transition are identical to the thermodynamics of two-state protein folding. Two-dimensional configurational and free energy landscapes reveal both a dominant “folding” pathway and a “dead-end” pathway resulting in a bimodal distribution of structures at the top of the free energy barrier. A simple AB-heteropolymer variant of this model leads to both rod-like and disk-like ground state structures while a fused sphere version of the model produces helical folded structures.


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P1.00212 Simulation of dynamics of disordered diblock copolymers near the order-disorder transition, PAVANI MEDAPURAM, DAVID MORSE, Univ of Minnesota - Twin Cities — We present a simulation study of the dynamics of composition fluctuations, chain conformations and stress for diblock copolymers near the order-disorder transition. Specifically, we study the behavior of the van Hove function S(r,t), which is a measure of structural relaxation, the linear response of the bond orientation tensor, which is closely related to optical birefringence, and the linear viscoelastic stress relaxation modulus G(t). We show how a slowly decaying mode associated with slow relaxation of composition fluctuations emerges as the degree of segregation is increased.

P1.00213 Conformation of Single Polymer Chains, HOWARD WANG, Binghamton Univ, XIAORONG WANG, Tongji University — Large biological molecules such as proteins and DNAs can be packed into condensed forms through hydrogen bonding and specific interactions; the conformation of an ultra-long single chain with no specific intra-chain interactions is considered here. We discuss three possible states, (1) uniformly compressed Gaussian, (2) totally irregular aggregates, and (3) long Gaussian sections separated by segments of frustrated local conformation, or “kinks.” Those states could be related to the methods of preparing the condensed form of the single chain globule. We argue that the Gaussian-Kink conformation is preferred and the segregation of kinks to the surface of globules would significantly alter the chain dynamics.

P1.00214 BIOPOLYMERS AND BIOHYBRID POLYMERS —

P1.00215 Binding Affinity Effects on Physical Characteristics of a Model Phase-Separated Protein Droplet, SARA CHUANG, Princeton University, SALMAN BANANI, UT Southwestern Medical Center, MICHAEL ROSEN, UT Southwestern Medical Center, HHHI, CLIFFORD BRANGWYNE, Princeton University — Non-membrane bound organelles are associated with a range of biological functions. Several of these structures exhibit liquid-like properties, and may represent droplets of phase-separated RNA and/or proteins. These structures are often enriched in multi-valent molecules, however little is known about the interactions driving the assembly, properties, and function. Here, we address this question using a model multi-valent protein system consisting of repeats of Small Ubiquitin-like Modifier (SUMO) protein and a SUMO-interacting motif (SIM). These proteins undergo phase separation into liquid-like droplets. We combine micro rheology and quantitative microscopy to determine affect of binding affinity on the viscosity, density and surface tension of these droplets. We also use fluorescence recovery after photobleaching (FRAP), fluorescence correlation spectroscopy (FCS) and partitioning experiments to probe the structure and dynamics within these droplets. Our results shed light on how inter-molecular interactions manifests in droplet properties, and lay the groundwork for a comprehensive biophysical picture of intracellular RNA/protein organelles.

P1.00216 Fluorescence microscopy techniques for characterizing the microscale mechanical response of entangled actin networks, SAVANNA BLAIR, TOBIAS FALZONE, RAE ROBERTSON-ANDERSON, University of San Diego — Actin filaments are semiflexible polymers that display complex viscoelastic properties when entangled in networks. In order to characterize the molecular-level physical and mechanical properties of entangled actin networks it is important to know the in-network length distribution and the response of entangled filaments to local forcing. Here we describe two single-molecule microscopy protocols developed to investigate these properties. Using confocal fluorescence microscopy and ImageJ image analysis we have developed a protocol to accurately measure the in-network actin length distribution. To characterize the deformation of actin filaments in response to perturbation, we trap micron size beads embedded in the network with optical tweezers and propagate the beads through the entangled filaments while simultaneously recording images of fluorescent-labeled filaments in the network. A sparse number of labeled filaments dispersed throughout the network allow us to visualize the movement of individual filaments during perturbation. Analysis of images taken during forcing is carried out using a combination of vector mapping and skeletonization techniques to directly reveal the deformation and subsequent relaxation modes induced in entangled actin filaments by microscale strains. We also determine the dependence of deformation modes on the relative filament position relative to the strain.

P1.00217 Assembly, Properties and Function of Synthetic Phase-Separated RNA/Protein Organelles, NICOLE TAYLOR, SHANA ELBAUM, HOWARD STONE, CLIFFORD BRANGWYNE, Princeton Univ — Non-membrane bound RNA/protein (RNP) bodies play a key role in cellular RNA processing steps. Many RNA helicases, required for RNA processing, are key components of RNPs. Consistent with this, a purified RNA helicase, Laf-1, exhibits a salt and protein concentration dependent phase separation in vitro, resulting in liquid-like droplets. We use such synthetic RNPs to study the biophysics of RNP assembly, and to elucidate the link between their physical properties and function. To accomplish this, we are developing custom microfluidic devices to measure biophysical properties, nucleation and growth kinetics, and RNA processing function of droplets. We measure droplet viscosity by applying a shear stress to protein droplets that adhere to the channel wall; measurements are consistent with those taken using a particle micro rheology approach. We also monitor and control protein droplet nucleation using oil/water emulsions. Our results provide a new platform for addressing how the cell regulates organelle assembly and properties through protein, RNA, and ATP concentration. We anticipate that these findings will offer insight into the contribution of RNPs in key RNA processing functions in the cell.

P1.00218 POLYMERS FOR SOLAR ENERGY —
P1.00219 Design of block and graft copolymers for use as compatibilizers in organic solar cell active layers. DYLAN KIPP, VENKAT GANESAN, University of Texas at Austin — Recent experiments have suggested that the use of block and graft copolymer compatibility in polymer-based donor-acceptor materials can improve the morphology and improve polymer of solar cells. Inspired by these successes, we use this framework of self-consistent field theory to study the influence of copolymer compatibilizers on the interfacial properties of donor-acceptor blends. First, we calculate the reduction in the interfacial tension (and hence the driving force towards macrophase segregation) brought by the copolymer compatibilizer as a function of the copolymer architecture. Second, we calculate the effective interaction between two copolymer monolayers at the interfaces between the donor and acceptor domains. The results of this second study allow us to comment on the expected ability of the copolymer compatibilizer to reduce the coalescence of domains. Overall, our results suggest important rules for designing copolymer compatibilizers to influence both kinetically-trapped and equilibrium morphologies of donor-acceptor blends.

P1.00220 Self-Assembly of Carotenoids During Solution Casting of Solar Devices. DUSANATHA ALWIS, DILRU RATNAWEERA, University of Sri Jayewardenepura, Sri Lanka, THUSITHA ETAMPAWALA, MARK DADMUN, University of Tennessee, Knoxville, UDUMALAGALA CHANDRIKA, PRADEEP JAYAWEERA, University of Sri Jayewardenepura, Sri Lanka — Self-assembly of carotenoids is a common phenomenon in nature and seems to be closely related to the functions of these natural dyes in solar devices. The large absorption coefficients in the visible region of carotenoids make them a well-suited natural resource for dye-sensitized solar cells (DSSC). The performance of carotenoid-based solar devices mainly depends on the photo-electrochemical properties of the active material (carotenoids) and their self-assembled morphology within solar devices. These associations of molecules will affect the light absorption, emission and energy harvesting abilities of these solar devices. Two types of highly conjugated natural carotenoids having mono and dicarboxy terminal groups, namely bixin and norbixin, were extracted from annatto seeds. In the current study, small angle neutron scattering experiments were carried out to examine the modes of assemblies of bixin and norbixin during solution processing of DSSCs. Spherical shape aggregates with rough interfaces were observed in acetonitrile medium, which is a good solvent for hydrocarbon chain. The shape of the aggregates slightly deviates from spherical to slightly elongated shape at high volume fractions of carotenoids. Bixin and norbixin show different association behaviors as a function of their concentration.

P1.00221 Hydrogen Bonding-mediated Conjugated Polymers for Bulk-Heterojunction Organic Photovoltaics. YEN-HAO LIN, Rice University, WAN-YI NIE, ADITYA MOHITE, GAUTAM GUPTA, Los Alamos National Laboratory, RAFAEL VERDUGO, Rice University — We use hydrogen bonding interactions to prevent large scale phase separation and improve polymer of organic solar cells. Poly(3-alkylthiophene) (P3HT) donor polymer and poly(2,7-(9′,9′-dioctyl-fluorene)-alt-5,5-(4′,7′-di-2-thienyl-2′-1′,3′-benzothiadiazole) (PFTBT) acceptor polymer with self-associating, quadruple hydrogen bonding end groups (2-ureido-4[H]-pyrimidinone, UPy) are used to explore the role of hydrogen bonding associations on blend morphology and photovoltaic performance. We study three systems: P3HT:PCBM, PFTBT:PCBM and P3HT:PFTBT and analyze by AFM, impedance, and device performance. In P3HT:PCBM, the performance is improved from 1.21% to 2.16% using UPy-terminated P3HT due to the enhanced long range order of semi-crystalline P3HT. In PFTBT:PCBM, the performance is decreased from 1.84% to 1.08% using UPy-terminated PFTBT due to entanglement of non-crystalline PFTBT chains. In P3HT/PFTBT system, the performance is improved from 0.43% to 0.77% with the use UPy-terminated P3HT and PFTBT because of suppressed macro-phase separation with maintained long range order of P3HT under annealing temperature. The impedance analysis under short circuit and illumination conditions indicates the faster charge transport and reduced charge recombination within the better performed devices. This study shows that the hydrogen bonding interactions can reduce phase separation but not produce better BHJ devices in all cases perhaps because some phase separation in blends is still required.

P1.00222 Side Chain Engineering of Naphthalenediimide-Based N-type Polymer for High-Performance All-Polymer Solar Cell near 6% Efficiency. CHANGYEON LEE, HYUNBUM KANG, WONHO LEE, TAEUS KIM, KI-HYUN KIM, KAIST, HAN YOUNG WOO, PNU, CHENG WANG, Lawrence Berkeley National Laboratory, BUMJOON KIM, KAIST, PUSAN NATIONAL UNIVERSITY (PNU) COLLABORATION, LAWRENCE BERKELEY NATIONAL LABORATORY COLLABORATION — Despite the attractive features of all-polymer solar cells (all-PSCs), i.e., enhanced absorption coefficients, the tunability of their energetic and chemical properties and their thermal and mechanical stabilities, they still face the great challenge of having significantly low power conversion efficiency (PCE) values of only 3-5%. The prominent origins of the poor efficiency of all-PSCs are the undesirable features of the bulk-heterojunction (BHJ) blend morphology including the phase-separated large-scale domain size, reduced ordering of the polymer chains. Tuning side alkyl chains of conjugated polymers is an effective route for manipulating the blend morphology in BHJ type solar cells. However, the role of side chains in all-PSCs is poorly understood. Herein, we report high-performing all-PSCs with 5.96% efficiency by developing a series of naphthalenediimide (NDI)-based polymer donors with different alkyl side chains. We demonstrated that the use of the PNDIT with hexadecyl side chains produced highly-ordered polymer stackings with strong face-on geometry and at the same time, forming the optimal BHJ morphology with finely separated phase domains, all of which contributed together to induce well-balanced μe/μh ratio and generate efficient all-PSCs with PCEs near 6%.

P1.00223 Fabrication of Organic Bulk Heterojunction Solar Cells on Flexible Substrates. GABRIEL CALDERON, MILZAIDA MERCED-SANABRIA, CAROLYN CARRADERO-SANTIAGO, JOSEE VEDRINE-PAULEUS, University of Puerto Rico-Humacao — The active layer for the organic solar cells fabricated is composed of P3HT:PCBM, poly(3-hexylthiophene) (P3HT) as electron donor and phenyl-C61-butyric acid methyl ester(PCBM) as electron acceptor. These polymers were used due to their promising characteristics for devices such as bulk heterojunction solar devices. We used polyethylene terephthalate (PET) substrates, a highly flexible plastic, with indium tin oxide (ITO) as the transparent conducting anode for the device, and UV lithography technique to pattern the ITO; this is to facilitate multiple devices on a single substrate. The fabrication process for pattern transfer incorporates developing and etching processes. We diluted the HCI and DI water to etch out the ITO. PEDOT:PSS and active layer of P3HT:PCBM were deposited on (3.0 sq-cm) patterned of ITO/PET by spin coating method. The cathode was thermally evaporated with Al. We characterized the device using a source meter. We also simulated portions of the device using PET on graphene as the substrate.

P1.00224 ORGANIC ELECTRONICS AND PHOTONICS —

P1.00225 Electroluminescent Molecule for DC-Driven, Sub-2V Solid-State Emissive Devices by Incorporating Redox Co-reactants. HONG CHUL MOON, TIMOTHY P. LODGE, C. DANIEL FRISBIE, University of Minnesota — We have demonstrated a solid-state DC-driven electroluminescent (ECL) device using a solution processable, emissive ECL gel based on polystyrene-based redox polymer molecules containing a one-electron acceptor (Ru(bpy)32+ and PFO2,2) and a two-electron donor (butylammonium oxalate (TBAOX)) was incorporated into the ECL gel for a co-reactant strategy. Oxalate can be viewed as a consumable fuel for the device providing reducing power and cutting the overall operating voltage. The device was fabricated by a simple two-step solution process. Application of 1.6 V DC bias across the device resulted in the onset of light emission. The maximum luminance was achieved at 1.5 mole ratio of ECL luminophore (Ru(bpy)32+) and TBAOX, and the turn-on voltage was independent of the composition. The simplicity of the ECL device and its low voltage operation characteristics make it potentially attractive as a display element for printed electronics.3

3 TPL and CDF acknowledge financial support from the Air Force Office of Scientific Research under FA9550-12-1-0067.
P1.00226 Ferroelectric switching behavior in morphology controlled ferroelectric-semiconductor polymer blends for organic memory. EUNHEE LIM, GREGORY SU, EDWARD KRAMER, MICHAEL CHABINYC, University of California, Santa Barbara — Memory is a fundamental component of all modern electronic systems. Organic ferroelectric memories are advantageous because they are thin and lightweight devices that can be made printable, foldable, and stretchable. Organic ferroelectric memories comprise a physical blend of an organic semiconducting polymer and an insulating ferroelectric polymer as the active layer in a thin film diode. Controlling the thin film morphology in these blends is important for electrical properties of the resulting device. We have found that when a semiconducting thiophene polymer with polar alkanoate side chains (P3EPT) is blended with well-studied ferroelectric polymer poly[(vinylenefluoride-co-trifluoroethylene] P (VDF-TrFE), the resulting film has low surface roughness and more controllable domain sizes compared to the widely used poly (3-hexylthiophene). This difference allows more reliable study of the ferroelectric switching behavior in devices with domain size of about 100nm. The influence of the 3D composition measured by a combination of methods, including soft x-ray microscopy, on the electrical characteristics will be presented.

P1.00227 Microscopic simulations of electronic excitations in donor-acceptor heterojunctions of small-molecule based solar cells. BJÖRN BAUMEIER, Max Planck Institute for Polymer Research — Fundamental processes involving electronic excitations govern the functionality of molecular materials, in which the dynamics of excitons and charges is determined by an interplay of molecular electronic structure and morphological order. To understand, e.g., charge separation and recombination at donor-acceptor heterojunctions in organic solar cells, knowledge about the microscopic details influencing these dynamics in the bulk and across the interface is required. For a set of prototypical heterojunctions of small-molecule donor materials with C80, we employ a hybrid QM/MM approach linking density-functional and many-body Green’s functions theory (DFT/GW-BSE) to polarizable force-fields and analyze the charged and neutral electronic excitations therein. We pay special attention the spatially-resolved electron/hole transport levels, as well as the relative energies of Frenkel and charge-transfer excitations at the interface. Finally, we link the molecular architecture of the donor material, its orientation on the fullerene substrate as well as mesoscale order to the solar cell performance.

P1.00228 Enhancing the Thermoelectric Characteristics of PEDOT:PSS Through the Incorporation of a Redox-Active Small Molecule. EDWARD TOMLINSON, MATTHEW WILLMORE, XIAOQIN ZHU, BRYAN BOUDOURIS, Purdue University — The polymer composed of poly(3,4-ethylene dioxythiophene) and poly(styrene sulfonate) (PEDOT:PSS) is a leading organic thermoelectric material due to its high-performance properties. Here, we establish the effect of incorporating the redox-active small molecule 4-hydroxy-2,2,6,6-tetramethylepiperidin-1-oxyl (TEMPO-OH) on the structural and thermoelectric properties of PEDOT:PSS. Specifically, the thermoelectric power factor (PF) was monitored as a function of TEMPO-OH loading, elucidating a clear trend in the PF. Importantly, at loadings as low as 5% TEMPO-OH, by mass, the thermopower of the sample was increased by a factor of two. Furthermore, the role of the TEMPO-OH on the thin film morphology of the composite material is examined through the use of grazing incidence-wide angle x-ray scattering (GI-WAXS) and atomic force microscopy (AFM). Despite the acidic conditions associated with the presence of PSS, the existence of radical functionality is confirmed through electron paramagnetic resonance (EPR) spectroscopy. Through careful tuning, the optimized conditions outlined within this work results in PF gains in excess of 40%.

P1.00229 Morphology optimization for enhanced performance in organic photovoltaics. OLGA WODO, JAROSŁAW ZOLA, State Univ of NY - Buffalo, BASKAR GANAPATYSUBRAMANIAN, Iowa State University — Organic solar cells have the potential for widespread usage due to their low cost-per-watt and mechanical flexibility. Their widespread use, however, is bottlenecked primarily by their low solar efficiencies. Experimental evidence suggests that a key property determining the solar efficiency of such devices is the morphological distribution of the electron-donor and electron-acceptor constituents. By carefully designing the morphology of the device, one could potentially significantly enhance their performance. This is an area of intense experimental effort that is mostly trial-and-error based, and serves as a fertile area for introducing mechanics and computational thinking. In this work, we use optimization techniques coupled with computational modeling to identify the optimal structures for high efficiency solar cells. In particular, we use adaptive population-based incremental learning method linked to graph-based surrogate model to evaluate properties for given structure. We study several different criterions and find optimal structure that that improve the performance of currently hypothesized optimal structures by 29%.

P1.00230 Facile Control of a Wide Range of Regioregularity: Significant Influence on Mechanical and Electrical Properties of Conjugated Polymers. JIN-SEONG KIM, JAE-HAN KIM, WONHO LEE, KAIJean, HOJEOUNG YU, POSTECH, HYEONG JUN KIM, KAIST, INHO SONG, JOON HAK OH, POSTECH, TAEK-SOO KIM, BUMJOON KIM, KAIST, POSTECH COLLABORATION — While regioregularity (RR) has been known to have a strong influence on inherent properties of conjugated polymer, systematic study of RR has been limited due to the lack of synthetic methodology. Herein, we prepared a series of poly(3-hexithiophenes) (P3HTs) having a wide range of RR from 64 to 96% by the modified Grignard metathesis method that utilizes the dimer moiety. We observed that the RR determines crystalline behavior, mechanical and electrical properties of P3HT. Although higher RR P3HT had higher hole mobility, its increased degree of crystallinity induced fragile nature of polymers (elongation break <1%). In contrast, lower RR had lower elastic modulus and thereby leading to significant reduction of fragility. Therefore, our finding suggested that the control of RR is critical to regulate the properties of conjugated polymers between electrical performance and mechanical resilience as depending on the purpose of the applications. (i.e flexible portable devices vs high performance panel)

P1.00231 Using COMSOL Multiphysics Software to Analyze the Thin Film Resistance Model of a Conductor on PET. CAROLYN CARRADERO-SANTIAGO, MILZAIDA MERCED-SANABRIA, JOSE VEDRINE-PAULÉUS, University of Puerto Rico-Humacao — In this research work, we will develop a virtual model to analyze the electrical conductivity of a thin film with three layers, one of graphene or conducting metal film, polyethylene terephthalate (PET) and Poly(3,4-ethylenedioxythiophene) Polystyrene sulfonate (PEDOT:PSS). COMSOL Multiphysics will be the software use to develop the virtual model to analyze the thin-film layers. COMSOL software allows simulation and modelling of physical phenomena represented by differential equations such as that of heat transfer, fluid movement, electromagnetism and structural mechanics. In the work, we will define the geometry of the model; in this case we want three layers-PET, the conducting layer and PEDOT:PSS. We will then add the materials and assign PET as the lower layer, the above conductor as the middle layer and the PEDOT:PSS as the upper layer. We will analyze the model with varying thickness of the top conducting layer. This simulation will allow us to analyze the electrical conductivity, and visualize the model with varying voltage potential, or bias across the plates.
P1.00232 Study of biodegradable polymers for “green” devices, CARLOS PEREZ, XIAOMEI JIANG, University of South Florida, JIANG GROUP TEAM — PI—conjugated polymers such as polythiophenes are conventional picks for cost-effective organic solar cells. However, these organic semiconductors are not environment-friendly since the polymer backbones require temperature higher than 300°C to be decomposed, thus will cause potential environmental problems upon disposal. In this work, the optical and electronic properties of biodegradable polymers, conjugated poly(disulfidediamine), were examined via continuous wave laser spectroscopy, FTIR spectroscopy and conductivity measurement. We found that the attachment of a side chain to aromatic ring increases both photo and thermal stability, as well as higher conductivity. Thermal annealing improved the film morphological, photophysical and electronic properties. Photo-induced Absorption (PIA) reveals different features comparing with conventional pi-conjugated polymers. No observation of long-lived photoexcitations such as polarons or triplets which are common with pi-conjugated polymers. Instead, we found the formation of low energy species upon thermal annealing in these biodegradable polymers.

P1.00233 Electron transport and light absorption/emission in molecular complexes, MIGUEL MARTINEZ. Bronx High School of Science, LEV MOUROKH, Physics Department, Queens College of CUNY — In this work, we address photo-assisted electron transport in molecular triads and tetrads connected to the leads. Donor-bridge-acceptor triads are promising candidates for efficient organic solar cells, as the photon absorption makes it possible to transfer electrons against the applied voltage. Deriving and solving numerically the equations of motion for electron creation/annihilation operators, we obtain the parameters of molecular complexes which are optimal for a maximal efficiency of the light harvesting. For donor-bridge-bridge-acceptor tetrads, we determine the conditions for another phenomenon, optical up-conversion. Electron transport along the applied voltage and the photon absorption at one of the bridges facilitates the photon emission at another bridge with higher frequency. Using the same equations of motion approach, we obtain the emitted electromagnetic energy and its dependence on the system parameters.

P1.00234 Nanostructural Patterning Improves the Performance of Non-volatile Polymer Memory Devices, SEUNG HYUN SUNG, BRYAN W. BOUDOURIS, Purdue University — Organic nonvolatile memory devices based on polymer ferroelectric materials are a promising approach toward the development of low-cost memory due to the ease of processing and flexibility associated with the device. Here, we focus on a memory device with a two-component active layer and a diode structure. This ferroelectric diode (FeD) has a nanostructured active layer, composed of ferroelectric and semiconducting polymers, and it can provide easy access to high-performance polymer-based memory devices. In order to create these nanostructured active layers, we have utilized electron beam (e-beam) lithography for the simple fabrication of a desired pattern on the ferroelectric polymer layer. Then, a semiconducting polymer was deposited into the nanoporous ferroelectric layer to complete the ordered heterojunction. By optimizing the nanostructure, the memory retention and ON/OFF current density ratio performance of FeD is greatly enhanced (e.g., the ON/OFF ratio is a factor of 3 greater) over a traditional blended diode. This ability to control the ferroelectric polymer morphology will open new fields of evaluating the relationships between structure and performance in organic memory devices.

P1.00235 Cross-linking high-K fluoropolymer gate dielectrics enhances the charge mobility in rubrene field effect transistors, JIHALA ADHIKARI, MATTHEW GADINSKI, QING WANG, ENRIQUE GOMEZ, Penn State University — Polymer dielectrics are promising materials where the chemical flexibility enables gate insulators with desired properties. For example, polar groups can be introduced to enhance the dielectric constant, although fluctuations in chain conformations at the semiconductor-dielectric interface can introduce energetic disorder and limit charge mobilities in thin-film transistors. Here, we demonstrate a photopatternable high-K fluoropolymer, poly(vinylidene fluoride-bromotrifluoroethylene) (P(VDF-BTFE)), with a dielectric constant between 8 and 11. The bromotrifluoroethylene moiety enables photolinking and stabilization of gate insulator films while also significantly enhancing the population of trans torsional conformations of the chains. Using rubrene single crystals as the active layer, charge mobilities exceeding 10 cm²/Vs are achieved in thin film transistors with cross-linked P(VDF-BTFE) gate dielectrics. We hypothesize that crosslinking reduces energetic disorder at the dielectric-semiconductor interface by suppressing segmental motion and controlling chain conformations of P(VDF-BTFE), thereby leading to approximately a three-fold enhancement in the charge mobility of rubrene thin-film transistors over devices incorporating uncross-linked dielectrics or silicon oxide.

P1.00236 Monte Carlo simulations of charge transport in heterogeneous organic semiconductors, PYIE PHYO AUNG, KIRAN KHANAL, JUTTA LUETTMER-STRATHMANN, Departments of Physics and Chemistry, The University of Akron, Akron, OH 44325-4001 — The efficiency of organic solar cells depends on the morphology and electronic properties of the active layer. Research teams have been experimenting with different conducting materials to achieve more efficient solar panels. In this work, we perform Monte Carlo simulations to study charge transport in heterogeneous materials. We have developed a coarse-grained lattice model of polymeric photovolaticcs and use it to generate active layers with ordered and disordered regions. We determine carrier mobilities for a range of conditions to investigate the effect of the morphology on charge transport.

P1.00237 ABSTRACT WITHDRAWN

P1.00238 ABSTRACT WITHDRAWN

P1.00239 ABSTRACT WITHDRAWN

P1.00240 The impact of P3HT molecular weight and solvent composition on P3HT films processed from binary solvent mixtures, LAWSON LLOYD, MADELEINE GORDON, DAVID BOUCHER, College of Charleston — Recent experimental endeavors have shown that well-ordered P3HT assemblies formed in solution can improve the crystallinity and morphological uniformity of thin films and composites, thereby providing a promising new route to more efficient polymeric optoelectronic materials. We have studied the assembly and crystallinity of two regioregular poly(3-hexylthiophene) (P3HT) samples, M_n ≈ 28 kDa and M_n ≈ 65 kDa, in several different binary mixtures of organic solvents. We use an excitonic coupling analysis of the UV/Vis absorbance spectra to assess the impact that the solvent and the molecular weight of P3HT have on the relative structural order of the polymer assemblies. In addition, we investigate the influence that the solvent composition and the structural order of P3HT aggregates have on the assembly and organization of P3HT films. We use optical and atomic force microscopy techniques to study thin films of P3HT processed from different solvent mixtures. Our results show that relatively small variations to the P3HT solutions can produce significant changes in the morphology and macromolecular structures of the P3HT films.

P1.00241 POLYMERS IN BATTERIES AND ELECTROCHEMICAL CAPACITORS —
P1.00242 In situ Mechanistic Investigation of an Organic Radical Polymer Cathode on Interfacial Charge Transport and Cycling Stability. FEI LI, JODIE LUTKENHAUS, Artie McFerrin Department of Chemical Engineering, Texas A&M University. Organic radical polymers have gained increased attention as cathodes for organic radical batteries due to their fast charge transport and high cycling stability. These features make them a promising alternative to conventional lithium-ion batteries. One polymer of interest is a nitroxide radical polymer, poly(2,2,6,6-tetramethylpiperidinyl-oxymethylacrylate) (PTMA), which is capable of a two-electron transfer process. The specific capacity of PTMA as cathode has a reported value between 77 to 220 mAh/g, depending on the charge/discharge conditions. Most work with PTMA has largely emphasized electrode optimization to improve its capacity by adding highly conducive materials or by designing new forms of radical polymers. There is little molecular level detail on the charge storage process and electrode/electrolyte interfacial activities in such systems. Here, we present the application of in situ characterization techniques towards the charge storage process in PTMA. Electrochemical quartz crystal microbalance with dissipation monitoring (EQCM-D) monitors various electrode physical properties (e.g. mass, shear viscosity) during controlled electrochemical interrogation (cyclic voltmmetry, charge discharge). Electrochemical impedance spectroscopy probes various charge storage and transport events at a range of frequencies and potentials. With this information attained, a clearer picture of charge storage in organic radical cathode batteries can be formed.

P1.00243 Flexible Hybrid Electrodes Containing Vanadium Pentoxide ($V_5O_8$) and an Electron- and Ion-Conducting Diblock Copolymer for Energy Storage. HYOSUNG AN, JARED MIKE, Texas A&M University, Chemical Engineering, KENDALL SMITH, LISA SWANK, YEN-HAO LIN, STACY PESEK, RAFAEL VERDUCZO, Rice University, Chemical and Biomolecular Engineering, JODIE LUTKENHAUS, Texas A&M University, Chemical Engineering. Vanadium pentoxide ($V_5O_8$) is a promising cathode material for lithium-ion batteries due to its high capacity, high energy density, and cost-effectiveness. However, its low lithium-ion diffusion coefficient ($10^{-12}$ - $10^{-13}$ cm$^2$/s), low electronic conductivity ($10^{-2}$ - $10^{-3}$ S/cm), and severe volumetric changes during cycling have hindered its application in practical devices. One way to address these challenges is to incorporate a second active material. For this purpose, poly(3-hexylthiophene)-block-poly(ethylene oxide) (P3HT-b-PEO) block copolymer containing electron- and ion-conducting polymer blocks was introduced to a $V_5O_8$ electrode system. Cathodes are prepared by mixing aqueous dispersions of block copolymer, $V_5O_8$-, and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) and drop casting. The $V_5O_8$ and P3HT-b-PEO hybrid electrode showed synergistic results, having improved electrochemical storage performance and mechanical property. We also demonstrated a flexible battery prototype using the P3HT-b-PEO/$V_5O_8$ cathode.

P1.00244 Phase Behavior and Electrical Characterization of Solid-State Magnesium Ion Electrolytes from Diblock Copolymers. JACOB THELEN, University of California Berkeley; Lawrence Berkeley National Laboratory, SEBNEM INCEOGLU, Lawrence Berkeley National Laboratory, NITASH BALSARA, University of California Berkeley; Lawrence Berkeley National Laboratory — Batteries utilizing magnesium metal anodes are considered a promising candidate for the next generation of energy storage with performance beyond lithium ion technology. The development of a safe, stable magnesium ion-conducting electrolyte represents one of the major barriers to the advancement of magnesium battery technology. One approach to increasing the safety and stability of electrolytes is to replace flammable organic solvents with more stable polymeric electrolytes. Here we report the synthesis and characterization of solid-state magnesium ion electrolytes derived from diblock copolymers.

P1.00245 Polyhedral Oligomeric Silsesquioxanes – Based Hybrid Electrolytes with Controlled Network Structure. QIWEI PAN, South China University of Technology; Drexel University, CHRISTOPHER LI, Drexel University, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, SOUTH CHINA UNIVERSITY OF TECHNOLOGY TEAM, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, DREXEL UNIVERSITY TEAM — High ion conductivity and mechanical integrity are the most important properties in the application of solid polymer electrolytes (SPEs). We herein report synthesis and characterization of hybrid electrolytes with inorganic polyhedral oligomeric silsesquioxanes (POSS) as the crosslinker. The SPEs were prepared by a facile one-pot reactions between octakis[3-(glycidyloxy)propyl(dimethyl/silyloxy)]silsesquioxane and bis(3-aminopropyl) terminated poly(ethylene glycol) (PEG) in the present of bis(trifluoromethanesulfonylimide) lithium salt (LiTFSI). Uniform distribution of POSS and LiTFSI in the SPEs were confirmed by SEM-BSD and SEM-EDX. We show that both ionic conductivity and mechanical properties of the SPE can be easily tuned by varying POSS contents. Correlation between the SPE network structure and the ionic conductivity and mechanical properties will be discussed.

P1.00246 HIERARCHICAL ASSEMBLY OF BLOCK COPOLYMERS AND SOFT NANOPARTICLES IN SOLUTIONS.

P1.00247 Structure and Ionic Conductivity Evolution of a Block Copolymer Electrolyte during Thermal Annealing. MAHADI CHINTAPALLI, NITASH BALSARA, Univ of California - Berkeley — Mixtures of block copolymers (BCPs) and lithium salts are promising materials for battery electrolytes because they exhibit high ionic conductivity and high modulus. However, since most polymer electrolytes show high conductivities only at temperatures above ambient, it is important to understand how the structure and ionic conductivity of BCP electrolytes evolve during thermal annealing. In situ small angle X-ray scattering and ac impedance spectroscopy were used to characterize a BCP electrolyte, lamellar polysiloxane-block-poly(ethylene oxide) mixed with lithium bis(trifluoromethanesulfonylimide) (LiTFSI), during thermal annealing. As annealing progressed, long range lamellar order and domain spacing increased, and scattering contrast between the two BCP phases decreased. A concomitant decrease in ionic conductivity was observed.

P1.00248 $\beta$-NMR Measurements of Lithium Ion Transport in Thin Films of Pure and Lithium-Salt-Doped Poly(ethylene oxide). IAIN MCKENZIE, TRIUMF, MASASHI HARADA, University of British Columbia, C.D. PHILIP LEVY, TRIUMF, W. ANDREW MACFARLANE, RYAN M.L. MCFADDEN, University of British Columbia, GERALD D. MORRIS, TRIUMF, SHIN-ICHI OGATA, Toyota Central Research and Development Laboratories, Inc., MATTHEW R. PEARSON, TRIUMF, JUN SUGIYAMA, Toyota Central Research and Development Laboratories, Inc. — $\beta$-Detected nuclear spin relaxation of $^{6}$Li$^+$ has been used to study the microscopic diffusion of lithium ions in thin films of poly(ethylene oxide) (PEO), PEO with lithium bis(trifluoromethanesulfonylimide) (LiTFSI), PEO with lithium trifluoracetate (LiTFA) and PEO with lithium trifluoroacetate (LiTFA) with monomer-to-salt ratios of 8:3:1. Hopping of Li$^+$ above ~ 250 K follows an Arrhenius law in all of the films. Diffusion of Li$^+$ is fastest in pure PEO and decreases in order LiTFSI $>$ LiTFA $>$ LiTFA. We observed the activation energy for hopping $(E_A)$ and the intrinsic hop rate (r$_0$) both increasing in order LiTFA $<$ LiTFSI $<$ PEO but the larger r$_0$ outweighs the larger $E_A$ and results in Li$^+$ motion being fastest in the pure polymer. The results will be discussed in terms of the ionicity of the salt.
P1.00249 Increase of the Effective Dispersity in ARB-Type Triblock Copolymer. SANGHOON WOO, HYUNJUNG JUNG, JUNE HUH. Department of Chemical and Biological Eng., Korea University, Seoul 136-713, Korea, DU YEOL RU, Department of Chemical and Biological Eng., Yonsei University, Seoul 120-749, Korea, JOONA BANG. Department of Chemical and Biological Eng., Korea University, Seoul 136-713, Korea — The domain spacing of block copolymer (BCP) has been mainly controlled by molecular weight and block immiscibility. Instead of these traditional variables, we designed a new type of BCP, namely ARB type triBCP, where the R represents the short middle block composed of A and B random copolymers. It was expected that the R block provide the effect of increased “effective” dispersity via compositional distribution leading to an increased domain size compared to the AB dibCP with same MW and dispersity. We prepared various ARB type triBCPs and AB dibCPs having the similar dispersity via living-radical polymerization, and their morphologies were characterized by TEM, SAXS, and GISAXS. As a result, it was shown that the ARB-type triBCP exhibited a significant increase in the domain spacing compared to the AB dibCPs with same MW and dispersity. These results were also compared with theoretical viewpoint.

P1.00250 Control Large Nanoparticle Assemblies in Suparmolecular Nanoparticle Thin Films. JINGYU HUANG, TING XU. University of California, Berkeley — Nanocomposites can generate new properties beyond those offered by organic and inorganic building blocks. Here we meet the demands in functional nanomaterials design. We study the self-assembly of nanoengineered building block and their spatial arrangements. With the recent development, colloidal synthesis and surface modification methods provide inorganic nanoparticles (NPs) with various sizes, shapes, compositions and properties in a facile manner. Block copolymer-based supramolecules further provide more versatile routes to control spatial arrangement of the nanoparticles over multiple length scales. Nanoparticle size is a critical parameter determining the optical and electronic properties. However, most of studies to date focused on nanoparticle smaller than 10 nm in size. Here, our recent studies showed that the assembly of nanoparticles with size larger than 10 nm can be achieved in the supramolecular nanocomposite thin films by finely tuning the ligand-polymer interactions and the sample treatment conditions. Both the overall morphology of the nanoparticle assemblies and inter-particle distances can be readily tailored. These new results opened a viable approach to construct functional materials using nanoparticles with different quantum confinement effects.

P1.00251 Crystallization Driven Responsive Janus Assembly. HAO QI, SHAN MEI, CHRISTOPHER LI, Drexel university, SOFT MATERIALS LAB TEAM — Responsive and dynamic nanostructures are ubiquitous in Nature, and they are also utter importance for applications such as sensing and drug delivery. Herein we report a series of hierarchical block copolymer nanostructure that is able to undergo 2D (sheet-like) to 3D (bowl-like) shape changing upon specific external stimuli. Freestanding Janus nanosheets were prepared via crystallization-driven self-assembly of poly(ε-caprolactone)-b-poly(acrylic acid) (PCL-b-PAA) and subsequent crosslinking and disassembly process. Due to the mechanical contrast between the two layers, and the chemical responsiveness of the PAA layer, such Janus nanosheets transform a mechanically stable nanobowl upon pH change. Atomic force microscopy and transmission electron microscopy results confirmed the Janus structure and bending property. Detailed structural characterization and shape changing mechanisms will be discussed.

P1.00252 Meso-scale Modeling of Self-assembly of Polymer-Grafted Nanoparticles. DERRICK MANCINI, Illinois Inst of Tech, SANKET DESHMUKH, SUBRAMANIAN SANKARANARAYANAN, Argonne National Laboratory — We develop meso-scale models to explore the self-assembly behavior of polymer-grafted nanoparticles. Specifically, we study nanoparticles with grafts of the thermo-sensitive polymer N-isopropylacrylamide (PNIPAM), which undergoes a coil-to-globule transition across the LCST at around 305 K. The atomic-scale mechanism of the coil-to-globule transition of polymers grafted nanoparticles and their interactions (agglomeration, assembly behavior) with other particles that are in its vicinity is poorly understood, yet knowledge about these interactions would enable designing novel self-assembled materials with well-defined structural and dynamical properties. Additionally, the effects of chemical nature, geometry, and morphology of the nanoparticle surface on the conformational transition of thermo-sensitive polymers is also unknown. We report on 1) development of all-atom models of polymer-grafted nanoparticles to conduct MD simulations at atomic-levels and 2) perform mesoscopic scaling of the conformational dynamics resulting from the atomicistic simulations with the aid of coarse-grained or meso-scale models of PNIPAM and its composites. Coarse-grained simulations allow modeling of larger assemblies of polymer-grafted nanoparticles over longer time scales.

P1.00253 Mesoscopic Polymer Assemblies. SATYAN CHoudhARY, JONATHAN PHAM, ALFRED CROSBY, University of Massachusetts Amherst — Materials encompassing structural hierarchy and multi-functionality allow for remarkable physical properties across different length scales. Mesoscopic Polymer (MSP) assemblies provide a critical link, from nanometer to centimeter scales, in the definition of such hierarchical structures. Recent focus has been on exploiting these MSP assemblies for optical, electronic, photonics and biological applications. We demonstrate a novel fabrication method for MSP assemblies. The current fabrication methods restrict the length scale and volume of such assemblies. A new method, which we developed uses a simple piezo-actuated motion for de-pinning of a polymer solution trapped by capillary forces between a flexible blade and a rigid substrate. The advantages of new method include ability to make MSP of monodisperse length and to fabricate sufficient volumes of MSP to study their physical properties and functionality in liquid dispersions. We demonstrate the application of MSP as filler for soft materials, providing rheological studies of the MSP with surrounding matrices.

P1.00254 SURFACES INTERFACES AND POLYMERIC THIN FILMS –

P1.00255 Structure of polymer brushes on flat substrates and its dependence on the conditions of the surface-initiated polymerization. ROHAN PATIL, JIRI SROGL, North Carolina State Univ, DOUGLAS KISEROW. US Army Research Office, JAN GENZER, North Carolina State Univ — We demonstrate an efficient method of degrafting surface anchored poly(methyl methacrylate) brushes using tetra butyl ammonium fluoride (TBAF). The grafted polymers are grown using standard atom transfer radical polymerization method which provides good control by varying the catalyst ratio (Cu(H):Cu(II)). The sample surface has been characterized before and after degrafting by means of X-ray photoelectron spectroscopy, ellipsometry, and time-of-flight secondary ion mass spectrometry. The degrafted polymer has been characterized using highly sensitive size exclusion chromatography, which provided information about the complete molecular weight distribution. The grafting density of PMMA chains is calculated as 0.517 chains/nm². The study of the dependence of the grafting density on the ATRP inhibitor/catalyst ratio evidences to an effect of early termination of the growing chains when a lower control on the polymerization step is exercised. Control of the degrafting process is provided by tuning time, temperature, concentration of the TBAF, which - in conjunction with spatial control - allows for the creation of polymer brush patterns and surface gradients.

P1.00256 Tribological properties of adsorbed PEO nanolayers on planar solids. WENDUO ZENG, NAISHENG JIANG, JAKE LINDBERG, MAYA K. ENDOH, TADANORI KOGA, State University of New York at Stony Brook — We report tribological properties of irreversibly adsorbed poly(ethylene-oxide) (PEO) nanolayers onto planar Si substrates. The adsorbed nanolayers (~ 3 nm in thickness) were derived from spin-coat polymer thin films (~ 50 nm in thickness) via thermal annealing and subsequent solvent leaching with water. We characterized the formation process of the adsorbed nanolayers and the detailed surface/film structures by using x-ray reflectivity, grazing incidence x-ray diffraction, and atomic force microscopy. In addition, the contact angle and adhesive property of the adsorbed layers were characterized. We will discuss the structure-property relationship of the adsorbed nanolayers.

1 T. K. acknowledges the partial financial support from NSF Grant No. CMMI-1332499.
P1.00257 Effects of the Adsorbed Polymer Nanolayers on the Dewetting of Polystyrene Thin Films. JUSTIN CHEUNG, JIAXUN WANG, NAISHENG JIANG, MAYA ENDOH, TADANORI KOGA, Stony Brook University — It was previously reported that irreversibly adsorbed polymer nanolayers can be produced on solid substrates by thermal annealing. This study sought to determine the impact of the adsorbed nanolayers on film stability of ultrathin polystyrene (PS) films. A series of bilayers composed of the bottom PS adsorbed nanolayers and PS overlayers with different molecular weights were prepared as model systems. The surface structures of the bilayer films annealed above the bulk glass transition temperature were analyzed by using optical and atomic force microscopes. We will discuss the unique roles of the adsorbed polymer chains in the stability of the liquid thin films. 1 T. K. acknowledges the partial financial support from NSF Grant No. CMMI-1332499.

P1.00258 Coatings with Thermally Switchable Surface Energy Produced From Block Copolymer Membranes. RALEIGH DAVIS, RICHARD REGISTER, Princeton University — Polymer-based coatings are employed across a wide array of sectors. One application of such coatings is to impart a prescribed surface energy, i.e., hydrophilic or hydrophobic character. The present work explores an approach to create surfaces with thermally switchable wetting behavior by employing coatings based on block copolymers which possess both hydrophilic and hydrophobic segments. The amphiphilic block copolymers were synthesized by coupling allyl-ended poly(ethylene oxide) (PEO) and hydride-ended poly(dimethylsiloxane) (PDMS) oligomers via a Pt catalyst. One PEO-PDMS diblock possessed an order-disorder-transition-temperature (T_{ODT}) of 64°C as characterized by small angle x-ray scattering. Above the T_{ODT} the polymer is a disordered melt, but below this temperature it self-assembles into alternating lamellae with a repeat spacing of 7.7 nm. When cooled through the T_{ODT} in vacuum or dry air, the PDMS-enriched domains wet the film's surface, producing a hydrophobic surface with a contact angle (CA) ≈ 90° as measured from CA goniometry. However, when cooled under water or in humid air, a PEO-rich hydrophilic surface is produced, yielding CAs ranging from 20-40°. The coatings can then be reversibly switched between the two states by reheating above the T_{ODT}, exposing to the appropriate environment, and re-cooling, ideally “locking in” the structure until the next processing cycle. The T_{ODT}, and thus the switching temperature, can be continuously tuned by blending with PEO-PDMS diblocks of different molecular weights.

P1.00259 Potential Energy Calculations for Water Adsorption on Poly (methyl methacrylate)$.^1$ MATEUSZ J. ZUBA, PATRICK HOWARD, BRIAN FAMILIO, THORIN KANE, ROSS L. NETUSIL, CAROLINA C. ILIE, State University of New York at Oswego — The generosity of the NOYCE Research Grant enabled me to focus on the study of various polymers. The main goal was to study the molecular orbitals of poly (methyl methacrylate) (PMMA) and calculate the energy band gap. We also performed the potential energy calculations for our system: two polymer chains and water molecules. We obtained the activation energy from thermal desorption spectra of water on poly (methyl methacrylate) by employing Arrhenius analysis. 1 NSF - Noyce Scholarship Program

P1.00260 Macroion Interaction at Polyelectrolyte Brush Interfaces. CHEN QU, Univ of Notre Dame — The effect of macromolecules, including synthetic polyelectrolytes, DNA and proteins, on the structure and surface properties of charged polymer thin films remains inadequately understood partially due to the complexity involving the hydrophobic effect and the conformational change of polymeric macromolecules. In this work, we explore a group of inorganic nanocluster based macromolecules, hydrophilic polyoxometalates (POMs) of robust nanocluster structure and carrying high surface charges (~ 2-42 negative charges) to investigate their interaction with surface tethered poly-2-vinylpyridine (P2VP) brush-like thin films immersed in aqueous solution. We observe the collapse of swollen P2VP chains by adding POM macroions of increased concentration by AFM, QCM and contact goniometer measurements, in sharp contrast to the increased chain stretching by adding monovalent salts. A careful comparison is made between distinct POMs based on their charge, size and chemical nature. These findings serve as a good reference for theoretical model modification and design of new mesoporous composite membranes.

P1.00261 Elastocapillarity: Adhesion and Wetting in Soft Polymeric Systems$.^1$ ZHEN CAO, Univ of Connecticut - Storrs, MARK STEVENS, Sandia National Laboratories, ANDREY DÖBRYNIN, Univ of Connecticut - Storrs — We study interactions of nanoparticles with adhesive elastic substrates by using molecular dynamics simulations and theoretical calculations. The deformation of nanoparticles and substrates are obtained as a function of the nanoparticle and substrate shear modulus, nanoparticle size, and strength of interactions. There are two different interaction regimes between nanoparticles and substrates. The classical JKR model can be applied to describe adhesion of strongly cross-linked large nanoparticles on rigid substrates when small nanoparticle deformations and substrate indentation take place. In this adhesion regime the deformation of nanoparticles and substrates is determined by balancing the elastic energy of deformation and the work of adhesion between a nanoparticle and a substrate. However, for the weekly cross-linked (soft) systems, the change of the surface energy of nanoparticle and substrate could play an important role in controlling nanoparticle-substrate interactions. In this so-called wetting regime the interaction between nanoparticle and substrate is determined by the surface tension of substrate or nanoparticle and the work of adhesion. We developed an analytical model describing crossover between adhesion and wetting regimes. In the framework of this model a crossover between different interaction regimes is controlled by a universal dimensionless parameter. 1 NSF # DMR-1004576 DMR-1409710

P1.00262 ABSTRACT MOVED TO V1.00023 —

P1.00263 Understanding “grafting through” polymerization reactions involving surface-bound monomers. PREETI DATTA, JAN GENZER, North Carolina State Univ — “Grafting through” polymerization is based on a bulk radical polymerization reaction utilizing a self-assembled monolayer that contain polymerizable units. Free polymer chains formed in solution can incorporate the surface-bound monomers, and thereby, get covalently bonded to the surface. As more growing chains attach to the surface-bound monomers, an immobilized polymer layer is formed on the surface. We use a combination of computer simulation and experiments to comprehend this process. Specifically, we report on the effect of spatial density of the surface-monomers on the formation of the surface-bound polymers. We use a lattice-based bond fluctuation model with periodic boundary conditions to simulate such systems. For experimental validation, we create gradients of density of methacrylate units on flat Si wafers using silane chemistry. The proximity of the surface-bound polymerizable units promotes the “grafting through” process but prevents more free growing chains to “graft to” the polymerizable units. Our studies indicate that these two counter-active effects balance each other and do not affect the overall density of the surface-bound polymer layer, except in case of the highest theoretical packing density of surface-bound monomers.

P1.00264
The work of adhesion and separation between soft elastomers is commonly used soft elastomers PDMS (Sylgard 184) and Ecoflex 0300 are obtained with the measured pull-in and pull-off forces using a dynamical mechanical analyzer (DMA). The effect of crosslinking density and solvent extraction are examined. It is found that the pull-in adhesion stays more or less constant for all contact pairs we measured. While the effect of crosslinking density is not significant for pristine PDMS, it is very obvious that the higher self-adhesion can be found in less crosslinked PDMS after solvent extraction. Such an effect is even more drastic for PDMS-to-Ecoflex adhesion. A unified adhesion mechanism is proposed to explain these complex adhesion behaviors. It is concluded that the chain-matrix interaction is the most effective adhesion mechanism compared to chain-chain or matrix-matrix interactions and the three interactions are exclusive to each other.

*This work is supported by the NSF CMMI award under Grant No. 1301335.

**P1.00265 Programming Surface Energy Driven Marangoni Convection in Polymer Thin Films to Generate Topographic Patterns**

CHAEBIN KIM, DUSTIN JANES, TALHA ARSHAD, JOSHUA KATZENSTEIN, NATHAN PRISCO, DANA MCGUFFIN, ROGER BONNCEACZE, CHRISTOPHER ELLISON, University of Texas at Austin - McKetta Department of Chemical Engineering — The Marangoni effect describes how fluid flows in response to gradients in surface energy. We recently developed a method for photochemically preprogramming spatial surface energy patterns in glassy polystyrene (PS) thin films. UV irradiation through a mask selectively dehydrogenates the PS, thus increasing surface energy in the UV exposed regions compared to the unexposed regions. After heating the film to the liquid state, transport of polymer occurs from regions of low surface energy to regions of high surface energy. This method can be harnessed to rapidly manufacture polymer films possessing prescribed three-dimensional topographies reflective of the original light exposure pattern. To quantify and verify this phenomenon, a theoretical model that gives a more thorough understanding of the physics of this process, its limits and ways to apply it efficiently for various target metrics will also be presented along with comparisons between theoretical predictions and experimental observations. Finally, while PS dehydrogenation can be used to produce a variety of topographical patterns, judicious selection of the photosensitizing compounds in an otherwise transparent polymer expands the use of this method to more readily available light sources.

**P1.00266 BLOCK COPOLYMER THIN FILMS —**

**P1.00267 Effect of Hydrogen Bonding on the interfacial width of PS-b-PMMA Block Copolymer Microdomains**

KYUSEONG LEE, SUNGHYUN HAN, SANGSHIN JANG, JICHEOL PARK, JONGHEON KWAK, JIN KON KIM, Pohang Univ of Sci & Tech — Sharp interface between two blocks in block copolymer nano pattern is one of the important issues because of strong demand in industrial applications to nano-patterning. We utilized hydrogen bonding between N-(4-aminomethyl-benzyl)-1-hydroxymethyl-bezamid (BA) and urea (U) at the interface of polystyrene-block-poly(methyl methacrylate) copolymer (PS-PMMA). For this purpose, we first synthesized PS by ATRP method, then the end group was converted to amino group. Next, it was reacted with BA, followed by reaction with 4-pentynoic acid, resulting in alkyne-terminated polymer/substrate interactions on silica substrates, and the other set possessing repulsive polymer/substrate interactions using poly(cyclohexylethylene) substrate. D was measured in the melt state (Tg = 48 K) and the D of thick films were identical to the bulk value regardless of the substrate type. The D of a ~19 nm thick film on a repulsive substrate was four times larger than its bulk value while Tg was increased by about 10-15 K. In contrast, attractive substrates typically do not affect D or Tg of PIbMA.

**P1.00268 Long-Range Ordering of Block Copolymers on Well-Controlled Patterned Substrates**

DONG-EUN LEE, NAM-KYUN KIM, JINA PARK, DONGHYUN LEE, Dankook University — In this study, we achieved long-range ordering of block copolymers (BCPs) by combining solvent-annealing process and well-controlled patterned substrates. Nano-lines of poly(tetrafluoro ethylene) (PTFE) were firstly fabricated in large area as a PTFE bar was rubbed on Si substrates at 340 °C. The amplitude and pitch distance of PTFE nanolines were around 17 nm and 150 nm, respectively. Then, asymmetric polystyrene-block-poly(2-vinylpyridine) copolymers (PS-b-P2VP) were subsequently spin-coated on the patterned substrates after a thin layer of poly(vinyl alcohol) (PVA) was prepared on the PTFE patterned substrates to enhance the wettability of BCP thin films. As BCP thin films were solvent-annealed in vapor of organic solvents, highly ordered BCP nanostructures oriented either parallel or perpendicular to the surface were generated in large area. In addition, the nanopatterns were successfully transferred to the underlying PVA layer or Si substrate by dry etching. Thus, the resulting nanopatterns were utilized as templates to synthesize inorganic nanostructures. The ordering behavior of BCP thin films on the patterned substrates was characterized by using AFM, SEM and GI-SAXS.

**P1.00270 Macroscopic Alignment of Cylindrical Block Polymer Thin Film via Raster Solvent Vapor Annealing with Soft Shear**

MING LUO, DOUGLAS SCOTT, THOMAS EPPS, University of Delaware — One challenge associated with the utilization of block polymer thin films in nanotechnology is the difficulty of orienting and aligning the self-assembled nanostructure on macroscopic length scales, as block polymers typically self-assemble in an isotropic manner in the absence of surface forces and external fields. In this work, macroscopic alignment of block polymer cylinders was achieved through raster solvent vapor annealing with soft shear. Spatial control over nanoscale structures was accomplished through the application of a solvent vapor delivery nozzle, poly(dimethylsiloxane) shearing pad, and motorized stage. Complex patterns such as dashes, cross-shapes, and curved structures were demonstrated along with the possibility of scale-up for industry production. The simplicity of instrumentation and the versatility of patterns possess advantages over other directed self-assembly methods that are currently available.
P1.00271 Tracking Solvent Uptake in Block Polymer Thin Films during Solvent Vapor Annealing. CAMERON SHELTON, University of Delaware, RONALD JONES, JOSEPH DURA, National Institute of Standards and Technology, THOMAS EPPS, University of Delaware — A key goal in the block polymer (BP) thin films community is the design of a template-free, universal annealing method to control nanoscale self-assembly over large length scales. Solvent vapor annealing (SVA) offers a unique solution to this challenge with its ability to tune substrate surface, free surface, and polymer-polymer interactions by exposing films to appropriate solvents. However, there is little understanding of how the solvent behaves during the SVA process. In this work, we utilized the combination of deuterated solvents with small-angle neutron scattering (SANS) and neutron reflectometry to track solvent uptake in poly(styrene-b-isoprene-b-styrene) thin films. Two solvents were chosen for this analysis: d-hexane (isoprene selective) and d-benzene (styrne selective). Our work has shown that solvent choice and partial pressure have a significant impact on how solvent segregates within individual polymer domains and the film as a whole, directly impacting the restructuring of polymer domains. This work provides further understanding of the mechanism behind SVA, thereby making it easier to select appropriate conditions for desired self-assembly control.

P1.00272 ABSTRACT WITHDRAWN

P1.00273 Optimization and Characterization of Self-assembled Triblock Polymer Membranes with Chemically-Tunable Pore Walls for Nanofiltration Applications. JESSICA SARGENT, RYAN MULVENNA, RAFAEL PRATO, Purdue University, JACOB WEIDMAN, WILLIAM PHILLIP, University of Notre Dame, BRYAN BOUDOURIS, Purdue University — The field of block polymer-based membranes for separation applications has grown considerably in the past several years. However, decreasing the domain sizes of these membranes to below 5 nm has proven to be a challenge in many instances. Here, we demonstrate that a triblock polymer, polyisoprene-polystyrene-block-poly(tert-butyl methacrylate) (PI-PS-PIBMA), can be utilized to form nanoporous membranes capable of high flux and high selectivity based on both size and chemical composition. By controlling the synthesis, solution self-assembly, and non-solvent induced phase separation of these polymers, a scalable fabrication process can produce the thin-film membranes that feature monodisperse pores approaching 1 nm in diameter, tunable pore-wall chemistry, good mechanical stability, and chlorine degradation resistance. The PI-PS-PIBMA functionality can further be converted to a number of side chain functionalities through simple coupling chemistry to produce membranes with specific chemical and structural characteristics tailored to meet the needs of various applications. In particular, these membranes provide a promising, inexpensive platform for chlorine degradation and fouling-resistant membranes for water purification that can be produced on an industrial scale.

P1.00274 Thin Films of Bottlebrush Block Copolymers with Homopolymer. GAJIN JEONG, Univ of Mass - Amherst, BENJAMIN R. SVEINBJORNSSON, ROBERT HOWARD GRUBBS, California Institute of Technology, THOMAS P. RUSSELL, Univ of Mass - Amherst, POLYMER SCIENCE AND ENGINEERING DEPARTMENT, UNIVERSITY OF MASSACHUSETTS AMHERST TEAM, CHEMISTRY DEPARTMENT, CALIFORNIA INSTITUTE OF TECHNOLOGY TEAM — We have investigated the self assembled structures of bottlebrush block copolymers (BrBCPs) in thin films by blending deuterated homopolymer. By use of neutron reflectivity (NR), the assemblies with microdomain oriented parallel to the substrate, the distribution of the homopolymer in the bottlebrush block copolymer was obtained. Polynorbornene-backbone-based bottlebrush BCPS with polylactide (PLA) and polystyrene (PS) side chains of different molecular weights were investigated. Small angle x-ray scattering was used to complement the NR studies.

P1.00275 Investigation of solvent annealing time dependence on morphology formation in polystyrene–block–polylactide thin films. RYAN GNABASIK, GUNNAR NELSON, ANDREW BARUTH, Creighton Univ — Solvent vapor annealing exposes a block polymer film to the vapors of one or more solvents, swelling the film. This process increases polymer mobility and can direct a self-assembly process by tuning the surface energy. Despite its efficacy to produce well-ordered, periodic nanostructures, no standardized production scheme exists. This is primarily due to a lack of understanding the intricate role multiple, incommensurate parameters play. By analogy to thermal annealing of elemental solids, the time a thin film spends in an equilibrium solvent concentration is one factor that will dictate the degree of ordering. To elucidate, optimized annealing conditions for perpendicular cylinder forming polystyrene-block-polylactide exist at solvent concentrations just below the order-disorder transition, where the kinetic and thermal processes required for recrystallization and crystal growth are optimally fast (similar to thermal annealing). By use of a purpose-built, climate-controlled solvent annealing chamber, we map out the annealing time dependence for non-optimized solvent concentrations. Namely, at lower solvent concentrations, where mobility is limited, longer times are required for large lateral correlation lengths. In situ spectral reflectance monitors solvent concentration, regulated via a mass-flow controlled solvent inlet, offering precision control over annealing. Atomic force microscopy, in conjunction with O2 plasma etching, provides 3-dimensional imaging of the nanoscale morphology. This work was funded by NASA Nebraska Space Grant.

P1.00276 Controlling Structure in Sulfonated Block Copolymer Membranes. PHUC TRUONG, GILA STEIN, Univ of Houston, JOE STRZALKA, Argonne National Lab — In many ionically block copolymer systems, the strong incompatibility between ionic and non-ionic segments will trap non-equilibrium structures in the film, making it difficult to engineer the optimal domain sizes and transport pathways. The goal of this work is to establish a framework for controlling the solid-state structure of sulfonated pentablock copolymer membranes. They have ABCBA block sequence, where A is polystyrene, B is poly(hydrogenated isoprene), and C is poly(styrene sulfonate). To process into films, the polymer is dissolved in toluene/n-propanol solvent mixtures, where the solvent proportions and the polymer loading were both varied. Solution-state structure was measured with small angle X-ray scattering (SAXS). We detected micelles with radii that depend on the solvent composition and polymer loading. Film structure was measured with grazing-incidence SAXS, which shows (i) domain periodicity is constant throughout film thickness; (ii) domain periodicity depends on solvent composition and polymer loading, and approximately matches the micelle radii in solutions. The solid-state packing is consistent with a hard sphere structure factor. Results suggest that solid-state structure can be tuned by manipulating the solution-state self-assembly.

P1.00277 Capillary forces induced wrinkling onto ultrathin single and bilayer polymer films. JOOYOUNG CHANG, JOSEPH PAULSEN, KAMIL TOGA,1 NARAYANAN MENON, THOMAS RUSSELL, Univ of Mass - Amherst — We have studied wrinkling phenomena on ultrathin polymer sheets floated onto the aqueous media. As previously studied (Science, 2007, 317(5838), 650–653, and Soft Matter, 2013, 9, 8289–8296), the capillary forces of a water droplet placed on a floating sheet generate compressive hoop stresses, causing the sheet to wrinkle. In our current work, we investigate this phenomenon over a broader range of film thicknesses (7 nm to 950 nm) of Polystyrene (PS), Poly(methyl methacrylate) (PMMA), as well as with PS/PMMA bilayers. We report that the Young’s modulus of PS (Mw: 97K) inferred from the wrinkle pattern is not significantly affected even if the thickness of PS is less than 10 nm. Furthermore, we also show that the type of the polymer (i.e. PS or PMMA) of the bottom layer of the bilayer system affects the length of the wrinkles.

1Keck Foundation
2Kamil Bugra Toga is currently working at Eastman Chemical Company.

P1.00278 POLYMER COMPOSITES —
P1.00279 Electrical Properties of PVDF Based Nanocomposites, JERRY CONTRERAS, HEINRICH D. FOLTZ, YUNPING DUAN, Dalian University of Technology, China, HASINA F. HHUQ, STEVEN C. TIDROW, MIRCEA CHIPARA, The University of Texas Pan American — Nanocomposites based on polyvinylidene fluoride (PVDF) have been obtained by melt mixing, loading the polymeric matrix with various weight fraction (between 0 % and 40 %) of different fillers (multiwalled carbon nanotubes, carbon nanofibers, and barium titanate). Pellets of nanocomposites have been obtained by hot pressing at about 175 °C. Copper contacts have been deposited on the as obtained pellets and the electrical features have been measured by using the two point technique. PVDF is a semicrystalline ferroelectric and piezoelectric polymer with a glass transition temperature of -35 °C and a melting temperature of about 175 °C. Electrical measurements have been performed in a wide range of frequencies starting from dc to ac (up to about 250 MHz). The dependence of the resistivity and dielectric constant on frequency and temperature (between -50 °C to 150 °C) was investigated in detail. Supplementary DSC, WAXS, and Raman data provided detailed information regarding the effect of fillers on phase transitions (glass, crystallization, and melting) and crystalline composition/structure of these nanocomposites.

P1.00280 Additive-Driven Assembly of Block Copolymer and Nanoparticles: Influence of Nanoparticle Size and Loading1, YUE GAI, Univ of Mass - Amherst, YING LIN2, 3M, JAMES WATKINS3, Univ of Mass - Amherst — Additive-driven assembly of block copolymer (BCP)/nanoparticle (NP) composites in which functionalized NPs exhibiting strong hydrogen bond interactions with one domain of the BCP has been shown to strengthen phase segregation and yield well-ordered materials at high NP loadings. Here we report a systemic study of how phase behavior and NP distribution in BCP/ NP composites are influenced by the NP size, NP loading and block copolymer domain size. 2nm, 5nm, 9nm and 15nm diameter Au nanoparticles at loadings ranging from 10% to 50% weight percent, in polystyrene-block-poly (2-vinyl pyridine) block copolymers with domain spacing ranging from 14 nm to 75 nm were used in the investigation. We find that strong interactions enable the incorporation of larger diameter NPs with respect to domain size as compared to systems in which interactions between the NP and BCP are weak or enthalpically neutral. 1This work was supported by NSF Center for Hierarchical Manufacturing at the University of Massachusetts, Amherst 2previous post-doc in Univ of Massachusetts, Amherst 3PI

P1.00281 Mechanically Robust Polymer-Graphene Aerogels, HEONJOO HA, University of Texas at Austin - McKetta Department of Chemical Engineering, KADHIRAVAN SHANMUGANATHAN, National Chemical Laboratory, Pune, Maharashtra, India, CHRISTOPHER ELLISON, University of Texas at Austin - McKetta Department of Chemical Engineering — Graphene oxide (GO) aerogels are particularly interesting due to their light weight and excellent performance in various applications, such as environmental remediation, super-hydrophobic and super-oleophobic materials, energy storage, etc. However, GO aerogels are generally weak and delicate which complicates their handling and potentially limits their application outside the research lab. The focus of this work is to synthesize mechanically stable aerogels that are robust and easy to handle without substantially sacrificing their low density. To overcome this challenge, we found that by intermixing a small amount of readily available and thermally crosslinkable manufacturing polymer can enhance the mechanical properties without disrupting other characteristic intrinsic properties of the aerogel itself. This method is a simple straightforward procedure that does not include any tedious chemical reactions or harsh chemicals. Furthermore, we will demonstrate the performance of these materials as a super-absorbent and pressure sensor.

P1.00282 Life-time of the bound layer in nanocomposites, DAN ZHAO, JACQUES JESTIN, SANAT K. KUMAR, Columbia University — It is now well accepted that an effectively irreversibly adsorbed monolayer of polymer forms when a polymer melt is intimately mixed with nanoparticles, in the limit where their enthalpic interactions are favorable. This bound layer has been postulated as being a central player in many of the highly favorable properties that result from polymer based nanocomposite materials. We investigated well-defined nanocomposites formed with different combinations of deuterated and hydrogenated polymers (P2VP and PMMA) and silica nanoparticles. SANS, in conjunction with contrast variation, then provides a direct means of probing the structure of the bound layer as a core-shell and its exchange kinetics with bulk (unbound) chains with annealing time and temperature. SAXS directly provides information on the particle-particle partial structure factor and particle dispersion. Thermodynamic equilibrium of the bound layer is reached one day at 150 °C while its exchange life time is ~ one hour at 180 °C.

P1.00283 POLYMER NANOCOMPOSITES: ACTIVE PARTICLES AND DYNAMICS —

P1.00284 Unusual dielectric loss properties of carbon nanotube - polyvinylidene fluoride composites in low frequency region (100 Hz < \( f < 1 \) MHz)1, GUANG-LIN ZHAO, YI ZHEN, JUAN ARREDONDO, Physics Department, Southern University and A&M College — Systematic investigations on the dielectric properties of multi-walled carbon nanotubes (MWCNTs)-polyvinylidene fluoride (PVDF) composites with a wide MWCNT concentration range (2-9wt%) have been carried out. It was revealed that the dielectric constant are increased by the addition of an appropriate amount of MWCNTs at room temperature. However, when the concentration of MWCNTs in the composites reaches above 5wt%, negative dielectric constants and large dielectric loss in the composites are observed in the low frequency range. The ferroelectric CNT-PVDF polymer composites containing more than 5 wt% MWCNTs have a strong dielectric absorption, which has the potential for acoustic applications. 1The work was funded in part by AFOSR (Award No. FA9550-09-1-0367) and by NSF LASIGMA Project (Award No. EPS-1003897, NSF92010-15-RII-SUBR).

P1.00285 Dispersion of bimodal polymer brushes functionalized anisotropic gold nanoparticles in polymer nanocomposites1, LILI ZHU, Peking University Shenzhen Graduate School, GI XUE, Nanjing University, LINDA REVEN, McGill University — Polymer nanocomposites (PNCs), which are composed of the nanofiller component and polymer matrix, have attracted growing interests due to their fascinating properties. Great efforts have been made to achieve high compatibility between the nanofillers and the polymer matrix. The dispersion of spherical gold nanoparticles (GNPs) in the matrix have been extensively studied, while there are few studies using anisotropic GNPs. The goal of this work is to produce homogeneous PNCs of anisotropic NPs in stimuli responsive polymer matrix. We compared the dispersion of gold nanoprisms (GNPRs) with single and bimodal poly(2-vinylpyridine) P2VP brushes. Bimodal brushes consisted of mixture of low and high molecular weight (Mw) polymers. GNPRs with P2VP were dispersed into polymer matrix and the Mw of the matrix was systematically varied to investigate the Mw effect. UV-Visible-Near Infrared spectroscopy was utilized to monitor the special plasmonic properties and architectures of GNPRs. The dispersion and morphology of PNCs were characterized by electron microscopy. This work will help to establish the correlations between the properties of anisotropic NPs (shape and protecting ligands) and the miscibility of corresponding PNCs. 1We gratefully acknowledge the National Science Foundation of China (nos.21404002)
P1.00286 Time-resolved WAXD studies on the crystallization of isotactic polypropylene/graphene nanocomposites. SHOTARO NISHITSUJI, MAYA ENDOH, YICHEN GUO, MIRIAM RAFAILOVICH, TADANORI KOGA, Department of Materials Science and Engineering, Stony Brook University — Graphene is one layer of carbon atoms, which has good electronic, thermal conductivity and mechanical properties. By adding graphene to isotactic polypropylene (iPP), the mechanical and electrical properties of the polymer are significantly improved. To further achieve high performance of iPP/graphene nanocomposites (“NCs”), it is important to investigate the relationship between the crystalline structure of iPP and the mechanical property of the iPP/graphene NCs. In this study, the effect of the graphene on the crystallization behavior of the polymer was investigated by using time-resolved wide angle X-ray diffraction (WAXD). The iPP/graphene NCs with different weight ratios of graphene were prepared by using a twin screw extruder. After temperature jump from 210 °C (>Tm) to 170 °C, the melt-crystallization process was observed by in situ WAXD. The results showed that the crystalline structure of all the samples was still α-form that is the same as the neat PP, while the ratios of the diffraction peaks are quite different from those of the neat PP. We will discuss the detailed structure in this presentation.

P1.00287 Rheology and Phase Transitions in Highly Filled Additive/Block Copolymer Composites. BENJAMIN M. YAVITT1, ROHIT KOTHARI2, H. HENNING WINTER3, JAMES J. WATKINS4, University of Massachusetts Amherst — We have recently demonstrated that strong, segment-specific interactions between multi-functional additives (organics, nanoparticles and nanotubes) and one segment of a block copolymer can yield highly filled, well-ordered composites. In this study we used rheology to determine phase transitions and materials properties in systems containing high volume fractions of nanoparticles that are not accessible in other ways. We utilized well-defined surface functionalized nanoparticle systems by which we can assess the role of the number, strength, and surface density of functional groups on the phase behavior and mechanical properties of the composites. From this study, we developed an understanding of the interactions and structure between nanoparticles and block copolymer, and the mechanisms by which these characteristics are affected by temperature.

P1.00288 PEO-MWCNTs Nanocomposites: The Effect of the Nature of Solvent on the Morphology and Physical Properties of Nanocomposites. ALFONSO SALINAS, CHARLES CARTWRIGHT, KEVIN L. NEWCOMBE, MIRCEA CHIPARA, IBRAHIM ELAMIN, JAMES HINTHORNE, DORINA M. CHIPARA, KAREN LOZANO, The University of Texas Pan American — Polyaniline (PANI) nanocomposites have been obtained by dissolving the polymer within selected solvents (water, ethanol, toluene, and chloroform), addition of the nanofiller (Multiwalled Carbon Nanotubes: MWCNTs), dispersion of the as obtained mixture by stirring at 500 rotation per minute for 1 h followed by a sonication for 30 minutes using a high power sonicator (500 W), and solvent evaporation in an oven at 110 °C, for 10 h. Nanocomposites containing 0 to 40 wt. MWCNTs have been obtained and investigated. Scanning Electron Microscopy was used to assess the dispersion of MWCNTs within the polymeric matrix. Wide Angle X-Ray Scattering, Raman, FTIR, and UV-VIS were used to characterize the crystalline structure and molecular/atomic motions in the as obtained samples. Differential Scanning Calorimetry was used to estimate the glass, crystallization, and melting temperatures. Thermal stability will be questioned by thermogravimetric analysis. The effect of the nature of the solvent on the dispersion of nanotubes and on the physical properties of the as obtained nanocomposites will be analyzed in detail.

P1.00289 Photo-actuating waveguiding fibers based on light responsive hydrogels. YING ZHOU, ADAM HAUSER, Uni of Mass - Amherst, NATHAN RASMUSSEN, MARK KUZYK, Washington State University, RYAN HAYWARD, Uni of Mass - Amherst — The combination of light-absorbing nanoparticles with thermally sensitive hydrogels has been widely explored as a strategy for photo-thermal actuation. Here, we employ a system of photo-crosslinkable copolymers containing pendant benzophenone units to prepare planar waveguiding polymethylmethacrylate(PMMA) fibers patterned with poly(N-isopropyl acrylamide) (PNIPAM) copolymer hydrogels containing Au nanoparticles. These structures show both thermally- and photo-actuated bending behavior due to swelling stresses developed in the PNIPAM gel layer. Further, we establish that light can be successfully guided through micro-patterned fibers, yielding a route to remotely controlled micro-actuators.

P1.00290 Polymer Crafted Nanoparticle-based Oil Dispersants. DAEHAK KIM, RAMANAN KRISHNAMOORTI, Univ of Houston — Particle-based oil dispersants mainly composed of inorganic nanoparticles such as silica nanoparticles are considered as environmentally friendly oil dispersants due to their biocompatibility and relatively low toxicity. The oil-water interfacial tension is reduced when nanoparticles segregate to the oil-water interface and this segregation is improved by grafting interfacially active polymer brushes. In this study, surfactant-like amphiphilic block copolymers were grafted from silica nanoparticles using an atom transfer radical polymerization (ATRP) method in order to increase their interfacial activity. We have studied the interfacial activity of such hybrid nanoparticles using pendant drop interfacial tension measurements, and their structure using small angle X-ray scattering. Amphiphilic copolymer grafted nanoparticles significantly reduced oil-water interfacial tension compared to the interfacial tension reduction induced by homopolymer grafted nanoparticles or the corresponding free ungrafted copolymer. Moreover, hard and stable oil-water emulsions were formed by applying the block copolymer grafted nanoparticles due to the formation of interfacial nanoparticle structures, which were observed by cryo-scanning electron microscopy (SEM) and small angle neutron scattering (SANS).

P1.00291 PNIPAM grafted on the surface of zirconium phosphate. HAI LI, XUEZHEN WANG, ZHENGDONG CHENG, Texas A&M Univ, DR.CHENG’S GROUP TEAM — We are reporting for the first time the grafting of the thermoresponsive polymer PNIPAM (poly N-isopropylacrylamide) on the surface of inorganic nanophases zirconium phosphate. Particularly, the grafting on inorganic nanophases using gamma rays has never scarcely been reported and yet proved to be successful in our synthesis. We proved that by gamma ray irradiation, the peroxide groups has been produced on the ZrP particles since that peroxide groups, on the surface of the hexagonal nanophases, which upon heating initiated the free radical polymerization and subsequent attachment of PNIPAM. The presence of covalent bond between ZrP and PNIPAM were observed and characterized by TGA, FTIR and solid state NMR respectively. The attachment of a thermoresponsive polymer to ZrP nanocrystals brings thus remarkable possibilities for their employment in the fields of medicine, oil industry, as well as physics.

P1.00292 Toward Designer Nanoparticle Assemblies: Supramolecular Nanocomposites on Patterned Surfaces. KATHERINE EVANS, JOSEPH KAO, TING XU, Univ of California - Berkeley — Nanoparticles have unique properties due to the quantum confinement effect. Controlled assemblies of nanoparticles of different sizes and chemical composition are predicted to have new optoelectronic properties. Supramolecules are ideal structural framework to guide nanoparticle assemblies in thin films without modifying the particle ligand chemistry. We recently showed that optically patterned trench patterns can effectively guide the assembly of supramolecular nanocomposites over micrometer to form aligned nanoparticle lines. I will report our recent investigation on more complex patterns to evaluate how the curvature of the pattern affects the nanoparticle assembly. Preliminary studies show potential for controlling and tailoring nanoparticle assemblies, and in turn, the optical properties of such assemblies.
P1.00293 Fluorescence in nanocomposites based on polyethylene oxides and block copolymers of polyethylene oxide-polypropylene oxide loaded with rare earth doped fluorides. BRIAN YUST, Univ of Texas, Pan American. FRANCISCO PEDRAZA, DHIRAJ SARDAR, University of Texas at San Antonio, AARON SAENZ, MIRCEA CHIPARA, Univ of Texas, Pan American — Rare earth doped fluoride nanoparticles with a size of about 25 nm have been synthesized by a solvothermal process. Polymer-based nanocomposites, containing various weight fraction of nanofillers, have been obtained by dissolving the polymeric matrix (polyethylene oxide) within a solvent (deionized water), adding the nanoparticles, sonicating the mixture, and finally removing the solvent. The complete removal of the solvent has been confirmed by Thermogravimetric Analysis. Additional information about the thermal features have been obtained by Differential Scanning Calorimetry, Wide Angle X-Ray Scattering, FTIR, UV-Visible, and Raman. The effect of the loading with nanoparticles on the glass, crystallization, and melting transition temperatures of the polymeric matrix are reported. Fluorescence of rare earth doped nanoparticles dispersed within the polymeric matrix has been tested by laser spectroscopy. The dependence of fluorescence intensity on the concentration of nanoparticles and on temperature in the range 300 to 400 K is analyzed.

P1.00294 Anisotropic Polymer Conformations in Aligned SWCNT/PS Nanocomposites, WEI-SHAO TUNG, RUSSELL COMPOSTO, University of Pennsylvania, NIGEL CLARKE, University of Sheffield, KAREN WINEY, University of Pennsylvania — In our previous study of isotropic SWCNT/polystyrene (PS) nanocomposites, we found that the polymer radius of gyration (Rg) increases and the SWCNT mesh size decreases with increasing SWCNT concentration. Here, we investigate the effect of aligning SWCNTs on Rg and the SWCNT mesh. SWCNT alignment was accomplished by melt fiber spinning or extrusion, and small angle neutron scattering was used to probe the structure. As expected, SWCNT alignment produces anisotropic meshes. Below 2 wt% SWCNT, no significant change in Rg is observed and Rg parallel and perpendicular to the direction of SWCNT alignment are comparable. More interestingly, at higher wt% SWCNT the polymer conformations are anisotropic with a larger Rg perpendicular to the SWCNT than along the SWCNT. For example, with 6 wt% SWCNT, the Rg perpendicular to the SWCNT is ~15% larger than parallel to the SWCNT. This anisotropy in the polymer conformation becomes more prominent at higher SWCNT concentrations, perhaps because at higher SWCNT concentrations the distribution of mesh shifts to smaller meshes (<2Rg) so that a single polymer chain interacts with multiple SWCNTs. Implications of this finding will be discussed.

P1.00295 THE PHYSICS OF CONFINED FLUIDS –

P1.00296 Capillary instability of periodic polymer structures: Influence of viscosity, substrate confinement and local curvature, ZHENG ZHANG, YIFU DING, Univ of Colorado - Boulder — We investigate the simultaneous capillary instability among periodic polymer lithographic structures supported on an immiscible viscous medium. The first system we studied was straight polystyrene (PS) stripes arranged in parallel in PMMA medium. When annealed at a temperature above the glass transition temperature of both polymers, the stripes undulated and then ruptured via capillary instability. We found that the PS-to-PMMA viscosity ratio strongly affected the rupture kinetics, while it had little influence on the rupture wavelength. The rupture behavior of those stripes could be drastically altered due to initial spacing and substrate confinement. For closely-neighboring stripes that were confined on a rigid substrate, the capillary waves became correlated in-phase among neighbors. Under strong confinement, the capillary rupture was always correlated, irrespective of the viscosity ratio. In addition, we examined the influence of in-plane curvature on capillary instability in concentrically arranged PS rings. When the rings were relatively far apart, their rupture behaviors were independent from each other; when they were close to each other, the primary mode in the capillary breakup became strongly correlated from the center towards the peripheral.

P1.00297 Static and Dynamic Capillary Forces in Pollen Adhesion and Detachment, CARSON MEREDITH, DONGGLEE SHIN, HAISHENG LIN, Georgia Tech — Nature provides remarkable examples of adhesive bioparticles including diatoms, pollens, and fungal spores, which are robust examples of nature’s solutions to particle adhesion. These particle’s interactions are often mediated by liquid films at micro- and nanometer length scales, and their study can lead to new physical insights into confined fluids. This talk will detail recent discoveries of the wet adhesive mechanisms of pollen, which provide useful insights into the role of capillary forces and confined fluids in nature. In particular, we describe how pollenkitt, a viscous fluid coating many pollen particles, forms nanoscale capillary bridges that mediate the adhesion and detachment of pollens from surfaces of insects and plants. We will present experimentally observed static and dynamic regimes of pollenkitt capillary forces. Models are utilized to understand the role of rheological properties of pollenkitt in creating these forces. Importantly, the forces generated by pollenkitt give pollen attachment and release from surfaces a sensitive dependence on humidity, rate, and surface morphology. This talk will explore how the physics of these forces contributes to pollination in nature and how they might be harnessed to engineer new materials.

P1.00298 EXTREME MECHANICS: CONTORTION OF RILAMENTS, RIBBONS AND BUNDLES –

P1.00299 EXTREME MECHANICS OF ORIGAMI: FOLDING, MECHANISMS AND MECHANICS –

P1.00300 Hysteretic self-folding of micro-scale polymer origami films, JUN-HEE NA, University of Massachusetts Amherst, JESSE SILVERBERG, Cornell University, ARTHUR EVANS, CHRISTIAN SANTANGELÒ, University of Massachusetts Amherst, THOMAS HULL, Western New England University, ITAI COHEN, Cornell University, RYAN HAYWARD, University of Massachusetts Amherst — Origami-inspired self-folding materials have attracted interest for the design of actuators and remotely deployable devices. While well-established geometric rules have been used to create rigidly self-foldable origami structures, the behavior of non-rigidly foldable crease patterns remains incompletely understood. In particular, understanding the relationship between crease geometry and the resulting elastic energy barrier remains a central challenge. Here, we describe a simple model system based on the well-known square twist folding pattern to explore how self-folding structures overcome such energy barriers, and the resulting hysteresis in the folding/unfolding behavior. We show that the magnitude of the hysteresis can be tuned by variations in the plane angle characterizing the crease pattern, as well as by selectively weakening the panel diagonals to reduce the energy cost of bending. These results provide insights into geometrically-controlled energy barriers in non-rigidly foldable origami and design rules for the construction of bistable self-folding systems.

P1.00301 CONFORMATIONS AND DYNAMICS OF BIOPOLYMERS –
**P1.00302 Conformations and dynamics of a translocating semi-flexible chain through a Nanopore facilitated by chaperones**, RAMESH ADHIKARI, ANIKET BHATTACHARYA, University of Central Florida — We have studied the translocation dynamics of a semi-flexible polymer through a nanopore from via to trans compartment containing binding particles (chaperones) which introduce a bias for the translocating chain. We have used a model semi-flexible polymer using excluded volume (Lennard-Jones), anharmonic spring (elasticity), and three-body bond bending (chain stiffness) potentials, and applied Langevin dynamics simulation to study various aspects of conformations and dynamics of the translocating chain. In particular, we have investigated the conditions for the most efficient translocation as a function of the chain stiffness, strength of the attractive interaction, and the density of the binding particles, reflected in the mean first passage time (MFPT) of translocating chain through the pore. We have observed that for certain binding strengths and concentrations of the chaperons, the translocation is faster than the ideal Brownian ratchet (BR) process [Simon et al., Proc. Natl. Acad. Sci. U.S.A. 89, 3770 (1992)].

**P1.00303 Uncovering the effect of DNA topology on the mobility and conformational dynamics of crowded DNA molecules**, STEPHANIE GORZCYZA, University of San Diego, COLE E. CHAPMAN, University of California, San Diego, RAE M. ROBERTSON-ANDERSON, University of San Diego — Using single molecule fluorescence microscopy and particle-tracking, we examine the effects of crowding on the diffusion and conformation of large, double-stranded circular DNA molecules. To determine diffusion, we track the mean-squared-displacement of single fluorescent-labeled DNA molecules embedded in solutions of different crowding agents. Using image analysis techniques, we also characterize the conformational change (from random coil configuration) induced in DNA by crowding. Our previous studies with linear DNA crowded by dextran reveal crowding-induced mobility reduction of DNA, dependent on crowder size, and elongation of DNA random coils, dependent on DNA size. Here, we compare our previous results to those for circular DNA crowded by varying crowding agents including dextran, Ficoll and Polyethylene Glycol. We determine the dependence of circular DNA mobility and conformation on the level of crowding, molecular weight of the crowding agent, structure of the crowder, and DNA length (11-115 kilobases). Thus, this research uncovers the underlying mechanisms responsible for observed DNA dynamics in crowded environments and biological cells.

**P1.00304 Dynamics of GLASSY POLYMERS UNDER CONFINEMENT** —

**P1.00305 Glass transition cooperativity from broad band heat capacity spectroscopy**, YEONG ZEN CHUA, GUNNAR SCHULZ, EVGENI SHOFIET, HEIKO HUTH, University of Rostock, REINER ZORN, Juelich Centre for Neutron Science, JUERN W.P. SCHMELZER, CHRISTOPH SCHICK, University of Rostock — Molecular dynamics is often studied by broad band dielectric spectroscopy (BDS) because of the wide dynamic range available and the large number of processes resulting in electrical dipole fluctuation and with that in a dielectrically detectable relaxation process. Calorimetry on the other hand is an effective analytical tool to characterize phase and glass transitions by its signatures in heat capacity. In the linear response scheme, heat capacity is considered as entropy compliance. Consequently, only processes significantly contributing to entropy fluctuations appear in calorimetric curves. The glass relaxation is prominent example for such a process. Here we present complex heat capacity at the dynamic glass transition (segmental relaxation) of polystyrene (PS) and poly(methyl methacrylate) (PMMA) in a dynamic range of 11 orders of magnitude, which is comparable to BDS [1]. As one of the results, we determine the temperature dependence of the characteristic length of the corresponding fluctuations. The characteristic length decreases from about 4 nm to about 0.7 nm in the temperature range from 370 K to 500 K. This proves an estimate for possible confinement effects on the segmental relaxation, which is different from vitrification as discussed by Cangialosi et al. [2]. [1] Y. Z. Chua et al., Col & Poly Sci 292, 2014. [2] D. Cangialosi, J of Phys: Cond Matt 26 (15), 2014.

**P1.00306 STABLE GLASSES, PROPERTIES AND ORIGINS** —

**P1.00307 Thermal Stability of Vapor-Deposited Stable Glasses of an Organic Semiconductor**, DIANE WALTERS, University of Wisconsin-Madison, RANKO RICHERT, Arizona State University, MARK EDIGER, University of Wisconsin-Madison — Organic glasses prepared by physical vapor deposition can be highly stable and resistant to transformation upon heating. Unlike ordinary glasses, transformation to the supercooled liquid is possible through the material at a constant velocity front. In this work, we show that an organic semiconductor commonly used as an active layer in organic electronics, TPD, transforms via propagating fronts when heated above the glass transition temperature. We measure transformation front velocities using spectroscopic ellipsometry. Using high-throughput preparation and annealing techniques, we find that front velocity can vary by over an order of magnitude depending upon the substrate temperature during the deposition of the glass. Transformation front velocity is also influenced by the mobility of the supercooled liquid at the annealing temperatures and, consistent with this view, transformation fronts have the same activation energy for stable glasses prepared with a wide range of the substrate temperatures. These results may aid in designing organic electronic devices with improved lifetimes.

**P1.00308 Effect of absorbed water on the thermodynamic and kinetic properties of vapor-deposited organic glasses**, MARTA GONZALEZ-SILVEIRA, CRISTIAN RODRIGUEZ-TINOCO, JOAN RAFOLS-RIBE, AJTOR F. LOPEANDIA, JAVIER RODRIGUEZ-VIEJO, Physics Dept. - Universitat Autonoma de Barcelona — Most organic glasses absorb water when exposed to ambient conditions. As a consequence, the glass can experiment changes in its physicochemical properties, being the triggering of crystallization one of the most inconvenient drawbacks. The amount of absorbed water depends on the partial pressure but also on the stability of the glass. Previous studies have shown that ultrastable indomethacin glasses absorb less water than the conventional counterpart. We show here how water absorption modifies the kinetic properties of the glass while, unexpectedly, the thermodynamic stability remains unaltered. By means of ex-situ and in-situ calorimetry, we analyze the relationship between water absorption and kinetic properties for glasses that are vapor-deposited at different temperatures around 0.85 Tg. Moreover, glasses exposed to water vapor exhibit a double glass transition, a clear indication of the presence in the glass of regions with different kinetic stability.

**P1.00309 Surface Self-diffusion of Organic Glasses and Low Molecular Weight Polystyrene**, WEI ZHANG, CALEB BRIAN, LIAN YU, Univ of Wisconsin, Madison — The study of surface self-diffusion of organic glasses and low molecular weight polystyrene help understand the formation of stable glasses by vapor deposition, the nature of surface mobility on polymer glasses and the fast surface crystal growth. Surface self-diffusion was measured via surface grating decay. Corrugated patterns were embossed on sample surfaces with master gratings at elevated temperatures. The smoothing of surface gratings was monitored with Atomic Force Microscopy or light diffraction. It was identified by Mullins' model that viscous flow dominates grating decay at high temperatures, but surface diffusion is the leading mechanism upon cooling. Surface diffusion coefficients were measured for organic glasses and polystyrenes with different glass transition temperatures and intermolecular forces. Surface diffusion is at least 10^5 times faster than bulk diffusion at T_g, and unlike bulk diffusion, surface diffusion exhibits strong material dependence. The fast surface diffusion implies fast rearrangement of molecules on surface during vapor deposition and helps the formation of stable glasses.

1 Now at 3 M Inc.
P1.00310 Infrared spectroscopic investigation of stable glasses of indomethacin. JING JIANG, MARK EDIGER, University of Wisconsin-Madison — Glasses with high density and kinetic stability can be prepared by physical vapor deposition. By varying the substrate temperature, stable glasses can be produced with an anisotropic distribution of molecular orientations. We use infrared transmission spectroscopy to investigate the effect of substrate temperature on the structure of indomethacin stable glasses. At normal incidence, height of peaks which are assigned to asymmetric hydrogen-bonded acid C=O stretching vary systematically with the substrate temperature. This indicates either more hydrogen-bonded acid carbonyl groups in the most stable glass or a dependence of molecular orientation upon substrate temperature can be shown by IR.

P1.00311 MANIPULATING GLASSES —

P1.00312 Non-affine reorganizations in glassy polymers under applied strain in the plastic regime. DIDIER LONG, LUCA CONCA, CNRS/Solvay, ALAIN DEQUIDT, Université de Clermont-Ferrand, JEAN-YVES DELANNOY, PAUL SOTTA, CNRS/Solvay, FRANÇOIS LEQUEUX, CNRS/ESPCI — A model for the dynamics of non-polar polymers, based on percolation of slow subunits, has been proposed and developed over the past ten years. This model has been extended for describing plastic deformation of glassy polymers. It has been proposed that the applied stress results in an acceleration of the dynamics of the subunits. At deformation amplitudes of a few percent, we can observe plastic yield. The onset of plasticity is accompanied by an increase of the non-affine nature of the deformation at microscopic scales. Localization phenomena are observed in the plastic regime. We present here a detailed study of the complex reorganization which takes place on a scale of a few nanometers. We show that the correlation length of non-affine deformation increases at yield, but remains finite, with typical value 10-20 nm, corresponding to typical distance between shear bands. We compare in detail the microscopic mechanisms at play during shear deformation, uni-axial extension and compression.

P1.00313 POLYMERIC GLASSES —

P1.00314 Volume Recovery of Polymeric Glasses, N. SAKIB, S.L. SIMON, Texas Tech University — Following the seminal work of Kovacs, capillary dilatometry has been used for the last fifty years to study volume recovery of polymeric glass formers. Our capillary dilatometer, which previously used a Linear Variable Differential Transducer (LVDT) to measure the height of the Hg column in the capillary, has been modified following the work of Richert. The current study demonstrates the use of a capacitance bridge as the transducer. A metallic layer of silver sputtered on the exterior of the dilatometer serves as the outer electrode, mercury (the confining fluid) serves as the inner electrode, and the glass in between serves as the dielectric of the capacitor. The Andeen-Hagerling 2550A 1kHz ultraprecision capacitance bridge is used for the measurements. Volume recovery of various glass formers will be used to test the new design; new measurements are planned to test models of structural recovery.

P1.00315 Cure Kinetics of the Hydroxyl-Epoxide Reaction in DGEBA Epoxy Hardened with Diethanolamine, LEBELO HAILESLASSIE, NARJES FREDJ, CAITLYN M. CLARKSON, JOHN D. MCCOY, New Mexico Tech, MATHEW C. CELINA, JAMIE M. KROPKA, Sandia National Laboratories — The curing of a diglycidyl ether of bisphenol-A Epoxy (Epon 828) with diethanolamine (DEA) involves a fast amine-epoxide reaction followed by a slower hydroxyl-epoxide reaction. At curing temperatures below 70°C, the time scales of these two reactions are well separated. This permits the study of the hydroxyl addition as an “isolated” reaction. The reaction is strongly auto-catalyzed and is well fit to a modified form of the Kamal equation. Here we study the temperature dependence of the Kamal parameters with modulated differential scanning calorimetry and infrared spectroscopy.

P1.00316 Liquid Substrate Effects on the Glass Transition Temperature of Nanoscopically Confined Polystyrene Spheres. DANE CHRISTIE, Princeton University, CHUAN ZHANG, Sphera Materials, RODNEY PRIESTLEY, Princeton University — The effect of the liquid-polymer interface on the glass transition temperature (T_g) of polystyrene (PS) was investigated using differential scanning calorimetry. Polystyrene nanoparticles of different radii were suspended in either water, glycerol or an ionic liquid. Particles suspended in water (or cast in film in air) exhibited a T_g-confinement effect consistent with that of freestanding films of PS. Particles suspended in an ionic liquid exhibited an invariant T_g with confinement while those suspended in glycerol exhibited a modest, depression in T_g with confinement. Upon re-suspension in water, particles formerly suspended in glycerol showed a partial recovery of their T_g in water. However, particles re-suspended in water from an ionic liquid showed no recovery of their T_g. These results are explained in the context of chain mobility and interfacial energy, and provide insight and a probable resolution to contradictory observations in the literature.

P1.00317 POSTDEADLINE ABSTRACTS —

P1.00318 Chirality Induced Spin Selectivity for Memory Applications. RAHAMIM GULIAMOV, SHINTO MATHEW, KIRAN VANKAYALA, Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel, HAGAY MOSHE, YITZHAK MASTAI, Department of Chemistry, Bar-Ilan University, Ramat-Gan Israel, RON NAAMAN, Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel, PROF. RON NAAMAN GROUP COLLABORATION1, PROF. YITZHAK MASTAI GROUP COLLABORATION2 — Creation and manipulation of spin current is one of major aspects of memory devices. In conventional devices spin-polarized current is created by permanent magnetic layer. Further miniaturization of the memory is limited by super-paramagnetic behavior of layer. Hence, high density memory requires out-of-plane geometry with perpendicular magnetic anisotropy. Achieving this goal with inorganic magnetic layers is a challenge. We present a new approach in which the permanent magnetic layer has been replaced with inorganic chiral film producing spin polarized current due to Chirality Induced Spin Selectivity (CISS) effect. Chiral Al2O3 film grown by ALD on self-assembled monolayer of chiral molecules acts as a spin filter. Spin polarization is parallel/antiparallel to the electron velocity depending on chirality. Devices show asymmetric magneto-resistance and slopes with opposite sign for left/right handed chirality. Hence, CISS-effect based device shows, for first time, an asymmetric magneto-resistance, which has potential application in magnetic memory and magnetic field sensors. Reference: Shint0 P. Mathew et al., Appl. Phys. Lett. 105, 242408 (2014)

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P1.00319 Proving grain boundaries and transport study of graphene grown on liquid Cu.
SEONG-YONG CHO, MIN-SIK KIM, KI-JU KIM, MIN-SU KIM, HYUN-MI KIM, SANG-HOON LEE, KI-BUM KIM, Seoul Natl Univ, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING TEAM — We revealed grain boundaries of graphene grown on liquid Cu via hydrogen etching and Cu oxidation, and found out that small gap and voids exist between graphene islands on liquid Cu due to small supersaturation ratio which was required for self-assembly to occur. Modified two-step growth was applied in order to fill the gap between graphene islands and continuous graphene was synthesized on liquid Cu. The continuity of the film was verified through hydrogen etching and NaCl assisted oxidation. Electrical resistance of graphene grown on liquid Cu was lower than graphene grown on solid Cu if there is no crack damage which might be resulted from thermal stress related solidification of Cu and wet-transfer. Also, Hall mobility of graphene grown on liquid Cu shows two times higher value compared to that of graphene grown on solid Cu. In order to verify the aligned grain boundary of graphene on liquid Cu, direct patterning enabled electrode deposition on two neighboring graphene single crystal which aligns in the same orientation. Grain boundary resistance was negligible based on our electrical measurement results which has a great potential impact on graphene growth on liquid Cu.

P1.00320 Enhancement of Electromagnetically Induced Transparency Cooling by an Optical Cavity1, WEI WU, JIE ZHANG, SHUO ZHANG, BAO-QUAN OU, PING-XING CHEN, National University of Defense Technology — One of the most popular methods for cooling trapped ions is to ground state cooling. However, carrier and blue sideband still exist, which are the obstacles for reaching lower phonon number. EIT cooling cancels the carrier transition and suppressed blue sideband transition to some extent, blue sideband transition still exists. To further suppress the blue sideband transition and improve EIT cooling, Introducing an optical cavity provides us a promising way to enhance the EIT cooling and reach lower phonon number for a trapped ion. A Λ-configuration ion with mass M is trapped in a Paul trap, we consider the situation that the radial confinement is much stronger than that of the axial direction, only one dimensional movement along the axis should be concerned. If we set the detuning properly, EIT effect occurs, canceling the carrier transition, while the heating effect from blue sideband transition can be suppressed by quantum interference between the laser and cavity. Analytical calculation shows that cooling limit of this new scheme is

$$\langle n_{st} \rangle = \frac{1}{C},$$

Numerical simulation shows that the standard EIT cooling is enhanced with the help of the high finesse cavity.

1National Natural Science Foundation of China (Grant Nos 11304387 and 61205108)

P1.00321 Properties of Transparent Conducting Oxides from First Principles: In-O, In-Zn-O, In-Sn-O, and Zn-In-Sn-O, RABI KHANAL, JULIA MEDVEDEVA, Missouri University of Science and Technology — Systematic investigations of amorphous In-based oxides, In-X-O with X=Zn and/or Sn, obtained via ab-initio molecular dynamics liquid-quench simulations, are performed to understand the role of composition in the structural, optical, transport, and mechanical properties of these oxides. First, the structural characteristics of the first, second, and third shells are compared between amorphous In-O, In-Zn-O, In-Sn-O, and Zn-In-Sn-O. The results reveal that the local Metal-Oxygen structure for both In and X cations — and hence, optical band gap and electronic effective mass governed by the metal-oxygen interactions — remains nearly intact upon the transition to amorphous state. In all amorphous oxides considered, Indium is undercoordinated with little dependence on X, whereas the X cations reach their natural coordination. This finding suggests that the carrier generation is primarily governed by In atoms, in agreement with transport measurements in the amorphous oxides. In contrast to the first shell, the composition affects the Metal-Metal distances, coordination, and oxygen sharing. The interconnectivity and spatial distribution of InO6 and XOx polyhedra limits the charge transport via scattering and ultimately determines the formation of the amorphous oxides and their properties.

P1.00322 Perovskite Structured Oxide Thin Film as Photocapacitor, JOYPROKASH CHAKRABARTTY, RIAD NACHACHE, FEDERICO ROSEI, INRS - Energie et Materiaux — Photocapacitor is a device that converts solar energy through photovoltaic effect, and stores the converted energy by maintaining the charge concentration difference across a membrane upon light irradiation. It eliminates additional storage devices, for example, extra battery towards device miniaturization by enabling generated charge storage facilities in the same system. Till to date published reports show those devices that used artificial layer within single structure to make storage facility. Here we show some preliminary results on Bi-Mn-O thin film systems that differ from others in such a way that it will employ self-assembled system to convert and to store solar energy.

P1.00323 Development of Magnetization Detecting Electron Spin Resonance Method, SATOSHI MATSUZAWA, HIROYUKI NOJIRI, Institute for Materials Research, Tohoku University, NOJIRI LAB TEAM — Electron spin resonance: ESR is a spectroscopy by using electromagnetic wave absorption in Zeeman spitted multiplet of spins. The split energy is determined by the resonance field and the line width is governed by relaxation and anisotropies. The absorption intensity is proportional to the population difference between the initial and the final states. These populations also determine the total z-component of magnetization of the system. It means that ESR absorption can be measured by magnetization under electromagnetic wave irradiation. This type of ESR is called magnetization detecting ESR: MDES. We have developed two types MDES, namely, SQUID-ESR and XMCD-ESR. XMCD is the abbreviation of X-ray Magnetic circular dichroism and is the method to measure magnetization in element and orbital selective manner. SQUID-ESR is easy to conduct by attaching radiation source to a conventional MPMS-SQUID machine. The advantage of SQUID-ESR is the evaluation of absolute value of ESR intensity. While, XMCD-ESR is very sensitive and can detect the magnetization of a few atomic layers. Details of the experimental systems and the test results will be presented.

P1.00324 Application of Scanning Probe Nanolithography to fabrication and study of large area graphene and Transition Metal Dichalcogenides heterostructures1, RUI DONG, LOGAN MOORE, IRMA KULJANSHVILI, Saint Louis University — Two-dimensional atomic crystals, such as graphene and layered transition metal dichalcogenides (TMDs), have drawn significant attention because of the unique physical and chemical properties. Recently developed graphene/TMDs stacking structures provide an attracting solution to design and fabricate unique electronic devices and nanostructures. In this study, we employ the “direct write” patterning technique, to fabricate Graphene/TMDs heterostructures. TMDs precursor is utilized as an “ink” to create the arrays of patterns employing multi-pen AFM cantilevers. The patterned structures of TMDs precursor on graphene /silicon oxide/silicon in processed in CVD to produce Graphene/TMDs heterostructures. Raman spectroscopy and AFM characterization demonstrates high quality of as-prepared Graphene/TMDs nanostructures. Mask free approach significantly reduces contamination of the graphene surface during patterning and demonstrates a promising unconventional technology for fabricating high quality Graphene/TMDs or other layered nanostructures in a convenient and economical manner with the nanoscale precision.

1IK acknowledges support from Saint Louis University’s President’s Research Fund
P1.00325 Geometric and Electromagnetic Field Effects on the Excitonic Properties of Core-multishell Semiconductor Quantum Wires1, JUŚCİANE ŚLІWA2, Sociedade Brasileira de Física, ANDREY CHAVES COLLABORATION1, GIL DE AQUINO FARIAS COLLABORATION1, SUBENIA MEDEIROS COLLABORATION2 — The effect of eccentricity distortions in the otherwise circular geometry of core-multishell quantum wires on their excitonic transitions is theoretically investigated. Within the effective mass approximation, the Schrödinger equation is numerically solved for electrons and holes in systems with single and double radial heterostructures, whereas the resulting exciton binding energy is calculated by means of a variational approach. Our results demonstrate that for a single shell heterostructure, in-plane electric fields applied in different directions produce qualitatively different energy spectra, which can be used to identify the eccentricity of the system. For a double heterostructure, the eccentricities of the inner and outer shells play an important role on the excitonic binding energy and on the oscillator strength. Our results also show that for a single shell heterostructure with a type-II confinement, i.e. with spatially separated electrons and holes, one of the carriers exhibits either a ring-like or a dot-like energy spectrum, depending on the radius of the system. In this case, a shell-to-core confinement transition for the electron can be induced also by an external magnetic field.

1Fundao de Apoio a Pesquisa do Rio Grande do Norte e UFERSA
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P1.00326 Final state lifetime effects in spectroscopic studies of iridium oxide , J. MATTHIAS KAHK, DAVID J. PAYNE, Imperial College London — Understanding the complex and varied electronic and magnetic properties of late 3rd row transition metal oxides is a topic of significant current interest. The technique of Resonant Inelastic X-ray Scattering (RIXS) is particularly valuable in this field as it provides element- and orbital-specific information about the occupied and unoccupied electronic states. A major advantage of RIXS over techniques such as nonresonant XAS and XES is the sharpening of spectral features due to the absence of a core hole in both the initial and the final states. In typical simulations of RIXS spectra, final state lifetime effects are thus neglected, but this also precludes the possibility to account for the finite lifetime of the excited electron-hole pair created in the RIXS process. Starting from the well-known Kramers-Heisenberg equation, we have developed a new formalism for RIXS simulations which does allow for the inclusion of final state lifetime effects. Results are shown for the O K-edge RIXS of IrO₂, and the new formalism leads to a vast improvement in the agreement between theory and experiment. A similar approach also yields excellent agreement between theory and experiment for the nonresonant XAS and XES of IrO₂, as well as the valence band region of the IrO₂ HAXPES spectrum.

P1.00327 Giant Spin Hall Effect in Perpendicularly Magnetized Ta/CoFeB/MgO Structure and Temperature Dependence1, QIANG HAO, GANG XIAO, Brown University — The Giant Spin Hall Effect (GSHE) in non-magnetic metals with strong spin-orbit coupling (SOC) has been found in various solids like Pt, beta-Ta, and beta-W. The spin current from GSHE solids yields a spin-transfer torque (STT) inside an adjacent ferromagnetic layer with perpendicular magnetic anisotropy (PMA) to effect a magnetization switching. The combination of PMA with STT-induced switching has the advantage of low power consumption, high reliability and durability and data non-volatility over earlier generations of MRAM. Here we first studied the post-annealing effect on achieving PMA in Ta/CoFeB/MgO multilayers. We achieved so far the lowest critical current density of 2.3 MA/cm² for the STT-induced switching in the presence of 5mT magnetic field created in the RIXS process. Starting from the well-known Kramers-Heisenberg equation, we have developed a new formalism for RIXS simulations which does allow for the inclusion of final state lifetime effects. Results are shown for the O K-edge RIXS of IrO₂, and the new formalism leads to a vast improvement in the agreement between theory and experiment. A similar approach also yields excellent agreement between theory and experiment for the nonresonant XAS and XES of IrO₂, as well as the valence band region of the IrO₂ HAXPES spectrum.

1This work was supported by Nanoelectronics Research Initiative (NRI) through the Institute for Nanoelectronics Discovery and Exploration (INDEX) and by National Science Foundation through Grant No. DMR-1307056.

P1.00328 Transition to Metallic Phase of Fluid Hydrogen at High Pressure and High Temperature1, MARI EINAGA, SHO KAWAGUCHI, KATSUYA SHIMIZU, KYOKUGEN, Osaka University, KENJI OHTA, Department of Earth and Planetary Sciences, Tokyo Institute of Technology, NAOHISA HIRAO, YASUO OHISHI, Japan Synchrotron Radiation Research Institute — We investigated the phase transition to the metallic fluid phase of hydrogen under high pressure and high temperature by the laser heated diamond-anvil cell (LHDAC) up to 100 GPa and 2500 K. Compressed hydrogen was heated by IR laser with a thin gold foil, acts as the laser absorber. The temperature of hydrogen was determined by National Science Foundation through Grant No. DMR-1307056.

1Japan Society for the Promotion of Science KAKENHI Grant Number 26000006

P1.00329 Spin Correlations in Quantum Wires , CHEN SUN, Texas A&M Univ, VALERY POKROVSKY, Texas A&M Univ, Landau Institute for Theoretical Physics — We consider theoretically spin correlations in an 1D quantum wire with Rashba-Dresselhaus spin-orbit interaction (RDI). The correlations of non-interacting electrons display electron-spin resonance at a frequency proportional to the RDI coupling. Interacting electrons on varying the direction of external magnetic field transit from the state of Luttinger liquid (LL) to the spin density wave (SDW) state. We show that the two-time total spin correlations of these states are significantly different. In the LL the projection of total spin to the direction of the RDI induced field is conserved and the corresponding correlator is equal to zero. The correlators of two components perpendicular to the RDI field display a sharp ESR driven by RDI induced intrinsic field. In contrast, in the SDW state the longitudinal projection of spin dominates, whereas the transverse components are suppressed. This prediction indicates a simple way for experimental diagnostic of the SDW in a quantum wire.
P1.00330 Few-layer-thin Two-dimensional Metallic Niobium Disulfide Nanosheets: Preparation, Optical Characterization and Transport Properties1. SIHAN ZHAO, TAKATO HOTT A, TAKUMI SAWAZAKI, MITSUHIRO OKADA, HISANORI SHINOHARA, RYO KITAURA, Nagoya Univ, SHINOHARA'S GROUP TEAM — The semiconducting two-dimensional (2D) transition-metal dichalcogenides (TMDs), such as MoS2, WS2 etc., have recently attracted tremendous research attention in the field of materials science. On the other hand, research work on 2D metallic TMDs, such as NbS2, NbSe2 etc., which show superconductivity and charge-density-wave (CDW) states in bulk, has been limited primarily due to the inaccessible transport behavior in ultrathin high quality samples. In this contribution, we report a direct chemical vapor deposition (CVD) growth of ultrathin 3R-NbS2 nanosheets down to 3 layers on the exfoliated hexagonal boron nitride (hBN) flakes. AFM data show that most of NbS2 samples grown are very thin with an average lateral size of ca. 2 × 3 μm. Detailed Raman spectroscopy studies on layer number-identified NbS2 samples reveal a systematic shift of out-of-plane vibration mode (A1g), which offers a reliable and rapid optical method for layer number identification. Two-terminal devices on thin-layered NbS2 were also fabricated and show a metallic transport behavior as predicted by DFT calculations. The metallic nature of thin-layered NbS2 has also been supported by absence of PL peaks regardless of number of layers. Exploration of 2D superconductivity and CDW states in this system is an on-going work.

1 This work was supported by a Grant-in-aid for Young Scientists (A) (No. 25708002), Scientific Research on Innovative Areas (No. 25107002), and Scientific Research S (No. 22225001) from MEXT, Japan, and the Global COE Program in Chemistry, Nagoya University.

P1.00331 A New Carbon Phase Constructed by Long-Range Ordered Carbon Clusters form Compressing C70 Solvates, WEN CUI, MINGGUANG YAO, SHI JIE LIU, FENGXIAN MA, QUANJUN LI, RAN LIU, BO LIU, BO ZOU, TIAN CUI, BINGBING LIU1. Jilin University, STATE KEY LAB OF SUPERHARD MATERIAL COLLABORATION — A novel carbon material has been recently reported from compressing C60 solvates (C60/m-xylene) and the obtained high pressure phase—the ordered amorphous carbon cluster (OACC) structure, breaks our inherent understanding of the categorization of various phases and adds a new member to the list of structures [L. Wang et al, Science 337, 825 (2012)]. Our study reveals that m-xylene plays an important role in both the structure and the property of the formed novel phase [M. Fujihara et al, App Phys Lett 103, 071913 (2013)]. Here, another example of OACC is also presented from compressing C70/m-xylene in which amorphized and highly compressed C70 units act as building blocks. The high pressure phase is exceptional incompressible, which can indent the (100) face of diamond. A new phase transition occurs in the compression process, which is very different from compressing C60/m-xylene, indicating OACC structure can be tuned by changing the initial fullerene molecules. The deformation of fullerene molecules under pressure and the formation mechanism of the high pressure hard phase have also been revealed in this study. Our study extends the OACC structure to larger fullerenes and suggests a universal rule for the high pressure behaviors of lower symmetry systems of solvated fullerenes [W. Cui et al, Adv Mater 26, 7257 (2014)].

Corresponding author

P1.00332 Optical properties of highly-extended, ultrathin graphene nanoribbons in carbon nanotubes. HONG EUN LIM, Department of Chemistry, Nagoya University, YASUMITSU MIYATA, Department of Physics, Tokyo Metropolitan University, MIHO FUJIHARA, Department of Chemistry, Nagoya University, SUSUMU OKADA, Graduate School of Pure and Applied Sciences, University of Tsukuba, HARUKA OMACHI, RYO KITAURA, HISANORI SHINOHARA, Department of Chemistry, Nagoya University — Growing graphene nanoribbons (GNRs) inside the carbon nanotubes (CNTs) [1, 2] is tempting, as it provides opportunities to tune the width and edge structure of the ribbons synthesized. To have a better insight into their intrinsic properties, it is therefore necessary to study the GNRs in such a confined state. Herein, we report the optical properties of the coronene-derived GNRs, confined in single-wall CNTs of 1.4-1.6 nm. The electronic structures of the outer CNTs were modified using diazonium chemistry [3], allowing clear absorption signals of the inner GNRs to be detected. The absorption bands around 1.5 and 3.4 eV can be related to the first and second transitions between the energy gaps of the valence and conduction bands, in qualitative agreement with the first principle calculations. Our study deepens the understanding on the ribbons fabricated, providing access towards the interesting physics of confined one-dimensional materials. References: [1] H. E. Lim et al. Nat. Commun. 2013, 4, 2548. [2] M. Fujihara et al. J. Phys. Chem. C 2012, 116, 15141-15145. [3] M. S. Strano et al. Science 2003, 301, 1519-1522.

P1.00333 Growth and Optical Properties of High-Quality WS2 Monolayers on Graphite. YASUMITSU MIYATA, YU KOBAYASHI, SHOGO SASAKI, SHOHEI MORI, YUTAKA MANIWA, Department of Physics, Tokyo Metropolitan University, KENJI WATANABE, TAKASHI TANIGUCHI, Department for Materials Science, HIROKI HIBINO, NTT Basic Research Laboratories, NTT Corporation — Atomic-layer transition metal dichalcogenides (TMDs) have attracted appreciable interest due to their tunable bandgap, spin-valley physics, and potential device applications. However, the quality of TMD samples available still poses serious problems, such as inhomogeneous lattice strain, charge doping, and structural defects. Here, we report on the growth of high-quality, monolayer WS2 onto exfoliated graphite by high-temperature chemical vapor deposition (CVD). Monolayer WS2 single crystals grown presents a uniform, single excitonic photoluminescence peak with a Lorentzian profile and a very small full-width at half maximum of 21 meV at room temperature and 8 meV at 7 K. Furthermore, in these samples, no additional peaks are observed for charged and/or bound excitons, even at low temperature. These optical responses are completely different from the results of previously reported TMDs obtained by mechanical exfoliation and CVD. Our findings indicate that the combination of high-temperature CVD with cleaved graphite surface is an ideal condition for the growth of high-quality TMDs, and such samples will be essential for revealing intrinsic physical properties and for future applications.

P1.00334 Energy landscape scheme for an intuitive understanding of complex domain dynamics in ferroelectric thin films1. JONG-GUL YOON, University of Suwon, T.H. KIM, W.K. PARK, S.M. YANG, S.Y. JANG, T. MIN, J.-S. CHUNG, Center for Correlated Electron Systems, Institute for Basic Science, S.H. BAEK, C.B. EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, T.W. NOH, Center for Correlated Electron Systems, Institute for Basic Science — Fundamental understanding of domain dynamics in ferroelectric thin films has been a longstanding issue because of its relevance to many systems and to the design of nanoscale domain-wall devices. Despite many theoretical and experimental studies, a full understanding of domain dynamics yet remains elusive due to complex interactions between domain-walls and disorder. In this work, by observing domain-wall breathing motion in ferroelectric BiFeO3 thin film using stroboscopic piezoresponse force microscopy, we demonstrate domain-shape-preserving deterministic domain-wall motion, confirming microscopic return point memory. We also map a spatial energy landscape that provides new insights into domain dynamics. The evolution of complex domain structure can be understood by the process of occupying the lowest available energy states of polarization in the energy landscape which is determined by defect-induced internal fields.

1 This work was supported by the Institute for Basic Science (IBS) and the National Research Foundation (RF) funded by the Ministry of Education, Science, and Technology (Grant No. 2010-0008341) in Korea. The work at t
P1.00335 Selective formation of zigzag-edges in graphene cracks, MIHO FUJIHARA, Nagoya University, RYOSUKE INOUE, YUTAKA MANIWA, Tokyo Metropolitan University, HISANORI SHINOHARA, Nagoya University, YASUMITSU MIYATA, Tokyo Metropolitan University — Graphene edges have attracted much attention due to their unique electronic and magnetic properties. To understand these properties, it is highly desired to prepare clean, smooth, and structure-controlled edges. However, structure selective preparation of zigzag or armchair edges has not been achieved yet. Here, we report the selective formation of graphene edges aligned in the zigzag orientation by cleavage with thermally-assisted tensile stress. Graphene grains were grown from methane on copper foil by using chemical vapor deposition. After cooling to room temperature, we occasionally observed zigzag-shaped cracks in graphene. Considering the grain edges which have the zigzag face, these cracks are found to propagate parallel to the zigzag edges. The origin of tension is probably due to the non-uniform lattice strain of graphene induced by thermal shrinking of Cu substrates as supported by Raman strain mapping. Furthermore, we demonstrate the carrier tuning around graphene edges by applying the electric field to the cracks. Our findings pave the way for the fabrication and applications of smooth, long zigzag edges of graphene and other two dimensional materials.

P1.00336 Thrust generation of thickness-varying flexible fins, YUANDI LI, PETER YEH, ALEXANDER ALEXEEV, Georgia Institute of Technology — We use three dimensional computer simulations to probe the hydrodynamics and thrust generation of an oscillating flexible fin with varying thickness. The fin is modeled as an elastic rectangular plate that plunges at its leading edge and is submerged in a viscous fluid. Since we assume that the thickest part of the fin is very small compared to its length and width, the plate is modeled as infinitely thin. We introduce an appropriate mass gradient and stiffness gradient in the plate to simulate the effects of the thickness gradient. As the fin flaps, fluid is displaced backwards and a net thrust is generated. We characterize this thrust generation as a function of driving frequency and find optimal conditions for largest propulsion. These findings are useful for designing biomimetic underwater propulsion devices.

P1.00337 Precise Analysis of Perfect Zero-Birefringence Polymer, YUKIYOSHI KADA, OSAMU URAKAWA, TADASHI INOUE, Osaka Univ — Control of strain-induced birefringence of amorphous polymers is an important issue for their optical applications. It is widely accepted that strain-induced birefringence of amorphous polymers has two origins, segment orientation and glassy deformation. The intrinsic birefringence, $\Delta n_{B}$ and the photoelastic coefficient, $C_{ij}$, are indexes of the two origins, respectively. $\Delta n_{B} - C_{ij}$ map help us to predict strain-induced birefringence of copolymers. Perfect zero-birefringence polymers, PZP, means $\Delta n_{B} = 0$ and $C_{ij} = 0$. One of the method to obtain the PZP is random copolymerization of three kinds of monomers. In a three components system, the birefringence of copolymers can be characterized by a point inside of the triangle region formed by three points for homopolymers of the three monomers in $\Delta n_{B} - C_{ij}$ map. In this study, PZP of MMA (Methyl methacrylate), TFEMA (Trifluoroethyl methacrylate) and BzMA (Benzy methacrylate) was synthesized and its birefringence behavior was analyzed. Following the reported composition, we synthesized PZP and conducted dynamic birefringence measurement. $\Delta n_{B}$ value of the synthesized PZP was unexpectedly large at high temperatures because $\Delta n_{B}$ of PMMA and PBzMA showed temperature dependence. More importantly, we found that zero birefringence of PZP is achieved only at a certain temperature. We will also discuss effect of sub relaxations in the talk.

P1.00338 Chaos and Big-Bang singularity in Bianchi type-IX universe for the Einstein equation, YUYA TAKEUCHI, Osaka Prefecture University, TOMIO PETROSKY, LINDA REICHL, The University of Texas at Austin, SATOSHI TANAKA, Osaka Prefecture University — Chaotic dynamics of a spatially homogeneous and anisotropic case in the Bianchi type-IX universe model for the Einstein equation has been studied for the vacuum case. There is a hyperbolic fixed point and a separatrix only for the type-IX model with positive cosmological constant. A difficulty in numerical analysis due to the Big-Bang singularity is avoided by constructing an analytical solution near the singular point. Thanks to the local analytic solution and by combining it with global numerical solution, we are able to construct Poincaré surfaces of a section near the separatrix. A new type of chaotic motion characteristics to the Einstein equation will be discussed.

P1.00339 NMR Spin-Lattice Relaxation Time T1 of Thin Films Obtained by Magnetic Resonance Force Microscopy, SUNGMIN KWON, SEUNGB-BO SAUN, SOONCHIL LEE, KAIST, SOONHO WON, Advanced Metallic Materials Division, Korea Institute of Materials Science — NMR spectrum and spin-lattice relaxation time(T1) of CaF2 thin films deposited on a silicon cantilever tip were obtained by magnetic resonance force microscopy(MRFM). Thickness of the thin films were 50nm and 150nm. In order to measure T1, a cyclic adiabatic inversion method was used with periodic phase inversion. A comparison of the bulk and two thin films showed that T1 becomes shorter as the film thickness decreases. To make the comparison as accurate as possible, all three samples were loaded onto different beams of a multi-cantilever array and measured in the same experimental conditions such as temperature and magnetic field.

P1.00340 Computational and Physical Analysis of Catalytic Compounds, RICHARD WU, JUNG JAE SOHN, RICHARD KYUNG, Choice Research Group — Nanoparticles exhibit unique physical and chemical properties depending on their geometrical properties. For this reason, synthesis of nanoparticles with controlled shape and size is important to use their unique properties. Catalyst supports are usually made of high-surface-area porous oxides or carbon nanomaterials. These support materials stabilize metal catalysts against sintering at high reaction temperatures. Many studies have demonstrated large enhancements of catalytic behavior due to the role of the oxide-metal interface. In this paper, the catalyzing ability of supported nano metal oxides, such as silicon oxide and titanium oxide compounds as catalysts have been analyzed using computational chemistry method. Computational programs such as Gamess and Chemcraft has been used in an effort to compute the efficiencies of catalytic compounds, and bonding energy changes during the optimization convergence. The result illustrates how the metal oxides stabilize and the steps that it takes. The graph of the energy computation step(N) versus energy(kcal/mol) curve shows that the energy of the titania converges faster at the 7th iteration calculation, whereas the silica converges at the 9th iteration calculation.

P1.00341 Superconductivity in Opal-based superconducting nanocomposites, M.K. LEE, MOST Instrument Center At NCKU, Tainan 70101, Taiwan, ÉV CHARNAIY, Institute of Physics, St. Petersburg State University, St. Petersburg, Petrovodets 198504 Russia, L.J. CHANG, Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan, YU. A. KUMZEROV, A. F. Ioffe Physico-Technical Institute RAS, St. Petersburg 194021, Russia, M. F. LÍN, Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — In this study, we investigate superconducting nanocomposites (SCNs) to elucidate superconductivity in nanostructured type I superconductor. In, Sn and Hg are loaded into opal matrices by high pressure up to 10kbar, in which introducing superconducting metals into templates preserves their own 3D nanostructures. The opal matrices is adopted because it is a well-developed nanoflafennement and widely used in the studies of photonics crystal due to its periodically-superlatticed nanoporous structure. The SCNs are then measured by Quantum Design MPMS 3 under different external magnetic fields reveal the field dependences of Tc and irreversibility field (Hirv). AC susceptibility measurements of SCNs determine strain coupling, vortex dynamics and field dependence of activation barrier (Ua) as well as Tc. Additionally, the phase diagrams of these SCNs are analyzed to study superconductivity for a system with similar nanogeometry. Exotic phase diagrams in the opal SCNs studies reveal an enhanced upper critical field (Hc2 (0)) and curvature crossover of upper critical field line. Additionally, according to the field dependence of Ua(H), curvature crossover of the upper critical field line can occur, owing to vortex phase transition.

P1.00342 The physics of a cell doublet: a minimal system to study early embryo morphogenesis, HERVE TURLIER, JEAN-ÉLON MAITRE, TAKASHI HIIRAGI, FRANCOIS NEDELEC, European Molecular Biology Laboratory — In early embryos, the shape of cells is determined in part by the actomyosin cortex and in part by interactions with the surrounding environment. Cell-cell adhesion, in particular, is determinant for the overall embryo organization. This complex interplay between cell autonomous mechanical properties and cell-cell interactions can advantageously be analyzed in paired isolated cells. We study theoretically and experimentally shape changes in doublets of mouse embryo blastomeres. Simple scaling analysis and numerical simulations can predict the various configurations adopted by blastomere doublets over different stages of embryo development. Our study provides a simple and robust physical framework to understand and characterize quantitatively diverse morphogenetic events such as compaction, entosis and cell internalization.
P1.00343 Calculation of modal contributions to thermal transport across Si/Ge and In\(_{0.53}\)Ga\(_{0.47}\)As/InP interfaces , KIARASH GORDIZ, ASEGUN HENRY, Georgia Institute of Technology — Reliable and quantitative calculation of the conductance of different phonons across an interface can have a significant impact on the applications where thermal interface resistance is limiting and can aid in the rational design of thermal interface materials. A new formalism for extracting the modal contributions to thermal interface conductance with full inclusion of temperature dependent anharmonicity and all of the atom level topography is presented. Application of the formalism to Si/Ge and In\(_{0.53}\)Ga\(_{0.47}\)As/InP interfaces reveals fundamental information on the nature of the vibrational modes involved in heat transfer and the interactions/correlations among them. Four distinct classes of vibrational modes are detected for the two interfaces. For Si/Ge interface, the density of states for these vibrational classes are completely mixed, while surprisingly for In\(_{0.53}\)Ga\(_{0.47}\)As/InP interface they are completely segregated. For Si/Ge interface, interfacial modes, located around 12THz, contribute near 20% to the total conductance, while for In\(_{0.53}\)Ga\(_{0.47}\)As/InP interface, low frequency extended modes contribute more than 50% to the total conductance. The temperature dependent anharmonicity analysis shows that increasing temperature decreases the contribution by extended modes and increases the contribution by partially extended modes. In both of the interfaces, interfacial modes exhibit the maximum per mode contribution.

P1.00344 Coherence lengths in attractively interacting Fermi gases with spin-orbit coupling , YU YIXIANG, JINWU YE, Mississippi State Univ, WUMING LIU, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences — Extensive research has been lavished on the effects of spin-orbit couplings (SOCs) in attractively interacting Fermi systems in both neutral cold-atom systems and condensed-matter systems. Recently, it was suggested that a SOC drives a class of BCS to Bose-Einstein condensate (BEC) crossover that is different from the conventional one without a SOC. Here, we explore what are the most relevant physical quantities to describe such a BCS to BEC crossover and their experimental detections. We extend the concepts of the coherence length and \(\xi_{\text{Cooper-pair size}}\) in the absence of SOC to Fermi systems with SOC. We investigate the dependence of chemical potential, coherence length, and \(\xi_{\text{Cooper-pair size}}\) on the SOC strength and the scattering length at three dimensions (3D) (the bound-state energy at 2D) for three attractively interacting Fermi gases with 3D Rashba, 2D Weyl, and 2D Rashba SOC, respectively. We show that only the coherence length can be used to characterize this BCS to BEC crossover. Furthermore, it is the only length which can be directly measured by radio-frequency dissociation spectra type of experiments. We stress crucial differences among the coherence length, \(\xi_{\text{Cooper-pair size}}\) and boundariesize. Our results provide the fundamental and global picture of the BCS to BEC crossover and its experimental detections in various cold-atom and condensed-matter systems.

P1.00345 Theory of Luminescent Emission in a Nanocrystal Doped by Co\(^{2+}\) , GEORGE CHAPPELL, QUE Huong NGUYEN, Marshall University — We theoretically study the effect on the electronic structures and optical properties of a Co-doped semiconductor nanocrystal (NC) of the interaction between the impurity atom and an electron existing inside the NC. The optical properties of impurity centers in NCs are very different from the bulk cases. Beside the strong hybridization of \(s\)-electrons of the semiconductor host and\(d\)electrons of the impurity due to confinement and the modification of the crystal field near the surface of the NCs, the Coulomb and exchange interaction of the \(d\)-electrons of the impurity centers with the confined electrons (or holes) existing inside the NCs could change the photoluminescence properties. In the strong confinement approximation, the boundary conditions enhance the coupling, and the effect on photoluminescence could be large. The transition \(4\text{f}^1\text{d}^1\text{S} \rightarrow 4\text{f}^0\text{d}^0\text{S}\) has been considered. The exchange interaction between the extra electron and the states of the impurity ion together with the confinement effect mix the wave functions, split the impurity energy levels, break the previous selection rules, and change the transition probabilities. Energy, wave functions, luminescence efficiency, and transition lifetime have been calculated. The results imply that the PL intensity increases and the lifetime is shortened inside the NC.

P1.00346 Role of precursor crystal structure on electrochemical performance of carbide-derived carbon electrodes , BENJAMIN PALAZZO, ZACH NORRIS, GREG TAYLOR, Department of Physics and Astronomy, Rowan University, LEI YU, Department of Chemistry and Biochemistry, Rowan University, SAMUEL LOFLAND, JEFFREY HETTINGER, Department of Physics and Astronomy, Rowan University — Binary carbides with hexagonal and cubic crystal structures have been synthesized by reactive magnetron sputtering of vanadium and other transition metals in acetylene or methane gas mixed with argon. The binary carbides are converted to carbide-derived carbon (CDC) films using chlorine gas in a post-deposition process in an external vacuum reaction furnace. Residual chlorine has been removed using an annealing step in a hydrogen atmosphere. The CDC materials have been characterized by x-ray diffraction, x-ray fluorescence, and scanning electron microscopy. The performance of the CDC materials in electrochemical device applications has been measured with the hexagonal phase precursor demonstrating a significantly higher specific capacitance in comparison to that of the cubic phase. We report these results and pore-size distributions of these and similar materials.

P1.00347 Stabilizing the false vacuum: Mott skyrmions\(^1\) , MÁRTÓN KANÁSZ-NAGY, Harvard University and Budapest University of Technology and Economics, BALÁZS DÓRA, Budapest University of Technology and Economics, EUGENE DEMLER, Harvard University, GERGELY ZARAND, Budapest University of Technology and Economics — Topological excitations keep fascinating physicists since many decades. While individual vortices and solitons have been observed in many areas of physics, their intriguing higher dimensional topological relatives, skyrmions remained mostly elusive. In particular, earlier attempts to create stable individual skyrmions in ultracold atomic experiments suffered from important instabilities: skyrmions have a tendency to shrink or expand, and to slip away from the atomic trap. In this work, we propose that loading a three-component nematic superfluid, such as \(^{23}\text{Na}\), into a deep optical lattice and thereby creating an insulating core, one can create topologically stable individual skyrmions, and investigate their properties in detail. Furthermore, the spectrum of the excitations of the superfluid and their quantum numbers change dramatically in the presence of the skyrmion, and they reflect the presence of a trapped monopole, as imposed by the skyrmion’s topology.

\(^1\)Acknowledgements: Hungarian Scientific Research Funds (K101244, K105149, CNK80991), the Bolyai Program of the Hungarian Academy of Sciences. E. A. D. acknowledges support through the DOE (FG02-97ER25308), the Harvard-MIT CUA, the ARO-MURI on Atomtronics, and the ARO MURI Quism program.

P1.00348 In Silico Discovery of High Deliverable Capacity Metal-Organic Frameworks\(^3\) , YI BAO, Rice Univ, RICHARD MARTIN, Lawrence Berkeley National Lab, CORY SIMON, UC Berkeley, MACIEJ HARANCZYK, Lawrence Berkeley National Lab, BEREND SMIT, UC Berkeley, MICHAEL DEEM, Rice Univ, MICHAEL W. DEEM TEAM, MACIEJ HARANCZYK TEAM, BEREND SMIT TEAM — Metal organic frameworks (MOFs) are actively being explored as potential adsorbed natural gas storage materials for small vehicles. Experimental exploration of potential materials is limited by the throughput of synthetic chemistry. We here describe a computational methodology to complement and guide these experimental efforts. The method uses known chemical transformations in silico to identify MOFs with high methane deliverable capacity. The procedure explicitly considers synthesizability with geometric requirements on organic linkers. We efficiently search the composition and conformation space of organic linkers for nine MOF networks, finding 48 materials with higher predicted deliverable capacity (at 65 bar storage, 5.8 bar depletion, and 298 K) than MOF-5 in four of the nine networks. The best material has a predicted deliverable capacity 8% higher than that of MOF-5.

\(^3\)US Department of Energy
P1.00349 Many-body calculation for charge transport through triangular quantum dot molecules

Many-body calculation for charge transport through triangular quantum dot molecules

CHIH-CHIEH CHEN, YIA-CHUNG CHANG, Department of Physics, University of Illinois Urbana-Champaign, DAVID M.T. KUO, Department of Electrical Engineering and Department of Physics, National Central University — We study the many-body effect of electron tunneling through the coupled quantum dot systems in the Coulomb blockade regime. Using the equation of motion method for the non-equilibrium Green’s function, we calculate the charge current and conductance of junctions consisting of metallic electrodes and a few quantum dots. Many-particle correlation functions are explicitly solved numerically. Quantum phenomena like quantum interference, Coulomb blockade and spin blockade for the triangular quantum dot molecules are discussed. Our work suggests a new method for the modeling of the mesoscopic transport.

1This work was supported in part by the Ministry of Science and Technology, Taiwan under Contract Nos. NSC 101-2112-M-001-024-MY3 and NSC 103-2112-M-008-009-MY3.
2Research Center for Applied Sciences, Academia Sinica, and Department of Physics, National Cheng-Kung University

P1.00350 Confinement of metal nanoparticles with various sizes in silica matrices

JEUN LEE, SHIN-HYUN KANG, SUNG-MIN CHOI, KAIST — Many studies have been focused on metal nanoparticles since they have interesting properties due to their high surface area to volume ratio. While bulk metals have constant properties regardless of their sizes, the noble properties of metal nanoparticles such as catalytic activity, magnetic, and electronic properties dramatically change depending on their sizes. Here, metal nanoparticles with various sizes are synthesized, functionalized, then confined in stable silica matrices and their physical and chemical properties are investigated. The structure of each system is characterized by transmission electron microscopy (TEM) and scanning electron microscopy (SEM).

P1.00351 Fitness, environmental changes and the growth of modularity- a quasispecies theory for the evolutionary dynamics of modularity

LIANG NISTEMSKI, Western New England University, JEONG-MAN PARK, The Catholic University of Korea, MICHAEL DEEM, Rice University — Although the modularity of a biological system is demonstrated and recognized, the evolution of the modularity is not well understood. We here present a quasispecies theory for the evolutionary dynamics of modularity. Complemented with numerical models, this analytical theory shows the calculation of the steady-state fitness in a randomly changing environment, the relationship between rate of environmental changes and rate of growth of modularity, as well as a principle of least action for the evolved modularity at steady state.

P1.00352 Pressure dependence of the nematic spin correlations in detwinned BaFe$_{1.97}$Ni$_{0.03}$As$_2$

WENLIANG ZHANG, XINGYE LU, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, JITAEPARK, Heinz Maier-Leibnitz Zentrum, Technische Universität München, Garching, Germany, PENGCHENG DAI, Department of Physics and Astronomy, Rice University, Houston — In the paramagnetic tetragonal phase of BaFe$_{2-x}$Ni$_x$As$_2$, inelastic neutron scattering shows a spin excitation anisotropy emerges at a temperature well above the structure transition temperature ($T_s$) [1], consistent with the onset of in-plane resistivity anisotropy [2]. However, how the applied uniaxial strain, which artificially breaks the four-fold symmetry, influences the observed anisotropy is still unclear. Here we studied the pressure dependence of the nematic spin correlations in detwinned BaFe$_{1.97}$Ni$_{0.03}$As$_2$. We find that the spin excitation anisotropy temperature ($T^*$) is largely enhanced when changing the pressure from a medium level (~8MPa) to a high level (~15MPa) [3]. Our results suggest the $T^*$ may be not a characteristic temperature where the system transit to a nematic phase, but a temperature the nematic fluctuations can reach under a uniaxial stress.

1Xingye Lu et al., Science 345, 657-660 (2014)
3Wenliang Zhang et al., unpublished manuscript (2015).

1Supported by MOST(973 programs), NSFC, CAS and CAEP

P1.00353 Evolution of sparsity and modularity in a model of living matter

MATHIEU HEMERY, Laboratoire Interdisciplinaire de Physique (Grenoble), OLIVIER RIVOIRE, CNRS & Université Grenoble Alpes — How much of the sequence of a protein is related to its evolutionary history? We present a theoretical model of a network of interacting proteins whose interactions are influenced by the environment. We show that the network becomes sparse and modular as the environment changes, and that the correlation between the environment and the network structure is related to the amount of information that is stored in the network.

P1.00354 Supramolecular Polymer Nanocomposites – Improvement of Mechanical Properties

JESSE HINRICHER, South Dakota Sch Mines & Tech, COLIN NEIKIRK, RODNEY PRIESTLEY, Princeton University — Supramolecular polymers differ from traditional polymers in that their repeat units are connected by hydrogen bonds that can reversibly break and form under various stimuli. They can be more easily recycled than conventional materials, and their highly temperature dependent viscosities result in reduced energy consumption and processing costs. Furthermore, judicious selection of supramolecular polymer architecture and functionality allows the design of advanced materials including shape memory and self-healing materials. Supramolecular polymers have yet to see widespread use because they can’t support much weight due to their inherent mechanical weakness. In order to address this issue, the mechanical strength of supramolecular polymer nanocomposites based on 1,4-diaminobenzene (DB) terephthalic poly(caprolactone) doped with surface activated silica nanoparticles was investigated by tensile testing and dynamic mechanical analysis. The effects of varying amounts and types of nanofiller surface functionality were investigated to glean insight into the contributions of filler-filler and filler-matrix interactions to mechanical reinforcement in supramolecular polymer nanocomposites.

1MRSEC NSF DMR 0819860 (PI: Prof. N. Phuan Ong) REU Site Grant: NSF DMR-1156422 (PI: Prof. Mikko Haataja)

P1.00355 Slip and flow dynamics of polydisperse thin polystyrene films

SEYED MOSTAFA SABZEVARI, Concordia university, JOSHUA D. MCGRaw, KARIN JACOBS, Saarland University, PAULA M. WOOD-ADAMS, Concordia university — We investigate the slip of binary and ternary mixtures of nearly monodisperse polystyrene samples on Teflon-coated (AF2400) silicon wafers using dewetting experiments. Binary mixtures of long and short chains along with ternary mixtures with a fixed weight-average molecular weight $M_w$ but different number-average molecular weight $M_n$ were prepared. Thin films of ca. 200 nm were spin coated on mica from polymer solutions and transferred to Teflon substrates. Above the glass transition temperature $T_g$ the films break up via nucleation and growth of holes. The hole growth rate and rim morphology are monitored as a function of $M_n$ and annealing protocol of the films before transfer to Teflon substrates. Slip properties, accessed using hydrodynamic models, and flow dynamics are then examined and compared. We found that the rim morphology and slip of polystyrene blends on Teflon depends on the molecular weight distribution. Similarly, flow dynamics is affected by the presence of short chains in mixture. Moreover, we can provoke differences in slip by choosing appropriate annealing and film transfer protocols for PS films that have first been spin cast on mica surfaces.
P1.00356 Particle-Laden Leidenfrost Droplets: Final-Stage Observations, ZECONG FANG, Washington State Univ, JIE XIU, University of Illinois at Chicago — Little interest has been paid to the final stage of a Leidenfrost droplet until a recent study by Celestini et al [Phys. Rev. Lett. 109, 034501 (2012)] reporting an unexpected take-off phenomenon of micrometer sized pure liquid droplets ($R_l < R < R_l$, where $R_l$ is the take-off radius, and $R_i$ is the critical radius above which droplets start to lose sphericity). In our study, we first report an unexpected observation on millimeter sized water Leidenfrost droplets ($R > R_l$), which behave quite differently from the previous study. While an originally micrometer sized Leidenfrost droplet takes off due to breakdown of lubrication regime, and hovers above its vapor layer until disappearing in the final stage of evaporation, an originally millimeter Leidenfrost droplet is observed to hover and oscillate, taking off and falling back consequentially. We further report another interesting observation, that just like pure droplets, these particle-laden drops create an unexpected explosive shoot-up at the end of evaporation.

P1.00357 Carbon Nanotubes Synthesis Through Gamma Radiation, PABLO TIRADO, RAFAEL GARCIA, Center of Research in Physics, University of Sonora, JORGE MONTES, Department of Nanotechnology, University of Sonora, RODRIGO MELENDEZ, MARCELINO BARBOZA, Center of Research in Physics, University of Sonora, OSCAR CONTRERAS, Center of Nano science and Nanotechnology, UNAM — Carbon nanotubes show a great potential of applications since there discovery by Iijima in 1991\(^1\) due to their numerous physical-chemical properties such as their high weight to strength relationship, which make them ideal to use in high resistance compound materials, and in many other applications\(^2\) In this work, a novel method for the synthesis of carbon nanotubes is presented, starting from an ultra-thin sheet of graphite synthesized by the chemical vapor decomposition technique (CVD), using ultra high purity methane and hydrogen at 1200°C in a horizontal quartz reactor. For the synthesis of carbon nanotubes, the graphite sheets were exposed to different doses of radiation, with the objective of breaking the graphite bonds and form carbon nanotubes; A Gammacell equipment model 220 Excel was used for the purpose, which counts with a radiation source of cobalt 60, and a current radiation rate of 0.9 Gy/seconds. The time of exposure to radiation was varied in each sample, according to the desired dose of radiation in each case, afterwards the samples were characterized using the Raman spectroscopy and TEM microscopy techniques with the objective of observing the kind of nanotubes formed, their morphology and their number of defects. Results will be shown during the poster session.

P1.00358 Hydration Layer of Enzymes Partially Controls Conformational Dynamics\(^1\), ZAHRA ALAVI, Student at UCLA, ZOCCHI TEAM — For a typical (20 kD, 4 nm size) monomeric enzyme, more than 50% of the residues are at the surface. The mechanics of these soft, heterogeneous nanoparticles was recently shown to be viscoelastic. Here we explore the contribution of the enzyme’s surface to the mechanics of the molecule. Nano-rheology provides sub-angstrom resolution measurements of the reversible deformation of the enzyme subject to an oscillatory mechanical stress. We perturb the surface of the enzyme by adding small amounts of DMSO, believed to affect ordering of the enzyme - water interface. We observe a dramatic though reversible change in the mechanics of the enzyme, which becomes more viscous. On the other hand, the catalytic speed is unaffected, while at higher DMSO concentrations (>1%) it even increases. Our measurements show that small (<1%) bulk concentrations of DMSO, which have negligible effect on the physico-chemical properties of bulk water, including the viscosity and dielectric constant, have nonetheless dramatic effect on the dynamics of the hydration layer of the enzyme, and ultimately on the enzyme’s mechanics. DMSO accumulates in the hydration layer (“binds to the surface of the enzyme”). Apparently the order - inducing (“kosmotropic”) quality of DMSO leads to a hardening of the enzyme - water interface.

\(^1\)US-Israel Binational Science Foundation

P1.00359 Effect of monomer sequence distribution in poly(vinyl alcohol-co-vinyl acetate) on the hydrogen bonding structure and physical properties, SHUN TASAKA, OSAMU URAKAWA, TADASHI INOUE, Department of Macromolecular Science, Graduate School of Science, Osaka University — It has been well known that hydrogen (H-) bonding interaction in polymer materials strongly affects their properties. For example, glass transition temperature ($T_g$) and terminal relaxation time increase by introducing H-bonding sites. This is because the molecular motion is restricted due to the formation of inter- and intra-chain H-bonds. For H-bonding copolymers in which H-bonding monomer and non-bonding one are incorporated, the fraction dependence of their properties has been examined so far. However, the influence of sequence distribution on their properties has not been studied in detail. In this work, we investigated the H-bonding structure and physical properties of molten poly(vinyl alcohol-co-vinyl acetate) with different monomer sequences to clarify the effect of the sequence distribution. We found that, with increasing the randomness in monomer sequences, the number of H-bonds between carbonyl group and hydroxyl (OH) group increased. Moreover, OH groups form linearly connected structure (OH-OH-OH) and its number also increases with the increase of randomness. $T_g$ for the samples with higher sequence randomness are higher than those with lower randomness for high VOH copolymers. These results indicate that formation of larger number of H-bonds makes $T_g$ higher.

P1.00360 Quantum Behavior of an Autonomous Maxwell Demon, ADRIAN CHAPMAN, AKIMASA MIYAKE, Univ of New Mexico — A Maxwell Demon is an agent that can exploit knowledge of a system's microstate to perform useful work. The second law of thermodynamics is only recovered upon taking into account the work required to irreversibly update the demon’s memory, bringing information-theoretic concepts into a thermodynamic framework. Recently, there has been interest in modeling a classical Maxwell demon as an autonomous physical system to study this information-work tradeoff explicitly. Motivated by the idea that states with non-local entanglement structure can be used as a computational resource, we ask whether these states have thermodynamic resource quality as well by generalizing a particular classical autonomous Maxwell demon to the quantum regime. We treat the quantum description using a matrix product operator formalism, which allows us to handle quantum and classical correlations in a unified framework. Applying this, together with techniques from statistical mechanics, we are able to approximate nonlocal quantities such as the erasure performed on the demon's memory register when correlations are present. Finally, we examine how the demon may use these correlations as a resource to outperform its classical counterpart.

Wednesday, March 4, 2015 2:30PM - 5:30PM –
Session Q0 APS: Kavli Foundation Special Symposium: Frontiers of Light Ballroom A –
2:30PM Q0.00001 The Optical Microscopy Revolution, STEFAN HELL, Max Planck Institute —
3:42PM Q0.00003 Developing Photo Activated Localization Microscopy, HARRALD HESS, Janelia Research Campus — Photo Activated Localization Microscopy, PALM, acquires super-resolution images by activating a subset of activatable fluorescent labels and estimating the center of the each molecular label to sub-diffractive accuracy. When this process is repeated thousands of times for different subsets of molecules, then an image can be rendered from all the center coordinates of the molecules. I will describe the circuitous story of its development that began with another super-resolution technique, NSOM, developed by my colleague Eric Betzig, who imaged single molecules at room temperature, and later we spectrally resolved individual luminescent centers of quantum wells. These two observations inspired a generalized path to localization microscopy, but that path was abandoned because no really useful fluorescent labels were available. After a decade of nonacademic industrial pursuits and the subsequent freedom of unemployment, we came across a class of genetically expressible fluorescent proteins that were switchable or convertible that enabled the concept to be implemented and be biologically promising. The past ten years have been very active with many groups exploring applications and enhancements of this concept. Demonstrating significant biological relevance will be the metric if its success.

4:18PM Q0.00004 History and Future Developments of Blue/Green/White LEDs and Laser Diodes, SHUJI NAKAMURA, University of California, Santa Barbara —

4:54PM Q0.00005 The Light Science of Coherent X-rays: How Quantum Dynamics Solved a 50 Year Challenge, MARGARET MURNANE, University of Colorado, Boulder —

Wednesday, March 4, 2015 2:30PM - 5:30PM –
Session Q1 DMP: Focus Session: Graphene: Moire, Superlattices, and Twisted Bilayers 001A -

Walt de Heer, Georgia Institute of Technology

2:30PM Q1.00001 Bilayer graphene moire pattern amplitude vs. twist angle identified using scanning tunneling microscopy1, JOSHUA THOMPSON, PIJUSH GHOSH, PAUL THIBADO, University of Arkansas, MEHDI NEEK-AMAL, FRANCOIS PEETERS, Universiteit Antwerpen, V.D. WHEELER, R.L. MYERS-WARD, C.R. EDDY, JR., D.K. GASKILL, U.S. Naval Research Laboratory — Twisted stacked layers of graphene have unique electronic properties. The layers produce a moire pattern with a wavelength determined by the twist angle. In addition, however, the surface of the moire pattern also has an increased corrugation amplitude when compared to untwisted AB-stacked graphene. The deformation strains the top-layer graphene lattice and realizes, in a natural way, triaxial stress creation as proposed by Guinea et al. Consequently, very large pseudo-magnetic fields can be created depending on the amplitude of the corrugations. Until now, no relation has been found between the moire twist angle and its corrugation amplitude. We found, using scanning tunneling microscopy, as the wavelength of the moire pattern increases so does its amplitude. Our experiments are supported by first-principles directed elasticity theory. The membrane corrugation amplitude at arbitrary twist angle is found to be a consequence of a competition between the van der Waals bonding energy and the energy required to bend the graphene.

1Financial support was provided, in part, by the Office of Naval Research under grant N00014-10-1-0181, the National Science Foundation under grant DMR-0855358.

2:42PM Q1.00002 Electronic properties and van Hove singularities of observed moiré patterns of dislocated graphene on HOPG, OGUZ GULSEREN1, H. SENER SEN, Bilkent University, DILEK YILDIZ, OGUZHAN GURLU, Istanbul Technical University — Highly Oriented Pyrolitic Graphite (HOPG) can be described as stacked graphene layers. Due the weak van der Waals interaction between the layers, topmost layer of HOPG can be rotated or shifted by chemical or mechanical means. With rotation of the topmost layer, super periodic structures called as moiré patterns are formed. In this work, moiré patterns on HOPG surfaces due to dislocated graphene layers were studied. A simple geometric investigation of the atomic structure of the moiré patterns revealed that different atomic moiré periodicities result in similar geometric moiré periods. Our calculations showed that the band structure of moiré patterns even though exhibits the fingerprints of those of twisted bilayer graphene system, like the preserved Dirac cone at the K point of moiré Brillouin zone, it has several new emerging features like van Hove singularities and linear or flat bands depending on the moiré periodicity. Our results show that most of the moiré patterns observed on graphene/HOPG system do not have a purely electronic or structural origin, but both. Moreover, our results show that van Hove singularities in these systems with different twist angles have different origins in their respective band structure.

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2:54PM Q1.00003 Transport measurements of van Hove singularity in twisted bilayer graphene, JUNXI DUAN, JINHAI MAO, YUHANG JIANG, GUOHONG LI, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, MONA ZEBARJADI, Department of Mechanical Engineering, Rutgers University, Piscataway, NJ, EVA Y. ANDREI, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ — Crossing between the Fermi energy and a van Hove singularity causes electronic instabilities which may result in new correlated phases such as superconductivity, magnetism and charge density waves. These crossings are usually rare and difficult to control as they are determined by the chemical composition and structure of the material. However, as was recently demonstrated in STM measurements, twisted graphene layers display van Hove singularities whose energy can be controlled by tuning the twist angle between them. Combining this flexibility with the ability to tune the Fermi energy by gating, makes it possible to bring these two energies together. But in order to induce an observable electronic instability the crossing energy must be uniform across the sample, which is difficult to achieve due to the potential fluctuation induced by insulating substrates. To investigate the possibility of a gate induced phase transition we fabricated devices with gated and precisely twisted graphene layers on minimally invasive substrates including hBN and suspended samples. We will report our findings on transport and STM measurements that revealed the global and local effects of gate induced band structure reconstruction.

1Work supported by DOE-FG02-99ER45742, NSF DMR 1207108 and FA9550-14-1-0316
3:06PM Q1.00004 Electronic signatures of stacking domain boundaries in twisted bilayer graphene¹. FERNANDO GARGIULO, BASTIEN GROSSO, GABRIEL AUTÉS, OLEG YAZYEV, EPFL — Experiments on bilayer graphene (BLG) show the coexistence of regions of inequivalent stacking order (AB and BA) separated by domain boundaries, topological defects akin to solitons [1]. The Frenkel-Kontorova model predicts that in-plane atomic displacements result in stacking domain boundaries of few nanometers width. We show how a hexagonal network of stacking domain boundaries naturally arises in twisted BLG in the limit of small twist angle (below ca. 1°). Equilibrium configurations of twisted BLG have been produced by means of classical force-field simulations. Atomic displacements diminish the area of AA stacking regions and extend the AB and BA stacking regions to triangular domains separated by boundaries of 7–8 nm width. Large-scale tight-binding simulations unveil the electronic properties of such twisted BLG models. A charge density depletion is the low-energy signature of stacking domain boundaries with electronic states mostly confined in AB and BA domains. Zero-energy states at the network nodes reach an asymptotic localization for vanishing twist angles. We propose STM experiments for confirming our predictions.


¹This work is supported by the Swiss NSF Grant no. PP00P2_133552.

3:18PM Q1.00005 Study of the optical phonons on gated twisted bilayer graphene , TING FUNG CHUNG, Purdue Univ, RUI HE, Univ of Northern Iowa, TAI-LUNG WU, YONG P. CHEN, Purdue Univ — In twisted bilayer graphene (tBLG), the low-energy van-Hove singularities (vHs) in the density of states (DOS) can be continuously tuned by twisting the two layers, leading to distinct electronic and optical properties compared to Bernal-stacked BLG (AB-BLG). This effect has been explored using resonance Raman scattering, showing enhanced Raman G and ZO' (low frequency, layer breathing vibration) bands when the vHs energy resonates with excitation laser energy. We have studied the influence on vHs and Raman bands in gated tBLG devices (at resonant twist angle ∼13° under a 532 nm laser light). We observed that the G band splits with increasing doping, attributed to asymmetric doping of charge carriers in the two layers. The strongly quenched G band intensity at high doping level is ascribed to the suppression of resonant interband transitions between the two saddle points (in conduction and valence bands) which are displaced in the momentum space by gate-tuning. We have also measured the doping dependence of ZO' band and R band in tBLG. Our results demonstrate that electric-field can be used to tune the optoelectronic and vibrational properties in tBLG devices.

3:30PM Q1.00006 Electronic Band Structure Modification upon Doping in Twisted Bilayer Graphene , SHENQIANG HUANG, MATTHEW YANKOWITZ, KANOKPORN CHATTRAKUN, ARVINDER SANDHU, BRIAN LEROY, Univ of Arizona — In twisted bilayer graphene, the electronic band structure and phonon dispersion depend on the rotation angle between the layers. From 9 to 15 degrees, the Raman G peak measured with a 532 nm laser is enhanced due to an increased density of states. The enhancement is a maximum at a critical angle of about 12 degrees where the laser energy matches the energy separation between the van Hove singularities in conduction and valence bands. We conduct a systematic study of the G peak enhancement upon doping up to charge densities of 2*10¹³ cm⁻². The G peak enhancement drops monotonously upon doping for angles smaller than the critical angle. In contrast, for angles larger than the critical angle, the G peak enhancement increases with doping at first before decreasing at higher doping levels. The charge density where the maximum enhancement occurs, scales with the rotation angle above the critical angle. This indicates that the band structure of twisted bilayer graphene is modified and the Fermi velocity is reduced upon doping.

3:42PM Q1.00007 The strong coupling limit of twisted bilayer graphene at large twist angles , HRIDIS PAL, STEPHEN SPITZ, MARCUS KINDERMANN, Georgia Institute of Technology — Using a recently proposed long-wavelength theory for twisted bilayer graphene near commensuration [1], we show that a strong distortion of energy bands can occur in such systems at large angles of twist. This is in contrast with the previously accepted belief that such non-trivial physics can arise only at extremely small angles of twist. At large angles, sufficiently close to commensuration, the system is driven to a non-perturbative regime (in the effective interlayer coupling), and it becomes locally gapped. We discuss the implications of this for the energy spectrum of the bilayer. [1] Theory of Twisted Bilayer Graphene Near Commensuration, Hridis K. Pal, Steven Carter, and M. Kindermann, arXiv:1409.1971.

3:54PM Q1.00008 Twisted Graphene Nanostructures , SATRIO GANI, YUDISTIRA VIRGUS, ENRICO ROSSI, College of William and Mary — Recent advances in fabrication techniques have made possible the realization of graphene nanostructures with atomic precision. Some of the nanostructures realized are completely novel. We study the electronic properties of such novel graphene nanostructures when deposited on two dimensional crystals. In particular we study the case when the two dimensional crystal is graphene, or bilayer graphene. We obtain results for the nanostructure electronic spectrum and find how the spectrum is affected by the coupling between the nanostructure and the two-dimensional substrate. In particular we study how the “twist” angle between the graphene nanostructure and the two-dimensional crystal affects the spectrum of the nanostructure.

¹Work supported by ONR-N00014-13-1-0321 and ACS-PRF # 53581-DNI5

4:06PM Q1.00009 The Interdependent Atomic and Electronic Structures of Graphene on Hexagonal Boron Nitride¹ , JEIL JUNG, Department of Physics, National University of Singapore, ASHLEY DASILVA, ALLAN MACDONALD, Department of Physics, The University of Texas at Austin, SHAFFIQUE ADAM, Yale-NUS college, Graphene Research Centre and Department of Physics, National University of Singapore — Recent progress in preparing well controlled 2D van der Waals heterojunctions has opened up a new frontier in materials physics. I will address the intriguing energy gaps that are sometimes observed when a graphene (G) sheet is placed on a hexagonal boron nitride (hBN) substrate, demonstrating that they are produced by an interesting interplay between structural and electronic properties, including electronic many-body exchange interactions. Our theory is able to explain the observed gap behavior by accounting first for the structural relaxation of graphene’s carbon atoms when placed on a hBN substrate and then for the influence of the substrate on low-energy π-electrons located at relaxed carbon atom sites. All three contributions of the moire pattern pseudospin Hamiltonian play a role in defining the features of the moire bands including the degeneracy of the mini-Dirac cones and the particle-hole asymmetry. We find that the effective anisotropic strains arising from virtual hopping are associated with effective magnetic fields on the order of ~10 T and they dominate over the pseudomagnetic vector potentials generated by the moire strains due to partial commensuration.

¹This work is supported by the Singapore National Research Foundation NRF-NRFF2012-01.
and identify the layer thickness of MX₂ properties distinctly different from those of bulk crystals, such as a direct rather than an indirect band gap, strong photoluminescence, and large exciton binding energy. For the twisted angle 30° or 60°, the photoluminescence spectra of twisted bilayer MoS₂ are investigated, revealing a tunability of the interlayer coupling of bilayer MoS₂. For the twisted angle 0° or 90°, the photoluminescence spectra of the trion and exciton of bilayer MoS₂ shows the highest intensity ratio, and the trion binding energy reaches its maximum value. For the twisted angle 30° or 90°, the situation is the opposite. These experimental observations are mainly attributed to the change of the interlayer coupling with the twisted angle. The first-principles density functional theory analyses further confirm that the band modification by the Moire superlattice is a promising material for optoelectronic devices due to its strong and stable photoluminescence emissions. In this work, the photoluminescence spectra of twisted bilayer MoS₂ materials, such as MoS₂, WS₂, MoSe₂, and WSe₂. Monolayers of these materials exhibit many physical properties distinctly different from those of bulk crystals, such as a direct rather than an indirect band gap, strong photoluminescence, and large exciton binding energies. Raman spectroscopy provides a powerful tool to characterize atomically thin 2D materials, having been utilized to probe the electron-phonon coupling and identify the layer thickness of MX₂ materials. To better understand Raman spectra, we perform systematic studies of Raman scattering in different MX₂ materials as a function of the photon excitation energy, light polarization, and spatial position. I will discuss their implications for quantitative characterization of MX₂ materials using Raman spectroscopy.
2:54PM Q2.00003 Characterizing and tuning excitons in monolayer and few-layer \( \text{MoS}_2 \). DIANA Y. QIU, FELIPE H. DA JORNADA, STEVEN G. LOUIE, Univ of California - Berkeley and Lawrence Berkeley National Lab — We use the GW-BSE method to study excitons arising from transitions in different regions of momentum space in mono- and few-layer \( \text{MoS}_2 \) and consider mechanisms to fundamentally change the features and character of the optical spectra. Our calculations show that sharp spatial variations in dielectric screening make 2D systems, such as \( \text{MoS}_2 \), computationally challenging, requiring very fine \( k \)-space sampling to resolve the structure of excitonic wave functions and converge binding energies. In highly converged calculations, we identify a series of excitons arising from transitions at the \( K/K' \) valleys in the Brillouin zone, a higher energy series arising from transitions in the valley of a Mexican hat potential centered at the \( \Gamma \) point, and transitions at the indirect gap from \( \Gamma \) to \( \Lambda \) in a few-layer \( \text{MoS}_2 \). As layer number changes, these states, which have varying character, momentum-space structure and real-space locations, are affected differently by changes in confinement and hybridization. By tuning layer number and strain, we find that we not only can tune the excitation energies but can also change the relative energies of the various excitonic series, allowing for movement of the lowest energy exciton between different regions of the Brillouin zone.

This work was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231.

3:06PM Q2.00004 Exciton band structure of monolayer \( \text{MoS}_2 \). FENGCHENG WU, Department of Physics, University of Texas at Austin, FANYAO QU, Department of Physics, University of Texas at Austin; Instituto de Física, Universidade de Brasília, ALLAN MACDONALD, Department of Physics, University of Texas at Austin — We describe a theory of the momentum-dependent exciton spectrum of monolayer molybdenum disulfide. Low-energy excitons occur both at the Brillouin zone center and at the Brillouin-zone corners. We find that binding energies at the Brillouin-zone center deviate qualitatively from the \( (n-1/2)^{-2} \) pattern of the two-dimensional hydrogenic model. Moreover, the four \( 2p \) states of \( A \) series are lower in energy than the corresponding \( 2s \) states and not degenerate. The two-fold ground-state valley degeneracy is lifted linearly at small momenta by electron-hole exchange processes that establish inter valley coherence. We conclude that although monolayer \( \text{MoS}_2 \) is a direct-gap semiconductor when classified by its quasiparticle band structure it may well be an indirect gap material when classified by its excitation spectra, and speculate on the role of this property in luminescence processes that establish inter valley coherence.

3:18PM Q2.00005 Helicity Resolved Raman Scattering of Atomic Layers of Transition Metal Dichalcogenides, SHAO-YU CHEN, JUN YAN, Univ of Mass - Amherst — Semiconducting transition metal dichalcogenides (TMDs) such as \( \text{MoS}_2 \), \( \text{MoSe}_2 \), \( \text{WS}_2 \) and \( \text{WSe}_2 \) are promising two dimensional (2D) materials for electronic and optoelectronic applications. Moreover, the unique capability to manipulate the valley degree of freedom with circularly polarized light has attracted widespread attention for potential applications in valley- and spintronics. In this talk we present helicity resolved Raman scattering of TMD atomic layers. The dominant first order Raman bands, including the low energy breathing and shear modes as well as the high energy zone center optical phonons, are found to either maintain or completely switch the helicity of incident photons. This helicity selectivity due to phonon scattering is interpreted by symmetry of lattice vibrations without involving intervalley scattering. Our results provide a useful tool for characterization of TMD atomic layers and offer new insights into the connection between photon helicity and valley polarization.

3:30PM Q2.00006 Energy splitting of excitons in gapped Dirac materials. DI XIAO, JIANHUI ZHOU, WENYU SHAN, Carnegie Mellon Univ, WANG YAO, Univ. of Hong Kong, SATOSHI OKAMOTO, Oak Ridge National Laboratory — We show that there is an energy splitting between excitons with opposite angular momentum in gapped Dirac materials, such as monolayers of transition metal dichalcogenides and gapped surface states of topological insulators. This splitting can be traced back to the chiral nature of Dirac electrons. We also discuss the optical selection rule of excitons in gap Dirac materials and clarify the relationship to its single-particle counterpart. A simple estimation of the splitting (~ 10 meV) in monolayer transition metal dichalcogenides is given. Our result reveals the limitation of the venerable hydrogenic model of excitons, and highlights the importance of the Berry phase in...
4:42PM Q2.00010 Temperature and polarization dependence of photoluminescence in monolayer tungsten diselenide. JIANI HUANG, THANG HOANG, MAIKEN MIKKELSEN, Department of Physics, Duke University — Two-dimensional transition metal dichalcogenides (TMDCs) have recently attracted considerable research interest, due to their plasmonic properties and applications in electronics, optics, and spintronics. Here, we experimentally study the evolution of photoluminescence (PL) from mechanically exfoliated monolayer tungsten diselenide (WSe$_2$) from $T = 10$ K to room temperature. At $T = 10$ K, we observe a clear free exciton ($X^0$) emission at 1.75 eV together with a charged trion emission at 1.72 eV, yielding a trion binding energy of 30 meV. Temperature dependent PL measurements show that both the free exciton and trion exist up to room temperature, as a result of the large exciton ($\sim 370$ meV) and trion binding energies of WSe$_2$, while other localized and defect-related emission peaks vanish above $T = 65$ K. Temperature dependent polarization of the exciton and trion emissions reveal a combined effect of large exciton binding energy, anisotropic thermal expansion and exciton-phonon interaction. These findings may provide a new platform to explore the valley polarization and valley-spin coupling in monolayer TMDCs.

5:06PM Q2.00012 Plasmonic enhanced Photoluminescence and absorption in MoS$_2$ single layers. ADNEN MLAYAH, CEMES-CNRS-Paul Sabatier University, Toulouse, SINA NAJMAEI, Department of Mechanical Engineering & Materials Science, Rice University, Houston, INES ABID, CEMES-CNRS-Paul Sabatier University, Toulouse, ARNAUD ARBOUET, CHRISTIAN GIRARD, CEMES-CNRS, Toulouse, JEAN LÉOTIN, LNCMI-CNRS, Toulouse, JUN LOU, Department of Mechanical Engineering & Materials Science, Rice University, Houston — We report the successful transfer of CVD grown MoS$_2$ to Au antenna fabricated using e-beam lithography, and we investigate the photoluminescence properties of this hybrid plasmonic-exciton system. The work is focused on the plasmonic mediated pumping of the MoS$_2$ photoluminescence emission. Off- and in-resonance excitation of the surface plasmons showed drastically different behaviors of the photoluminescence emission from the MoS$_2$. For plasmonically mediated pumping, we found a significant enhancement of the photoluminescence intensity, emission peak broadening and red-shift. Based on numerical simulations of the plasmonic properties of the Au antenna, combined with heat dissipation calculations, we found that the results can be interpreted in terms of efficient light absorption by the plasmonic antenna and conversion into electron-hole pair excitations of the 2D MoS$_2$ layer thus producing a photo-induced heating.

5:18PM Q2.00013 Correlative confocal Raman Imaging for 2D materials. JIANYONG YANG, WEI LIU, WITec Instruments Corp., THOMAS DIEING, HARALD FISCHER, MARIUS HENRICH, OLAF HOLLRICHER, WITec GmbH — Graphene was one of the first two-dimensional materials which soon after its mono-layer production received much attention by many researchers worldwide. Its properties vastly differ from bulk graphite and its potential for applications ranges from transistors to transparent conducting electrodes and solar cell applications. While graphene is arguably the most prominent two-dimensional material there are to date many more that are subject to current research such as MoS$_2$, WS$_2$ or MoSe$_2$. Graphene has been already and still is extensively studied using a variety of characterization techniques. Raman spectroscopy and more importantly still, Raman imaging proved to be of great value due to the clearly different spectra obtained from single, double, triple and multi-layered Graphene. This and more information that can be extracted from Raman spectroscopy and imaging can be well be complemented with various forms of atomic force microscopy (AFM), Scanning Nearfield Optical Microscopy (SNOM), and scanning electron microscopy (SEM). In this contribution we illustrate the benefit of correlating said techniques with confocal Raman imaging in order to deepen the understanding of the samples in question.

Wednesday, March 4, 2015 2:30PM - 4:54PM — Session Q3 FIP: Invited Session: Condensed Matter Physics in Latin America II 002AB - Edmond L Berger, Arqonne National Laboratory

2:30PM Q3.00001 Spin dynamics with Solid State NMR and GPU calculations: Loschmidt Echoes, Intrinsic Decoherence and Quantum Dynamical Phase Transitions. HORACIO M. PASTAWSKI, Instituto de Física Enrique Gaviola, Universidad Nacional de Cordoba — After overviewing argentine Condensed Matter Physics outside the Metropolitain area I will focus on the Loschmidt Echo (LE), a concept developed and pursed at Córdoba. It is the recovered fraction of a localized excitation after a spreading protocol followed by an imperfect time reversal procedure [1]. In Solid State NMR, the LE has allowed us to quantify the decoherence and irreversibility induced by an uncontrolled environment. Notably complex many-body dynamics makes the system particularly sensitive to environmental disturbances presenting a decoherence rate much slower than decoherence expected beyond some small threshold. These experiments and the theoretical analysis based on the Feynman’s path integral, summarized at a tutorial level, fueled the field of dynamical quantum chaos [4]. The quest for a perturbation independent decoherence as an emergent phenomenon in thermodynamic limit, lead us to discuss other dynamical observables that depend non-analytically on the environment strength, i.e. that undergo a quantum dynamical phase transition QDPT [2]. GPU based high performance computing boosts the evaluation of the LE [3], allowing us to asses thermalization and how the Metal-Insulator transition (also a QDPT) emerges in interacting many-body systems.


1Financing institutions: CONICET, SeCyT-UNC, ANPCyT, MinCyT-Cor and Antorchas
3:06PM Q3.00002 An Upgrade for the Brazilian Synchrotron Light Source: Are you Sirius? ANTONIO JOSÉ ROQUE DA SILVA, Laboratório Nacional de Luz Síncrotron – LNLS — The application of synchrotron radiation in a great variety of fields in general, and condensed matter in particular, has increased steadily worldwide. This, to a large extent, is a result of the availability of the much brighter third-generation light sources, which opened up new experimental techniques. Recently, new developments in accelerator technology are paving the way for even brighter sources, which are being named fourth-generation light sources. Sirius, the future new Brazilian synchrotron, is one of the first two such machines being currently constructed in the world. Its first light is expected by 2018. It is being planned to be a state of the art machine, providing tools for cutting edge research that are non-existent today in Brazil. It is a project designed and executed by the Laboratório Nacional de Luz Síncrotron – LNLS, which was also responsible for the construction of the current second generation Brazilian light source, the first synchrotron in the southern hemisphere, still the only one in Latin America. In this talk an overview of the status of Sirius will be provided.

3:42PM Q3.00003 Large area radiation detectors based on II VI thin films, MANUEL QUEVEDO-LOPEZ, University of Texas at Dallas — The development of low temperature device technologies that have enabled flexible displays also present opportunities for flexible electronics and flexible integrated systems. Of particular interest are possible applications in flexible, low metal content, sensor systems for unattended ground sensors, smart medical bandages, electronic ID tags for geo-location, conformal antennas, neutron/gamma-ray/x-ray detectors, etc. In this talk, our efforts to develop novel CMOS integration schemes, circuits, memory, sensors as well as novel contacts, dielectrics and semiconductors for flexible electronics are presented. In particular, in this presentation we discuss fundamental materials properties including crystalline structure, interfacial reactions, doping, etc. defining performance and reliability of II-VI-based radiation sensors. We investigate the optimal thickness of a semiconductor diode for thin-film solid state thermal neutron detectors. Besides II-VI materials, we also evaluated several diode materials, Si, CdTe,GaAs, C (diamond), and ZnO, and two neutron converter materials, 10B and 6LiF. We determine the minimum semiconductor thickness needed to achieve maximum neutron detection efficiency. By keeping the semiconductor thickness to a minimum, gamma rejection is kept as high as possible. In this way, we optimize detector performance for different thin-film semiconductor materials.

4:18PM Q3.00004 Condensed Matter Physics in Colombia is in its forties, ANGELA CAMACHO, Universidad de Los Andes — Physics in Colombia started to develop in the 70’s as a research part of basic sciences with the acquisition, at that time, of large research equipments such as x-rays and EPR. Experimental work was soon supplemented by theoretical investigations, which led to the formation of research groups in condensed matter in the early 80’s. The early 80’s existed such groups in five universities. In this report we present, after a short history of the main steps that guided the initial research subjects, the major areas already developed and the minor research groups that are in the stage of consolidation. Currently this type of work is done at least in 20 universities. We also show the actual numbers of researchers, publications, PhD students and laboratories discriminated in gender to complete an overview of Condensed Matter Physics in Colombia. Finally, we present a short review of the main theoretical issues that have been worked in the last decade focusing on low dimensional systems, their structural and optical properties.

Wednesday, March 4, 2015 2:30PM - 5:30PM – Session Q4 DCMP: Invited Session: Fractional Quantum Hall Effect: New Directions Mayor Cockrell Room 004 - Jainedra Jain, Pennsylvania State University

2:30PM Q4.00001 Interacting Flatland Electrons Never Stop Surprising, MANSOUR SHAYEGAN, Princeton University — I will present the highlights of several new magneto-transport experiments that probe the physics of interacting two-dimensional (2D) electrons (or holes) at high magnetic fields and low temperatures. These include: (1) observation of rare fractional quantum Hall states at even-denominator (1/2) filling factor in 2D hole systems at an unusual crossing of the two lowest Landau levels [1,2]; (2) tuning and measuring the shape and anisotropy of the composite fermion (CF) Fermi contours [3-5], and (3) data suggesting that CFs themselves can be interacting and form their own fractional quantum Hall and Wigner solid states [6]. I will also discuss a bilayer experiment where the CFs in one layer are used to probe an electron Wigner solid in the other layer [7]. (Work done in collaboration with Yang Liu, D. Kamburov, M.A. Mueed, S. Hadsenir, I. Jo, H. Deng, L.N. Pfeiffer, K.W. West, and K.W. Baldwin. Supported by the NSF, DOE, Keck, and Moore Foundations.)


3:06PM Q4.00002 Composite Fermions and Broken Symmetries in Graphene, DAVID GOLDHABER-GORDON, Stanford Univ — No abstract available.

3:42PM Q4.00003 Even-denominator fractional quantum Hall physics in ZnO, JURGEN SMET, Max Planck Institute for Solid State Research — The study of even denominator fractional quantum Hall physics has for a long time been the exclusive privilege of the III-V semiconductor community. Its discovery at filling 5/2 and 7/2 in GaAs unleashed a flood of theoretical as well as experimental work, because these states are in essence thought to be p-wave superconducting ground states possessing non-abelian excitations. Recently however even-denominator fractional quantum Hall physics has been observed outside of the realm of III-V heterostructures in the emergent ZnO 2D electron system. ZnO not only exhibits a robust quantum Hall state at filling 7/2, but also at unconventional fillings. There is an incipient 9/2 state in perpendicular field and a fully resolved 3/2-state emerges when tilting. The latter is believed to be, just like the 7/2 state, a genuine single component state analogous to the 5/2 and 7/2 states in GaAs. Alternatively, it could be a two component spin state, a variant two-component state that has not previously been reported. The use of ZnO for investigating this even denominator FQH-physics offers a powerful additional degree of freedom. Because the Zeeman splitting and the cyclotron energy are comparable, it is possible to alter the orbital character of the partially filled level at fixed filling by tilting the sample. Our studies show unequivocally that the orbital nature of the partially filled level is crucial for the appearance of even-denominator fractional quantum Hall physics. While a basic understanding has been developed, key features remain to be understood with the spin degree of freedom likely playing a prominent role. This work has been performed together with J. Faison (University of Tokyo), D. Maryenko (RIKEN), B. Friess (MPI-FKF), D. Zhang (MPI-FKF), Y. Kozuka (University of Tokyo), A. Tsukazaki (Tohoku University and JST), M. Kawasaki (University of Tokyo and RIKEN).
4:18PM Q4.00004 Proliferation of Neutral Modes in Fractional Quantum Hall Regimes, HIROYUKI INOUE, Braun Center for Submicron Research, Department of Condensed Matter Physics, Weizmann Institute of Science — The fractional quantum Hall effect (FQHE) is a canonical example of 2D topological phases. Being incompressible in the bulk, available low-energy charged excitations are only at the edge: gapless chiral 1D edge channels. Various collective phenomena can emerge when interactions take place between coexisting multiple edge channels. Recently, there is a surge of energy transport in FQHEs besides the charge transport. A notable example is upstream neutral edge modes in so-called hole-like fractional FQHEs, arising from the interacting channels, which remained elusive despite of an early theoretical prediction. In this talk, I will describe the observation of such neutral modes stabilized via our sensitive shot noise measurements. Surprisingly, they were found not only in the hole-like FQHEs, as theoretically expected, but also in particle-like FQHEs and, furthermore, in the bulk. Our result presents a new picture of energy transport in FQHEs. The presence of various neutral modes may imply their unfavorable roles as potential decoherers for fractional quasiparticles. Hence, understanding the properties of the neutral modes may allow us to control decoherence and thus to conclusively observe quantum oscillations of the fractional quasiparticles.

In collaboration with Anna Grivnin, Yuval Ronen, Moty Heiblum, Vladimir Umansky, Diana Mahalu, Braun Center for Submicron Research, Department of Condensed Matter Physics, Weizmann Institute of Science.

1Present affiliation: Department of Physics, Princeton University

4:54PM Q4.00005 NMR probing of quantum electron solids in high magnetic fields, TREvor DAVID ROHNE, NTT and ERATO-JST — In the presence of a high magnetic field, a two dimensional electron system (2DES) is expected to manifest Wigner crystal phases. Over thirty years ago, the search for the Wigner solid led to the discovery of the fractional quantum Hall effect (FQHE). Since then, with the advent of GaAs quantum wells with increasingly high mobility, 2DESs in the quantum Hall regime have proved to be a hunting ground for exceedingly rich many-body physics. Incompressible liquid FQHE states were found to occur in the first Landau level at several fractional filling factors \( v \) with odd-denominator. The sequence of FQHE states is truncated by the formation of a Wigner crystal of electrons at very low filling factors, the transition being affected by disorder. In the second Landau level, composite fermions, the quasiparticles of the FQHE, can pair to yield a remarkable even-denominator FQHE state, whose properties are at the forefront of investigation. More recently, electronic solid phases have been shown to emerge among integer quantum Hall states. In this talk, I will discuss a new tool, resistively detected NMR, which serves as a direct local probe of in-plane charge density modulations in the 2DES. In our recent work we probe the local charge density landscape of Wigner solids in the vicinity of \( v = 2 \) and \( v < 1/3 \) revealing quantum correlations. This unprecedented access to the microscopic behavior of these exotic solid phases opens up new venues in FQHE studies. Furthermore, our NMR technique can probe in-plane charge density fluctuations due to disorder, allowing increased access to understanding roles of disorder in quantum Hall systems. In addition, our latest NMR measurements reveal evidence for charge inhomogeneity in the third Landau level which leads to the possibility of studying bubble and stripe phases in this regime. Future directions may find our NMR technique applied to other exotic phases such as quasiparticle solid phases, which have been proposed to emerge near the \( v = 1/3 \) and 5/2 FQHE states.


Wednesday, March 4, 2015 2:30PM - 5:18PM – Session Q5 DMP DCOMP: Focus Session: Search for New Fe-based Superconductors II

2:30PM Q5.00001 Itinerant magnetism in metallic CuFe2Ge2\(^2\), K. V. SHANAVAS, D. J. SINGH, Oak Ridge National Laboratory — Discovery of superconductivity in iron pnictides and chalcogenides has generated interest in the coexistence and interplay of superconductivity and magnetism. Antiferromagnetic spin fluctuations are believed to be mediating superconductivity in these systems. The large spin-fluctuations may arise as a consequence of nearness to a quantum critical point (QCP), which can also lead to non-Fermi liquid behavior, unusual transport and novel ground states. Thus, it is of interest to look for other materials that share similar characteristics. Using density functional theory based calculations we have studied the electronic structure and magnetic properties of CuFe2Ge2 based on it’s structural similarities with recently discovered YFe2Ge2. We find large density of states at the Fermi level \([N(E_F)]\), consistent with itinerant character. Fermi surfaces in this system have a sheet like structure amenable to nesting and consequently to magnetic instabilities. Our results suggest that CuFe2Ge2 is an antiferromagnetic metal, with similarities to the Fe-based superconductors; such as magnetism with substantial itinerant character and coupling between magnetic order and electrons at the Fermi energy.

2This research was supported by the US Department of Energy, Basic Energy Sciences, Office of Science, Materials Sciences and Engineering Division

2:42PM Q5.00002 Universal V-shaped phase diagram in the iron-based superconductors XFe2As2 (X = K, Rb, Cs) , ALEXANDRE OUELLET, FAZEL FALLAH TAFTI, ALEXANDRE JUNEAU-FECTEAU, SAMUEL FAUCHER, MAXIME LAPOINTE-MAJOR, NICOLAS DOIRON-LEYRAUD, LOUIS TAILLEFER, University of Sherbrooke, AIFENG WANG, XIGANG LUO, XIANHUI CHEN, University of Science and Technology of China — Following the discovery of a sharp reversal in the dependence of \( T_c \) on pressure in KFe2As2 [1] and CsFe2As2 [2], we report a similar behavior in RbFe2As2. The application of hydrostatic pressure initially decreases \( T_c \), until a critical pressure \( P_c = 11 \) kbar where \( T_c \) suddenly starts to increase. For the three materials, we find a universal V-shaped temperature-pressure phase diagram, with identical slopes above and below \( P_c \). Upon crossing \( P_c \), the upper critical field \( H_{c2} \) is observed to jump, by a similar factor for KFe2As2 and RbFe2As2. We interpret these universal features in terms of a pressure-induced change in the pairing state of these superconductors. [1] F. F. Tafti et al., Nature Physics 9, 349 (2013). [2] F. F. Tafti et al., Physical Review B 89, 134502 (2014).

2:54PM Q5.00003 Field dependence of thermal conductivity in XFe2As2 (X = K, Rb, Cs), PATRICK BOURGEOIS-HOPE, F. F. TAFTI, B. VINCENT, N. DOIRON-LEYRAUD, L. TAILLEFER, University of Sherbrooke, Sherbrooke, Canada, A.F. WANG, X.-G. LUO, X.H. CHEN, University of Science and Technology of China, Hefei, China — There is ongoing debate over the pairing symmetry in the hole-overdoped iron-based superconductor KFe2As2. While thermal conductivity [1] and penetration depth [2] data have been taken as evidence of a d-wave pairing state, heat capacity [3] and ARPES [4] have been interpreted within an s-wave state with accidental nodes on some parts of the Fermi surface. Here we report a complete study of the magnetic field dependence of thermal conductivity in the \( T = 0 \) limit for the isostructural materials XFe2As2 with X = K, Rb and Cs. Extending our previous results of KFe2As2 to RbFe2As2 and CsFe2As2 reveals a universal behaviour, implying that all three materials must have a very similar nodal structure. All data are found to be in excellent agreement with calculations for a d-wave superconductor. A similar nodal quasiparticle behaviour across different materials is natural within a d-wave state, a common nodal structure being automatically imposed by symmetry. By contrast, such similarity would be highly coincidental if nodes are accidental, as in an s-wave state.

3:06PM Q5.00004 Novel Materials & Multi-scale Analysis of the Superconducting State in Iron Based Superconductors1, ATHENA S. SEFAT, Oak Ridge National Laboratory — The understanding of the fundamental nature of a material's superconducting state is of crucial importance, if superconductors are to fulfill their promise for widespread use in energy-related needs. Our research applies multi-scale characterization techniques to study and probe the nuclear, electronic, and magnetic details of single crystals. The importance of such broad investigative work is demonstrated in our recent publication on praseodymium-doped BaFe2As2 for which non-uniform local distortions through isolated Pr atoms do not provide percolation path superconductivity [1]. For CaFe2As2, it is found that large Fermi-surface reconstruction in the non-magnetic phase causes a non-superconducting ground state [2], while different crystalline domains with varying lattice parameters are identified [3]. For Co-doped BaFe2As2 it is found that orthorhombic distortion below Tc leads to magnetically ordered state of FeAs planes, hence no superconductivity [4]. Studies of this nature can yield groundbreaking results by demonstrating that many parameters can compete in a bulk material and even be spatially and electronically non-homogeneous on nanometers.


1This work was primarily supported by the U. S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division.

3:42PM Q5.00005 Enhancement of transition temperature in iron based superconductor KFe2As2 under pressure, YASUYUKI NAKAJIMA, RENXIONG WANG, TRISTIN METZ, XIANGFENG WANG, Univ of Maryland-College Park, JASON JEFFRIES, Lawrence Livermore National Laboratory, JOHNPIERRE PAGLIONE, Univ of Maryland-College Park — Superconducting pairing symmetry in the iron pnictides is one of the key issues to clarify the origin of high Tc superconductivity. The versatile pairing symmetry, including sign-reversed full gap, symmetry-imposed, or accidental nodal states, has been proposed theoretically and experimentally [1,2], and it can undergo a transition from one to another by chemical substitution or pressure. For instance, recent pressure study on heavily hole-doped KFe2As2 may imply a possible symmetry change accompanied by sudden reversal in pressure dependence of Tc [3]. To explore the phase diagram of KFe2As2 in a wider pressure range, we here report low-temperature transport study under high pressure up to 33 GPa by utilizing a designer diamond anvil cell. We will discuss the evolution of the superconducting and structural properties of this material, highlighting novel changes in the system at high pressure. [1] J.P. Reid et al., PRL 109, 087001 (2012). [2] T. Shibauchi et al., Annu. Rev. Condens. Matter Phys. 5, 113 (2014). [3] F. Tafti et al., Nat. Phys. 6, 349 (2013).

3:54PM Q5.00006 Fermi-Surface Reconstruction in the collapsed-tetragonal phase of KFe2As2, LIMIN WANG, YASUYUKI NAKAJIMA, XIANGFENG WANG, Univ of Maryland-College Park, JASON JEFFRIES, Lawrence Livermore National Laboratory, JOHNPIERRE PAGLIONE, Univ of Maryland-College Park — Recent experiments reveal that applying pressure to KFe2As2 produces a rich phase diagram that includes the reversal in pressure dependence of Tc and without electronic structure change [1] and evolution of structural properties. Inspired by these, we investigate the electronic structure of KFe2As2 as a function of pressure using first-principles theory. Comparing with the ambient pressure tetragonal phase, we find that the Fermi surface topology undergoes significant changes at high pressures, with possible Lifshitz transition in the Fermi surface at high pressure. Together, our results suggest an interesting scenario of superconductivity in this material. [1] F. Tafti et al., Nat. Phys. 6, 349 (2013).

4:06PM Q5.00007 Microscopic, Transport and Thermodynamic properties of Ca10(2Pt5As5)((Fe1-xTMx)2As2)5 (TM=Co, Ni) single crystals, SHAN JIANG, NI NI, Univ of California - Los Angeles — Here we report detailed microscopic, transport and thermodynamic measurements on two series of high quality single crystals Ca10(2Pt5As5)((Fe1-xTMx)2As2)5 (TM=Co, Ni). With electron doping on Fe sites, the structural/magnetic phase transitions in the parent compound were suppressed at a rate of roughly -7K per 0.01Co doping and -9K per 0.01Ni doping. Superconductivity emerges in the region of 0.048 < x < 0.20 for Co doping with optimal Tc of 13.5K (x = 0.11) while it occurs in the region of 0.035 < x < 0.11 for Ni doping with optimal Tc of 9.6K (x = 0.064). No coexistence of AFM and SC is observed, which is different from the well-studied 122 Fe-pnictides but reminiscent the one of La1111. The comparison of the effect between Co- and Ni- doping on 10-3-8 shows that rigid band approximation is likely working for these two dopants in this superconducting family.

4:18PM Q5.00008 Vortex Lattice Anisotropy and Pauli Limiting in KFe2As2, S.J. KUHN, M.R. ESKILDSEN, University of Notre Dame, H. KAWANO-FURUKAWA, M. ONO, Ochanomizu University, Japan, E.M. FORGAN, E. JELLYMAN, R. RIYAT, University of Birmingham, United Kingdom, C.H. LEE, K. KIHOU, AIST, Japan, J. GAVILANO, Paul Scherrer Institute, Switzerland — In superconducting KFe2As2 (KFA), Hc2 (in Tesla) parallel to the basal plane is much larger than Hc1 (in Kelvin) suggesting Pauli limiting. We have used small-angle neutron scattering (SANS) with H applied close to the basal plane to study the vortex lattice (VL) anisotropy and scattered intensity in KFA. The VL anisotropy reflects the intrinsic anisotropy of the superconducting state (Γac), and may differ significantly from the Hc2 anisotropy (ΓHc2) as recently seen in Sr2RuO4 [C. Rastovsky et al., Phys. Rev. Lett. 111, 087003 (2013)]. Our data indicates a field dependent VL anisotropy in KFA, increasing with H, possibly caused by multi-band effects. At high fields Γac > ΓHc2, supporting Pauli limiting. Due to the moderately high anisotropy, both the longitudinal and transverse VL field modulation may contribute to the SANS signal, occurring as non-spin-flip and spin-flip scattering respectively. This allows us to determine the possible Pauli paramagnetic effects (spin polarization of un-paired quasiparticles in the vortex cores) along the two different directions.

1This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences under Award DE-FG02-10ER46783.

4:30PM Q5.00009 Influence of doping on the physical properties of Ca10-xRExPt5As5(Fe2-yPyAs2)5, JIAYUN PAN, AMAR KARKI, RONGYING JIN, Louisiana State Univ - Baton Rouge — Ca10-xRExPt5As5(Fe2-yPyAs2)5 is a new FeAs-based superconductor. We report the change of its superconducting transition temperature Tc and physical properties upon chemical doping in either Ca (using La or Gd) or Fe (using Pt) site. While partial replacement of Fe by Pt results in Tc up to 21K, we find that the substitution of Ca by La is most effective pushing Tc to 30 K. The doping dependence of electrical transport properties will be presented and discussed.
4:42PM Q5.00010 Field dependence of thermal conductivity in the iron-based superconductor KFe$_2$As$_2$: Evidence of a $d$-wave state. FAZEL FALLAH TAFTI, ALEXANDRE JUNEAU-FECTEAU, PATRICK BOURGOIS-HOPE, SAMUEL RENE DE COTRET, JEAN-PHILIPPE REID, NICOLAS DOIRON-LEYRAUD, LOUIS TAILLEFER, Univ of Sherbrooke, AIFENG WANG, XINGANG LUO, XIANHUI CHEN, University of Science and Technology of China — Pairing symmetry in the iron-arsenide superconductor KFe$_2$As$_2$ is the subject of active debate. Thermal conductivity at milliKelvin temperatures is a sensitive and directional probe of the superconducting gap structure. Thermal conductivity measured along both [100] and [001] directions reveal that Fermi surfaces in KFe$_2$As$_2$ must have vertical line nodes. This stringent constraint is automatically satisfied by $d$-wave symmetry, but not likely to be satisfied by an $s$-wave state, where nodes are accidental. Here, we report a detailed study of the magnetic field dependence of thermal conductivity in KFe$_2$As$_2$, measured in the $T = 0$ limit. The data are found to be in excellent agreement with $d$-wave calculations. Our data are also compatible with low-temperature specific heat data as a function of field, within a multi-band $d$-wave scenario. Using Fermi surface parameters from quantum oscillations, we estimate the thermal conductivity expected of the gap structure extracted from ARPES measurements on KFe$_2$As$_2$ for the different Fermi surface sheets. We find a result that is incompatible with our thermal conductivity data, and conclude that the superconducting state at the surface, accessed by ARPES, must be different from the state in the bulk, accessed by transport and thermodynamic measurements.

4:54PM Q5.00011 Huge enhancement of superconductivity in the collapsed tetragonal KFe$_2$As$_2$. JIANJUN YING, LING-YUN TANG, Center for High Pressure Science and Technology Advanced Research, HO-KWANG MAO, VIKTOR STRUZHZKIN, Geophysical Laboratory, Carnegie Institution of Washington, AI-FENG WANG, XIAN-HUI CHEN, University of Science and Technology of China, XIAO-JIA CHEN, Center for High Pressure Science and Technology Advanced Research — Recent work (F. F. Tafit, et al. Nature Phys. 9, 349 (2013)) on hole-doped iron pnictide KFe$_2$As$_2$ indicated a paring symmetry change at pressure of around 1.7 GPa. The investigation for the low-pressure region (below 7 GPa) revealed oscillation of $T_c$ with pressure. Here we report results of high-pressure transport and XRD measurements on KFe$_2$As$_2$ single crystals at high pressures up to 30 GPa. We map out the phase diagram of KFe$_2$As$_2$ and find a huge enhancement of $T_c$ in the collapsed tetragonal phase. The correlation between $T_c$ electronic and crystal structures is discussed. The strong electronic correlations are proposed to account for such an unexpected $T_c$ enhancement in KFe$_2$As$_2$.

5:06PM Q5.00012 Superconducting Properties of KFe$_2$Se$_2$. YOSHIHIKO TAKANO. National Institute for Materials Science (NIMS) — Layer structured iron selenide, FeSe has the simplest crystal structures among iron-based superconductors. It shows superconductivity with transition temperature ($T_c$) of 13 K under ambient pressure. The $T_c$ increases up to 37 K by applying high pressure [1-3]. These facts indicate that the FeSe-layers are favorable structures to show superconductivity. When potassium is doped to the interlayer of FeSe, the resulting compound KFe$_2$Se$_2$ shows superconductivity at around 31 K under ambient pressure. However, the superconducting properties have no consensus even in the ambient pressure condition, because of its reproducing, inhomogeneity, and instability, and so on. It is necessary to obtain the high-quality single crystals to clarify the intrinsic properties. In this study, we cultivate the preparation method for the single crystalline KFe$_2$Se$_2$ [4], and investigate its superconducting properties by electrical properties using ARPES, magnetic susceptibility and transport properties, and single crystal structural analysis. [1] Y. Mizuguchi et al., Appl. Phys. Lett. 93, 152505 (2008). [2] S. Margadonna et al., Phys. Rev. B 80, 064506 (2009). [3] S. Masaki et al., J. Phys. Soc. Jpn. 78, 063704 (2009). [4] T. Ozaki et al., Euro. Phys. Lett., 98, 27002 (2012).

Wednesday, March 4, 2015 2:30PM - 5:30PM — Session Q6 DMP DCOMP: Focus Session: Coupling Polarization and Magnetism II 060A - Haidan Wen, Argonne National Laboratory

2:30PM Q6.00001 Magnetically induced ferroelectricity in single crystalline Lu$_2$CoMnO$_6$. SHA-LINEE CHIKARA, JOHN SINGLETON, National High Magnetic Field Lab, Los Alamos Natl Lab, HWAN YOUNG CHOI, NARA LEE, YOUNG J CHOI, Yonsei University, South Korea, VIVIEN ZAPF, National High Magnetic Field Lab, Los Alamos Natl Lab — We present pulsed-magnetic-field measurements on Lu$_2$CoMnO$_6$ single crystals. We are able to resolve electric polarization in single crystals for the first time. The bulk hysteric magnetization couples to the electric polarization resulting in a hysteretic, ferroelectric behavior. The alternating $S = 3/2$ Co$^{2+}$ and Mn$^{4+}$ ions sit in a corner-sharing octahedral oxygen environment. The Co-Mn-Co-Mn spins order in an up-up-down-down (uudd) arrangement along the $c$-axis. The ferroelectricity was believed to originate from the exchange striction due to the uudd spin arrangement. However, recent dielectric measurements suggest polarization along the $b$- not the $c$-axis. Our results confirm that ferroelectricity is indeed observed along the $b$-axis and not along the uudd spin-ordering direction. This indicates a different origin for the multiferroic behavior. The frustrated spin system displays an incommensurate long-wavelength modulation that may play a role in inducing ferroelectricity.

2:42PM Q6.00002 Multiferroicity in HoFeO$_3$. PRATIK DHUVD, XIFAN WU, Physics Department, Temple University, Philadelphia, PA 19122 — Rare-earth ferrites are becoming popular among multiferroic materials due to its spontaneous magnetic and electric orderings. After discovery of new family of multiferroic RFeO$_3$(R=Lu,LuF) which shows simultaneous ferroelectricity and weak ferromagnetic moment, HoFeO$_3$(HFO) is explored as a potential candidate in multiferric materials. Combined theoretical and experimental study has been done to understand ferroelectric and ferromagnetic properties of HFO. Our calculations suggest that iron in HFO exhibits very large canting, about one order of magnitude, compared to canting of iron in LFO, which is consistent with experimental findings. Analysis of structural phase transitions and calculation of phonon modes governing this ferroelectric transition revealed that HFO is improper ferroelectric with ferroelectric polarization about 8.3 $\mu$C/cm$^2$. These ferroic properties advocate HFO to be a useful multiferroic among other rare-earth ferrites.

2:54PM Q6.00003 ABSTRACT WITHDRAWN

3:06PM Q6.00004 A study of the origin of large magnetic field coupled electric polarization in HoAl(BO$_3$)$_4$. TIAN YU, HAN ZHANG, TREVOR TYSON, New Jersey Institute of Technology, ZHIQIANG CHEN, State University of New York at Stony Brook, MILINDA ABEYKOON, CHRISTIE NELSON, Brookhaven National Laboratory, LEONARD BEZMATERNYKH, L. V. Kirensky Institute of Physics — The multiferroic system RAl(BO$_3$)$_4$ is known to exhibit a strong coupling of magnetic field to the electrical polarization. Recently a giant magnetoelectric effect was found in HoAl(BO$_3$)$_4$. This phenomenon is considered quite interesting because the value discovered is significantly higher than reported values of linear magnetoelectric or even multiferroic compounds. We are conducting detailed structural measurements to understand the coupling. We are exploring the local and long range structure in these systems using x-ray PDF, XAFS and single crystal diffraction measurement between 10 K and 400 K. Structural parameters including lattice parameters and ADPs are being determined over the full temperature range. This work is supported by DOE Grant DE-FG02-07ER46402.

3:18PM Q6.00005 High Pressure Study on the Multiferroic State in Mn1-xCoxWO4: x = 0.135 and x = 0.15, MELISSA GOOCH, NARAYAN POUDEL, BERND LORENZ, K.C. LIANG, Y.Q. WANG, Y.Y. SUN, Texas Center for Superconductivity at the University of Houston, JINCHEN WANG, FENG YE, Oak Ridge National Laboratory, JAIME FERNANDEZ-BACA, Oak Ridge National Laboratory and Department of Physics and Astronomy at The University of Tennessee, CHING-WU CHU, Texas Center for Superconductivity at the University of Houston and Lawrence Berkeley National Laboratory — Mn1-xCoxWO4 has an interesting and complex phase diagram where 2 multiferroic phases coexist at x = 0.15. For x < 0.15 a spiral spin structure forms, while in contrast a conical spin is observed for x > 0.15. High pressure polarization measurements on x = 0.135 observed a polarization flop and an increase in the polarization, indicating the a-c spiral is converted to the conical spin. An enhancement of the polarization by ∼ 400% is seen for x = 0.15, at the highest pressure measured. High pressure neutron measurements found supporting results.

3:30PM Q6.00006 Temperature and high-pressure dependent X-ray absorption of SmNiO3 at K-Ni and Sm-L3 edges , N.E. MASSA, LANAIS EFO-CQUEINOR, UNLP, La Plata, Argentina, A.Y. RAMOS, H.C.N. TOLENTINO, Inst. Neu-CNRS, F-38042 Grenoble, France, N. SOUSA NETO, J. FONSECA JR., NLNS, 13084-971, Campinas, Sao Paulo, Brazil, M.J. MARTINEZ-LOPE, J.A. ALONSO, ICMC-CSIC, Madrid, Spain — We report XANES and EXAFS measurements of SmNiO3 from 20 K to 600 K and up to 38 GPa done at NLNS, Campinas, Brazil, in the DXAS energy dispersive beamline. SmNiO3 undergoes an atmospheric pressure insulator to metal transition at TMI ∼ 400 K, orders magnetically at T N ∼ 205 K, and shares with all RNiO3 (R = Rare Earth) a negative ∆TMI/∆P slope. Ni white line peak energies show an abrupt 2.4 GPa and 8.11 GPa valence discontinuity at 300 K and at 20 K respectively, due to non-equivalent Ni sites with Ni++ and Ni−− charge disproportion in a monoclinic distortion turning at TMI into Ni+3+ in the orthorhombic Pbnm metal oxide phase. Increasing pressure induces Ni-O-Ni angle increments toward more symmetric NiO6 octahedra of rhombohedral R−3c space group (metallic LaNiO3). At 38 GPa, there is a clear split of the main EXAFS band according to the cell volume decrease due to contraction. Pre-edge tail accounts for e−-t2g splitting and a stronger band growing in intensity in the higher symmetry metallic phases associated to e− electron delocalization hopping conductivity. The Ni+3+ post-edge becomes smoother and intensity increased by the reduction of electron-phonon interaction as the pressure-induced phases set in. We also found that Sm L1-edge does not show distinctive behaviors either at 300 K or 20 K up about 35 GPa.

3:42PM Q6.00007 Driving the magnetic response of BiFeO3 by hydrostatic pressure . C. TOULOUSE, J. BUHOT, Y. GALLAIS, A. SACUTO, Laboratoire Matériaux et Phénomènes Quantiques - Université Paris Diderot-Paris7, A. FORGET, D. COLSON, DSM/DRECAM/SPEC - Service Physique de l’Etat Condensé - CEA Saclay, R. DE SOUSA, Department of Physics and Astronomy - University of Victoria, D. WANG, Electronic Research and Development Center - Xi’an Jiaotong University, L. BELLACHE, Physics Department and Institute for Nanoscience and Engineering - University of Arkansas, M. BIBES, A. BARTHELÉMY, Unité Mixte de Recherche CNRS/Thales, M. CAZAYOUS, M. MEASSON, Laboratoire Matériaux et Phénomènes Quantiques - Université Paris Diderot-Paris7, — BiFeO3 exhibits ferroelectric and magnetic orders at room temperature, which makes it an ideal candidate for spintronics, electro-optics and data storage applications. Most of its properties are related to its ferroelectric character, especially studied under electric or magnetic fields, however the antiferromagnetism has not been extensively investigated, in particular under pressure. Here, we bring insight into the rich spin physics of BiFeO3 in a detailed study of the dynamic magnetic response of bulk BiFeO3 under pressure up to 12GPa measured by Raman spectroscopy. As pressure increases, multiple spin excitations associated to non-collinear cycloidal magnetism collapse into two excitations, which show jump discontinuities at some of the ensuing crystal phase transitions. Using effective hamiltonian simulations of both the structure and the magnetism and Ginzburg-Landau theoretical calculations we show that the pressure controls both the structural phase and the magnetic anisotropy that drives the spin excitations.

3:54PM Q6.00008 Multiferroicity in Ni doped MnWO4 , N. POUDEL, B. LORENZ, B. LV, TcSUH and Department of Physics, University of Houston, F. YE, Neutron Scattering Science Division, Oak Ridge National Laboratory, Y.Q. WANG, Y.Y. SUN, TcSUH and Department of Physics, University of Houston, J.A. FERNANDEZ-BACA, Neutron Scattering Science Division, Oak Ridge National Laboratory and Dept. of Physics and Astronomy, Univ. of Tennessee, C.W. CHU, TcSUH and Department of Physics, University of Houston and Lawrence Berkeley National Laboratory — In this work, we studied the multiferroic properties of MnWO4:Ni for Ni content up to 0.30 with ferroelectric, magnetic and heat capacity measurements. For x = 0.05 and 0.10, the maximum polarization is 38 μC/m2 and ferroelectric transition temperature (Tc) is 13.2 K which is 0.5 K higher than in parent compound. For other increasing values of x, the polarization decreases. For x = 0.15, due to onset of AF4 collinear phase, the polarization becomes maximum and then decreases at lower temperature. A small polarization of 2.3 μC/m2 is observed for x = 0.20 with Tc lowered at ~9.5 K and the polarization is completely suppressed for x = 0.30. Unlike in Co doped MnWO4, neutron scattering reveals only two AF2 and AF4) AF magnetic phases and the onset of the AF4 phase shift to higher temperatures with increasing value of x.

1 supported by DOE, the AFOSR, the T.L.L. Temple Foundation, the J.I. and R. Moores Endowment and the State of Texas/TcSUH

4:06PM Q6.00009 A second ferroelectric transition induced by pressure in multiferroic GdMn2O5 , BERND LORENZ, NARAYAN POUDEL, MELISSA GOOCH, CHING-WU CHU, Texas Center for Superconductivity and Department of Physics, University of Houston, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University — In multiferroic materials different magnetic and ferroelectric states compete for the ground state and are usually close in energy. This results in a high sensitivity of the multiferroic state to external perturbations, such as magnetic fields or pressure, which has been demonstrated, e.g. in Fe3V2O8, MnWO4, and RMn2O5 (R = Tb, Ho, Dy, Y). Here we report the results of a high-pressure study of the multiferroic and ferroelectric properties of GdMn2O5, the RMn2O5 compound with the highest value of the polarization. The ferroelectric polarization below 29 K is enhanced upon application of pressure. Above a critical pressure, a second ferroelectric transition at even higher temperature is detected through a sizable increase of the polarization and a second peak of the dielectric constant. The ferroelectric polarization at high pressures exhibits two step-like increases upon decreasing temperature. This work was supported by the US AFOSR, the T.L.L. Temple Foundation, the John J. and Rebecca Moores Endowment, and the State of Texas through TcSUH.

4:18PM Q6.00010 Evolution of weak ferromagnetism in BiFeO3 under applied epitaxial strain , HEMANT DIXIT, JUN HEE LEE, VALENTINO R. COOPER, Oak Ridge National Lab — The magnetoelectric effect has been a focus of research in multiferroic materials due to potential applications in magnetic data storage, spintronics and memory devices. We perform first principles calculations based on density functional theory to explore the evolution of weak ferromagnetism under compressive and tensile strains in BiFeO3. An isosymmetric phase transition between the rhombohedral ground state and strained phases (Cc space group) is considered which confines the polarization vector to rotate in the (110) plane. For the ground state, we find that the easy spin axis is degenerate in a plane perpendicular to the polarization direction. This weak ferromagnetic moment also persists for the tested strain values (up to ±5%). Under compressive strains, the easy spin axis is also degenerate in a plane perpendicular to the polarization vector. On the other hand for tensile strain the weak ferromagnetic ordering is stabilized along the [1-10] direction. Further, calculated Dzyaloshinskii-Moriya interactions help us to understand the stabilization of weak ferromagnetic moments in the tensile region. Our study thus offers useful insights for manipulating the magnetic response and utilizing the magnetoelectric effect.

1 Acknowledgement: Research supported by Office of Science of the U.S. Department of Energy, Basic Energy Sciences (BES) and Materials Sciences and Engineering Division.
4:30PM Q6.00011 Control of oxygen octahedral rotation in BiFeO$_3$ films using modulation of SrRuO$_3$ bottom electrode layer, Sungsu Lee, Ji Young Jo, School of Materials Science and Engineering, Gwangju Institute of Science and Technology (GIST), Gwangju 500-712, Korea — Oxygen octahedral rotation of multiferroic BiFeO$_3$ (BFO) has attracted great attention due to changes of electrical and magnetic properties. Coupling of octahedral rotation in BFO-bottom electrode layer interface remains unexplored. Recently, there have been reported the control of octahedral rotation in SrRuO$_3$ (SRO) film on SrTiO$_3$ (001) substrate by coherently controlling the oxygen pressure during growth and interfacial coupling [1]. Here we demonstrate that the octahedral rotation of BFO film is changed using tetragonal a$_x$I$a$-c$_x$ tilted-SRO bottom electrodes. In this work, BFO/SRO heterostructure is fabricated to SrTiO$_3$ (001) single crystal substrates by pulsed laser deposition at different oxygen partial pressures. The rotation pattern of FeO$_6$ and the structural symmetry are identified from half-integer reflections using high-resolution X-ray diffraction. The effects depending on octahedral tilting of BFO films on the magnetic and ferroelectric properties will be presented.


4:42PM Q6.00012 Predicting a Ferrimagnetic-Ferroelectric Phase of Zn$_2$FeOsO$_6$ with Strong Magnetoelectric Coupling, Hongjun Xiang, P.S. Wang, Fudan University, Wei Ren, Shanghai University, L. Bellaiche, University of Arkansas — Multiferroic materials, in which ferroelectric and magnetic order coexist, are of fundamental interest for the development of novel memory devices that allow for electrical writing and non-destructive magnetic readout operation. The great challenge is to create room temperature multiferroic materials with strongly coupled ferroelectric and ferromagnetic (or ferrimagnetic) orderings. BiFeO$_3$ has been the most heavily investigated single-phase multiferroic to date due to the coexistence of its magnetic order and ferroelectric order at room temperature. However, there is no net magnetic moment in the cycloidal (antiferromagnetic-like) magnetic state of bulk BiFeO$_3$, which severely limits its realistic applications in electric field controlled spintronic devices. Here, we predict that double perovskite Zn$_2$FeOsO$_6$ is a new multiferroic with properties superior to BiFeO$_3$. First, there are strong ferroelectricity and strong ferrimagnetism at room temperature in Zn$_2$FeOsO$_6$. Second, the easy-plane of the spontaneous magnetization can be switched by an external electric field, evidencing the strong magnetoelectric coupling existing in this system. Our results suggest that ferrimagnetic 3d-5d double perovskite may therefore be used to achieve voltage control of magnetism in future spintronic devices.


4:54PM Q6.00013 Prediction of electromagnons in BiFeO$_3$ from atomistic simulations, Brajesh Mani, Chun-Min Chang, Sergey Lisenkov, Inna Ponomareva, Department of Physics, University of South Florida, Tampa, Florida 33620, USA — We developed a first-principles-based computational approach to study the finite-temperature complex dynamics in multiferroics. Application of this technique to one of the most well-known multiferroic, BiFeO$_3$, revealed that the most general form of the magnetoelectric coupling that is allowed in any multiferroic, may produce an electromagnon in antiferromagnetic ferroelectric. Such an electromagnon shares most of the features with the magnon, but is activated by an electric, rather than magnetic, field. We also found that the A$_1$ phonon mode is repelled by the magnon mode, while the E phonon modes is rather insensitive to the presence of electromagnons. We believe that our findings will aid to a deeper understanding of electromagnon modes and their origin in multiferroics as well as provide a computational methodology for further research.


5:18PM Q6.00015 Magnetic structures in potential multiferroic GdCrO$_3$, Pascal Manuel, ISIS Pulsed Neutron and Muon Facility, Laurent Chapon, Institut Laue Langevin, Dmitry Khalyavin, ISIS Pulsed Neutron and Muon Facility, Wang Xueyun, Sang-Wook Cheong, Rutgers University — For the past decade, multiferroics materials have attracted a lot of attention in the condensed matter community because of potential applications for devices. A somewhat ambiguous addition to the multiferroics family was recently reported in the perovskite based GdCrO$_3$, in both bulk and thin film samples. Indeed, ferroelectricity was evidenced by a strong enhancement of the capacitance in a field but significant leakage and no well developed P-E hysteresis blurred the picture. Our own measurements clearly indicate the existence of a polar phase below 2K. To complete the understanding of this material, the determination of the magnetic structure is required but is hampered by the fact Gd is a strong neutron absorber. We will present some neutron diffraction data collected on an isotopic $^{160}$GdCrO$_3$ sample at the WISH diffractometer at ISIS which confirm the presence of three successive magnetic phases, previously only seen by magnetization, as a function of temperature. We will compare our determined structures against predictions based on group theoretical considerations and experimental work on other rare-earth ortho-chromates and discuss the mechanism for multiferroicity.

Wednesday, March 4, 2015 2:30PM - 5:30PM
Session Q7 DCMP: Topological Insulators: Theory and Experiment 006B - Ken Burch, Boston College

2:30PM Q7.00001 Magnetic ordering on edges of topological insulator, Yea-Lee Lee, Seoul Natl Univ, Hee Chul Park, Korea Institute for Advanced Study, Jisoon Ihm, Seoul Natl Univ, Young-Woo Son, Korea Institute for Advanced Study — Based on first-principles calculations, we show that the B$_2$I$_3$Se$_3$ crystal, which is a prototypical topological insulator, with different crystal-face orientation surfaces generates a built-in electric field around the facet edges due to the work function differences. For a given broken time reversal symmetry in the crystal, the electric field, in turn, induces a net magnetic ordering along the edges by the topological magnetoelectric coupling. The predicted magnetic ordering depending on the work function differences between facets would be a unique manifestation of the axion electrodynamics in real solids and suggests a route to reveal novel properties of macroscopic topological edge states.
2:42PM Q7.00002 Exotic quantum phase transitions of 2+1d Dirac fermions, and connections to 2d and 3d topological insulators, KEVIN SLAGLE, YI-ZHUANG YOU, CENKE XU, Univ of California - Santa Barbara — Using determinant quantum Monte Carlo simulations, we demonstrate that an extended Hubbard model on a bilayer honeycomb lattice has two novel quantum phase transitions, each with connections to symmetry protected topological states. 1) The first is a continuous phase transition between the weakly interacting gapless Dirac fermion phase and a strongly interacting fully gapped and symmetric trivial phase. Because there is no spontaneous symmetry breaking, this transition cannot be described by the standard Gross-Neveu model. We argue that this phase transition is related to the Z_{16} classification of the topological superconductor 2He-B phase with interactions. 2) The second is a quantum critical point between a quantum spin Hall insulator with spin S^z conservation and the previously mentioned strongly interacting gapped phase. At the critical point the single particle excitations remain gapped, while spin and charge gaps close. We argue that this transition is described by a bosonic O(4) nonlinear sigma model field theory with a topological O(2)-term.

2:54PM Q7.00003 Phase diagrams of disordered 3D topological insulators and superconductors, TOMI OHTSUKI, Sophia University, KOJI KOBAYASHI, Sophia University, KEN-ICHIRO IMURA, Hiroshima University, KEN NOMURA, Tohoku University — A global phase diagram of disordered weak and strong topological insulators belonging to the class AII is obtained by numerically calculating the conductance, the Lyapunov exponents and the density of states. The location of the phase boundaries, i.e., the mass parameter, is renormalized by disorder, a feature recognized in the study of topological Anderson insulator. We report quantized conductance on the phase boundaries between topologically distinct phases, which is interpreted as the robustness of conductance against disorder. This robustness is also confirmed by the large-scale numerical calculation of the density of states, which remains parabolic up to certain strength of disorder with renormalized Dirac electron velocity. From the size dependence of the conductance, we also point out that the surface states of weak topological insulator are either robust or “defeated”. The nature of the two distinct types of behavior is further revealed by studying the Lyapunov exponents. (K. Kobayashi et al., Phys. Rev. Lett. vol. 110, 236803 (2013)). We also obtain the phase diagram of disordered topological superconductors belonging to the class DIII. Similar renormalization of mass and velocity due to disorder is found.

3:06PM Q7.00004 Surface-to-bulk scattering in topological insulator films, KUSH SAHA, ION GARATE, University of Sherbrooke, Sherbrooke, Quebec, Canada — We present a quantitative microscopic theory of the disorder- and phonon-induced coupling between surface and bulk states in topological insulator (TI) films. We find a simple mathematical structure for the surface-to-bulk scattering matrix elements and confirm the importance of bulk-surface coupling in transport and photoemission experiments, assessing its dependence on temperature, carrier density, film thickness and film-hole asymmetry.

3:18PM Q7.00005 Sum rule constraints on the surface state conductance of topological insulators, K.W. POST, B.C. CHAPLER, M.K. LIU, H.T. STINSON, M.D. GOLDFLAM, Univ of California - San Diego, A.R. RICHARDELLA, J.S. LEE, Pennsylvania State University, A.A. REJINDERS, University of Toronto, K.S. BURCH, Boston College, N. SAMARTH, Pennsylvania State University, D.N. BASOV, Univ of California - San Diego — We report the Drude oscillator strength (D) and the magnitude of the bulk band gap of the epitaxial topological insulator alloy (Bi,Sb)_{1-x}Te_{x}. The bulk band gap is used in conjunction with f-sum rules to establish an upper bound for the D expected in a typical Dirac like system composed of linear bands. We expand our result from the linear band model to include both hexagonal warping and electron-hole asymmetry, as is typical in topological insulator systems. The corresponding maximum value of D arising from Dirac bands in this more complex system is also determined. The observed D is found to be close to this upper bound, demonstrating the effectiveness of alloying in eliminating bulk charge carriers. Moreover, Hall effect parameters and the weak anti-localization observed in transport on the same sample support assignment of the low-energy conduction to topological surface states.

3:30PM Q7.00006 Many-Body Effects in 2D Topological Kondo Insulators, JASON IACONIS, Univ of California - Santa Barbara, LEON BALENTS, Kavli Institute for Theoretical Physics - Univ of California - Santa Barbara — Recently there has been an immense amount of interest in studying the effect of interactions on systems with a nontrivial topology. Perhaps the simplest manifestation of this phenomena, and that which is most closely related to experimental materials, can be found in the so called topological Kondo insulators. In our work we study a model of graphene which is doped with localized partially filled d-shell electron moments. We model this system using a simple Hamiltonian in which the Kondo interaction can lead to the formation of a topological insulating phase with many-body correlations. I will discuss a mean field treatment of this model where we map out the different possible interacting phases of the system. It is of particular interest to study the effect of interactions on the symmetry protected gapless edge states, as such edge states are perhaps the most dramatic consequence of having a band structure with a nontrivial topology. We discuss the possibility that the Kondo interaction leads to edge states which spontaneously break time-reversal symmetry, while preserving the symmetry within the bulk.

3:42PM Q7.00007 Quantum criticality in Kondo quantum dot coupled to helical edge states of interacting 2D topological insulators, CHUNG-HOU CHUNG, SALMAN SILOTRI, Department of Electrophysics, National Chiao-Tung University, HsinChu, Taiwan, R.O.C. — We investigate theoretically the quantum phase transition (QPT) between the one-channel Kondo (1CK) and two-channel Kondo (2CK) fixed points in a quantum dot coupled to helical edge states of interacting 2D topological insulators (2DTI) by tuning Kondo couplings at a fixed Luttinger parameter K < 1. The system can be mapped onto an anisotropic two-channel Kondo Hamiltonian, and the 2CK fixed point was argued to be stable for infinitesimally weak tunnelings between dot and the 2DTI. We re-examine this model beyond the bare scaling dimension analysis via a controlled perturbative renormalization group (RG) approach combined with bosonization and re-fermionization techniques near weak-coupling and strong-coupling (2CK) fixed points. For $K$ close to but less than 1, we find the 2CK fixed point can be unstable towards the 1CK fixed point and the system is expected to undergo a quantum phase transition between 1CK and 2CK fixed points. Our system serves as the first example of the 1CK-2CK QPT that is accessible by the controlled RG approach though this transition has been known to exist in Kondo dot coupled to two conventional Luttinger liquid leads with a critical value $K_c = 1/2$. We extract quantum critical and crossover behaviors from various observables near criticality.

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1 Grants-in-Aid No. 23540376, Grants-in-Aid No. 2400013.

2 This work is supported by the NSC grant No.98-2918-I-009-06, No.98-2112-M-009-010-MY3, the NCTU-CTS, the MOE-ATU program, the NCTS of Taiwan, R.O.C..
3:54PM Q7.00008 Electrical Detection of Spin-Polarized Surface States Conduction in (Bi$_{0.53}$Sb$_{0.47}$)$_2$Te$_3$ Topological Insulator$^1$, JIANSHI TANG, LI-TE CHANG, XUFENG KOU, KOICHI MURATA, MURONG LANG, YABIN FAN, MOHAMMAD MONTAZERI, WANJIUN JIANG, LIANG HE, KANG L. WANG, Univ of California - Los Angeles, EUN SANG CHOI, National High Magnetic Field Laboratory, YING JIANG, YONG WANG, Zhejiang University — Strong spin-orbit interaction and time-reversal symmetry in topological insulators enable the spin-momentum locking for the helical surface states. Here we report the electrical detection of spin-polarized surface states conduction using a Co/Al$_2$O$_3$ ferromagnetic tunneling contact, in which the compound topological insulator (Bi$_{0.53}$Sb$_{0.47}$)$_2$Te$_3$ was used to achieve low bulk carrier density [1]. Resistance (voltage) hysteresis was observed when sweeping the magnetic field to change the relative orientation between the Co electrode magnetization and the spin polarization of surface states. The two resistance states were reversible by changing the electric current direction, affirming the spin-momentum locking in the topological surface states. Angle-dependent measurement was also performed to further confirm that the abrupt change in the voltage (resistance) was associated with the magnetization switching of the Co electrode. Our results show a direct evidence of spin polarization in the topological surface states conduction. It might open up great opportunities to explore energy-efficient spintronic devices based on topological insulators. This work is supported by DOE-BES (Grant No. DE-FG02-04ER46148) and NSF-MRSEC (Grant No.DMR-1121252).


4:06PM Q7.00009 Tuning Topological Edge States of Bi(111) Bilayer Film by Edge Adsorption, ZHENGFEI WANG, University of Utah, LI CHEN, Linyi University, FENG LIU, University of Utah — Based on first-principles and tight-binding calculations, we report that the topological edge states of zigzag Bi(111) nanoribbon can be significantly tuned by H/S element adsorption. The Fermi velocity is increased by 1 order of magnitude, as the Dirac point is moved from the Brillouin zone boundary to the Brillouin zone center, and the real-space distribution of Dirac states are made twice more delocalized. These intriguing changes are explained by an orbital filtering effect of edge H atoms, which pushes certain components of the p orbital of edge Bi atoms out of the band gap regime that reshapes the topological edge states. In addition, the spin texture of the Dirac states is also modified, which is described by introducing an effective Hamiltonian. Our findings not only are of fundamental interest but also have practical implications in potential applications of topological insulators. This work is supported by DOE-BES (Grant No. DE-FG02-04ER46148)

4:18PM Q7.00010 Crossover between Weak Antilocalization and Weak Localization of Bulk States in Ultrathin Bi$_2$Se$_3$ Films, HUICHAO WANG, HAIWEN LIU, YANFEI ZHAO, YI SUN, X.C. XIE, JIAN WANG, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China, CUIZU CHANG, KE HE, XUCUN MA, QI-KUN XUE, State Key Laboratory of Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University, Beijing 100084, China, HUAUKAN ZUO, ZHENGCAI XIA, Wuhan National High Magnetic Field Center, Huazhong University of Science and Technology, Wuhan 430074, China — We report studies on the 5 nm thick Bi$_2$Se$_3$ topological insulator films which are grown via molecular beam epitaxy technique. The angle-resolved photoemission spectroscopy data show that the Fermi level of the insulator films which are grown via molecular beam epitaxy technique. We observed a clear distinction in the phases of emitted terahertz electric field and azimuth-dependent second harmonic generation techniques. We reported the topological edge states of zigzag Bi(111) nanoribbon can be significantly tuned by H/S element adsorption. The Fermi velocity is increased by 1 order of magnitude, as the Dirac point is moved from the Brillouin zone boundary to the Brillouin zone center, and the real-space distribution of Dirac states are made twice more delocalized. These intriguing changes are explained by an orbital filtering effect of edge H atoms, which pushes certain components of the p orbital of edge Bi atoms out of the band gap regime that reshapes the topological edge states. In addition, the spin texture of the Dirac states is also modified, which is described by introducing an effective Hamiltonian. Our findings not only are of fundamental interest but also have practical implications in potential applications of topological insulators. This work is supported by DOE-BES (Grant No. DE-FG02-04ER46148) and NSF-MRSEC (Grant No.DMR-1121252).

4:30PM Q7.00011 Crossover from 3D to 2D Quantum Transport in Bi$_2$Se$_3$/In$_2$Se$_3$ Superlattices, ZHAO YANFEI, LIU HAIWEN, ICQM, Peking University, GOU XIN, Physics Department, The University of Hong Kong, JIANG YING, Department of Materials Science and Engineering, Zhejiang University, SUN YI, WANG HUICHAO, ICQM, Peking University, WANG YONG, Department of Materials Science and Engineering, Zhejiang University, LI HAN DONG, University of Electronic Science and Technology of China, XIE MAO HAI, Physics Department, The University of Hong Kong, XIE XINCHE NG, WANG JIAN, ICQM, Peking University — The topological insulator/normal insulator (TI/Ni) superlattices (SLs) with multiple Dirac channels are predicted to offer great opportunity to design novel materials and investigate new quantum phenomena. Here, we report first transport studies on the SLs composed of TI/Bi$_2$Se$_3$ layers sandwiched by Ni In$_2$Se$_3$ layers artificially grown by molecular beam epitaxy (MBE). The transport properties of two kinds of SL samples show convincing evidence that the transport dimensionality changes from three-dimensional (3D) to two-dimensional (2D) when decreasing the thickness of building block Bi$_2$Se$_3$ layers, corresponding to the crossover from coherent TI transport to separated TI channels. Our findings provide the possibility to realizing 3D surface states in TI/Ni SLs.

4:42PM Q7.00012 Surface state of Bi$_{1.5}$Sb$_{0.5}$Te$_{1.7}$Se$_{1.3}$ investigated by terahertz emission and visible second-harmonic generation techniques, SOON-HEE PARK, S.Y. HAMH, J.S. LEE, Gwangju Inst of Sci & Tech, JOONBUM PARK, JUN SUNG KIM, Pohang Univ. of Sci & Tech — One of the key issues in three-dimensional topological insulators is to separate a response of the surface from the bulk to exploit novel spin-momentum-locked Dirac fermionic surface state, and Bi$_{1.5}$Sb$_{0.5}$Te$_{1.7}$Se$_{1.3}$ is one of such materials having a negligible contribution of the bulk conduction. We investigate the surface state of Bi$_{1.5}$Sb$_{0.5}$Te$_{1.7}$Se$_{1.3}$ single crystals by using terahertz emission spectroscopy and second harmonic generation techniques. We observed a clear distinction in the phases of emitted terahertz electric field and azimuth-dependent second harmonic intensity in different pieces of the sample, and found their clear correlation with carrier types which can be attributed to upward or downward band bending. We examined variations of such optical responses after the cleavage of the samples under different atmospheric environments, and discussed the time-evolution of the surface state particularly in comparison with previous results on n-type Bi$_2$Se$_3$.

4:54PM Q7.00013 Parity blocking in quenching dynamics of Majorana wires, SUraj HEGDE, Univ of Illinois, Urbana-Champaign, VASUDHA SHIVAMOGGI, Northrop Grumman Electronic Systems, SMITHA VISHVESHWARA, Univ of Illinois, Urbana-Champaign, DEPTMANN GE, ICQM, Peking University for High Energy Physics, Indian Institute of Science, Bangalore, India. — We study the point where the ground state changes parity. We develop a real-space formalism for calculating the dynamics of excited state, even when the quenching is very slow. Termed as “parity-blocking,” this happens when the fermion parity of the ground state is changing with time. This change in parity is related to the oscillation of near zero energy mid-gap states of the end Majorana modes. Using exact Majorana wave functions and transfer matrix techniques, we track the points where the ground state changes parity. We develop a real-space formalism for calculating the dynamics of quantities such as the many-body wavefunction overlap and residual energy. Using these techniques for numerical calculations, we demonstrate parity blocking and other scaling effects with the quench rate and length of the chain.

5:06PM Q7.00014 Chiral electromagnetic waves in Weyl semimetals, ALEXANDER ZYUZIN, University of Basel, VLADIMIR ZYUZIN, University of Florida — We show that Weyl semimetals with broken time-reversal symmetry is an optically gyrotropic medium and can host chiral electromagnetic waves. The magnetization in the system that results in a momentum space separation of a pair of opposite chirality Weyl nodes is also responsible for the non-zero gyration vector in the system. We show that in the region where the magnetization flips its directions (magnetic domain wall) there exist a chiral electromagnetic field localized at the domain wall and propagating along it. The direction of propagation is determined by the sign of the gyrotyro factor. Such magnetic domain walls might appear naturally in the Weyl semimetal materials, or, for example, they can be created with a help of a ferromagnetic material placed in proximity. The chiral electromagnetic wave propagating at the domain walls is an analog of quantum Hall state for photons.
**Effects of indistinguishability and interaction**, JOSEF MICHL, MARKUS BIBERGER, Institute of Theoretical Physics - University of Regensburg

**Wave Scattering through Mesoscopic Chaotic Cavities: Universal Effects of Indistinguishability and Interaction**, JOSEF MICHL, MARKUS BIBERGER, Institute of Theoretical Physics - University of Regensburg

**Many-Body Scattering through Mesoscopic Chaotic Cavities: Universal Effects of Indistinguishability and Interaction**, JOSEF MICHL, MARKUS BIBERGER, Institute of Theoretical Physics - University of Regensburg

**Wave Scattering through Mesoscopic Chaotic Cavities: Universal Effects of Indistinguishability and Interaction**, JOSEF MICHL, MARKUS BIBERGER, Institute of Theoretical Physics - University of Regensburg

**Luukko Scars - a New Mechanism for Wavefunction Scar Formation**, ERIC HELLER, Harvard University

**Focusing Waves at Arbitrary Locations in a Ray-Chaotic Enclosure Using Time-Reversed Synthetic Sonas**, STEVEN ANLAGE, BO XIAO, THOMAS ANTONSEN, EDWARD OTT, Physics and ECE Departments, University of Maryland

**Eigenfunction Scarring in Distorted Quantum Wells**, ESA RASANEN, Tampere University of Technology, PERTTU LUUKKO, University of Jyvaskyla, ANNA KLAES, Harvard University, BYRON DRURY, Massachusetts Institute of Technology, LEV KAPLAN, Tulane University, ERIC HELLER, Harvard University - Conventional scarring refers to pronounced localization of eigenfunctions along unstable classical periodic orbits [1]. Here we apply a highly efficient eigenvalue solver of arbitrary two-dimensional (2D) systems [2] to study scarring phenomena in generic situations. In particular, we report unexpectedly strong scarring in 2D quantum wells perturbed by random potential bumps of variable characteristics [3]. The scars resemble classical periodic orbits of the unperturbed system (no bumps), but there appears to be no clear connection to the periodic orbits of the perturbed system, as would be the case for conventional scarring. The scars are also robust to increasing distortion amplitude, and show a tendency to pin to the potential bumps. We have used a variety of tools to analyze the origin of the scarring, in particular its relation with Anderson localization. [1] E. J. Heller, Phys. Rev. Lett. 53, 1515 (1984); [2] P. J. J. Luukko and E. Rasanen, Comp. Phys. Comm. 184, 769 (2013); [3] P. J. J. Luukko, A. Klaes, B. Drury, L. Kaplan, E. J. Heller, and E. Rasanen (2015).
4:06PM Q8.00007 Semiclassical propagation of correlation functions in closed electromagnetic environments\textsuperscript{1}, GABRIELE GRADONI, STEPHEN CREAGH, GREGOR TANNER, University of Nottingham, United Kingdom — Field-field correlation functions can be propagated efficiently within confined systems through the Wigner-Weyl formalism. A semiclassical Frobenius-Perron operator is derived for the propagation of Wigner functions as a solution of the associated boundary integral equation. This idea is used to study the effect of non-integrable (chaotic) dynamics on the propagation of classical noisy fields. Model systems for quantum mechanics are used to mimic the radiation into closed spaces. A realistic model of statistical sources into a semi-open polygonal billiard is also presented. We find that the simplest description in terms of the classical Frobenius-Perron operator provides a description of the frequency-averaged correlation function but that wave-resonant and interference effects can also be accounted for. Application of the theory focus on the prediction of energy distribution through electromagnetic environments in electromagnetic compatibility, wireless communication systems, and imaging optics.

\textsuperscript{1}Work supported by the UK Engineering and Physical Sciences Research Council

4:18PM Q8.00008 ABSTRACT WITHDRAWN

4:30PM Q8.00009 Massive simulation of complex electromagnetic cavities\textsuperscript{1}, FRANCO MOGLIE, LUCA BASTIANELLI, VALTER MARIANI PRIMIANI, Universita Politecnica delle Marche - DII, Ancona — The analysis of the chaotic behavior of complex electromagnetic cavities benefits from the availability of a large amount of data on field samples. The application of a code running on a supercomputer is able to reproduce accurately electromagnetic simulations of electrically large structures. The simulations of mode-stirred reverberation chamber (RC) were performed using an in-house parallel finite-difference time-domain (FDTD) code. The code is divided into three modules that are managed by a unique, single-step job: the electromagnetic solver based on the FDTD method; a fast Fourier transform (FFT) to obtain the frequency domain behavior; a statistical tool to obtain the RC properties. A tool allows for the saving of intermediate data. The code implements a hybrid parallelization as function of the number of processors and the cavity volume. Specifically, such a computation is known to be “embarrassingly parallel” with respect to the cavity angle. The excitation is a Gaussian pulse modulated sinusoid at 1.1 GHz: the 95% bandwidth is 0.2 and 2 GHz. After the FDTD simulation is completed, the FFT module gives the frequency behavior of the fields in each point with a resolution of about 50 kHz.

\textsuperscript{1}We acknowledge PRACE for awarding us access to resource FERMI based in Italy at CINECA

4:42PM Q8.00010 Nonlinear elastic waves in solids: Deriving simplicity from complexity, MAHMOUD I. HUSSEIN, ROMIK KHAJEHTOURIAN, University of Colorado Boulder — The introduction of nonlinearities to the dynamics of a homogeneous elastic medium alters the underlying wave dispersion characteristics. In this work, we present an exact formulation for the treatment of geometric nonlinearity in one-dimensional elastic wave propagation in a rod, considering both a thin rod where the thickness is small compared to the wavelength and a thick rod where lateral inertia is accounted for. Our derivation starts with the implementation of Hamilton’s principle and terminates with an expression for the finite-strain dispersion relation in closed form. We explore the effect of wave amplitude on the derived dispersion relation and compare with results obtained by direct time-domain simulations followed by Fourier transformations. While often dispersion is attributed to only linear mechanisms, here we show that an otherwise linearly non-dispersive elastic solid may exhibit dispersion solely due to the presence of a nonlinearity. This work provides insights into the fundamentals of nonlinear wave propagation in solids, which represents one of the agents of wave chaos in complex systems.

5:06PM Q8.00012 Non-Harmonic Pressure Fluctuations by the Self-Excited Oscillations in a Reactor-Column, HASSON M. TAVOSSI, Valdosta State University, Department of Physics, Astronomy, and Geosciences — Self-excited non-harmonic pressure oscillations that result from non-linearity in the system are generated in an air-flow in a reactor column. The uniform steady flow is converted spontaneously into an oscillatory flow, under the especial experimental conditions in a reactor column that includes a thin layer of dissipative porous medium. The uniform steady flow is converted spontaneously into an oscillatory flow, under the especial experimental conditions in a reactor column that includes a thin layer of dissipative porous medium. The resulting large-amplitude non-harmonic pressure fluctuations in the air-flow are similar to the bifurcation in chaotic systems; where two or more energy states can occur simultaneously, with the system oscillating between them. Experimental results will be presented to demonstrate this abrupt change in flow-regime, from steady-flow to chaotic turbulent vibrations. Our results show that a low-pressure shock-wave-front is established in the column and precedes the self-excitation oscillations in the system. Results show that there exists a threshold for flow-rate, beyond which the transition from steady-flow to pulsating-flow occurs. A numerical model is developed to express this behavior terms of system variables, such as; dominant frequencies, obtained from fast-Fourier-transforms of time-domain pressure signals, flow-rate, dimensionless aerodynamic characteristic numbers, relaxation-time, and energy dissipation in the system.

5:18PM Q8.00013 A spectral force based version of the Wigner-Liouville equation, MAARTEN VAN DE PUT, WIM MAGNUS, BART SOREE, Univ of Antwerp, imec — Traditionally, a direct numerical solution of the Wigner-Liouville (WL) equation has been plagued with high computational burden and instability inherent to the integration of the highly oscillatory Wigner potential kernel. We have developed a method based on the spectral decomposition of the force which recasts the WL equation into a manageable form. By removing one integral, this new form is computationally less demanding. Furthermore a damping term naturally appears which reduces the instability caused by the oscillatory terms. Finally, the new form is local in position as opposed to the original WL equation which is non-local in both position and momentum. The spectral force WL equation is interpreted as a representation of a classical evolution with a constant force, and a local quantum generation term with positive and negative contributions mediated by the spectral components of the force. This interpretation allows for a straightforward implementation using a finite difference scheme for the classical evolution coupled with direct evaluation of the discretized generation terms. We observe a good match between results obtained using our method and theoretical results.

Wednesday, March 4, 2015 2:30PM - 5:30PM – Session Q9 DCMP: Semiconductor Thermodynamic & Transport Properties 006D - Selman Hershfield, University of Florida - Gainesville
2:30PM Q9.00001 Anomalous pressure dependence of thermal conductivities of large mass ratio compounds

L. LINDSAY, Oak Ridge National Laboratory, D.A. BROIDO, Boston College, J. CARRETE, N. MINGO, CEA-Grenoble, T.L. REINECKE, U.S. Naval Research Laboratory — The lattice thermal conductivities \( k \) of binary compound materials are examined as a function of hydrostatic pressure, \( P \), using a first-principles approach. Compound materials with relatively small mass ratios, such as MgO, show an increase in \( k \) with \( P \), consistent with measurements. Conversely, compounds with large mass ratios (e.g., BiSb, BAs, BeTe, BeSe) exhibit decreasing \( k \) with increasing \( P \), a behavior that cannot be understood using simple theories of \( k \). This anomalous \( P \) dependence of \( k \) arises from the fundamentally different nature of the intrinsic scattering processes for heat-carrying acoustic phonons in large mass ratio compounds compared to those with small mass ratios. This work demonstrates the power of first principles methods for thermal properties and advances the understanding of thermal transport in non-metals. * * *J. L. acknowledges support from the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division for work done at ORNL. D.A.B acknowledges support from the National Science Foundation under Grant No. 1402949. NM and JC acknowledge support from Institut Carnot through project SIEVE. T.L.L. acknowledges support from ONR and DARPA.

2:42PM Q9.00002 Numerical solution of the drift-diffusion equation for a p-i-p diode

ANGEL MANCEBO, SELMAN HERSHFIELD, Univ of Florida — In low carrier density semiconductors such as organic semiconductors the leads supply carriers to the sample. The extra charge flowing into the sample causes the phenomena of space charge build up. In its simplest form this is characterized by the Mott-Gurney law, where the current is proportional to the voltage squared. The Mott-Gurney law as usually derived includes the drift term for the current but omits the diffusion term. The diffusion term cannot be neglected as the diffusion coefficient is proportional to the mobility by the Einstein relationship. We numerically solve the drift-diffusion equation and Poisson’s equation for a p-i-p diode, where \( p \) refers to a p-type semiconductor and \( i \) to an intrinsic semiconductor with very few charge carriers. The model includes no charge traps. By including both the drift and the diffusion terms we find that the current is no longer proportional to the voltage squared but primarily linear with a slight upturn at higher voltages. Furthermore, by examining the carrier density vs. electric field in the sample, we are able to show that for fixed length, there is a maximum current for which there is a physical steady state solution. We will discuss the implications of our results for using the Mott-Gurney law to fit for carrier mobility.

1Supported by the UF Physics REU program NSF grant DMR-1156737

2:54PM Q9.00003 Theory of multiphonon inelastic scattering and carrier capture by defects in semiconductors - Application to capture cross sections

GEORGIOS D. BARMPARIS, YEVGENY S. PUZYREV, Vanderbilt University, X.-G. ZHANG, University of Florida, SOKRATES T. PANTELIDES, Vanderbilt University — Inelastic scattering and carrier capture by defects in semiconductors are the primary causes of hot-electron-mediated degradation of power devices. At the same time, carrier capture is a major issue in the performance of solar cells and light-emitting diodes. First-principles, parameter-free calculations of inelastic-scattering and capture cross sections as functions of carrier energy can provide guidance for modeling device degradation based on atomic-scale physical mechanisms. Here we report the construction of a comprehensive theory of multiphonon inelastic scattering by defects, with carrier capture being a special case. We resolve the old debate about what constitutes a correct theory of capture cross sections and report first-principles density-functional-theory calculations of capture cross section for three prototype defects. A Monte Carlo algorithm has been developed to obtain converged sum over all possible phonon configurations. The results reveal that the capture cross section depends strongly on the energy of the incoming electron.

2:54PM Q9.00003 Theory of multiphonon inelastic scattering and carrier capture by defects in semiconductors - Application to capture cross sections

1Supported by the Samsung Advanced Institute of Technology (SAIT)’s Global Research Outreach (GRO) Program and by the LDRD program at ORNL

3:06PM Q9.00004 Giant thermal resistivity of interlaced nanoparticles

YEVGENY S. PUZYREV, XIAO SHEN, SOKRATES PANTELIDES, Vanderbilt University — We present a theoretical study of thermal resistivity of “interlaced crystals,” recently discovered in hexagonal-CuInS\(_2\) nanoparticles [1]. Interlaced crystals exhibit a perfect global Bravais lattice with two cations and multiple ordering patterns within the cation sublattice. The interlaced crystal consists of interlaced domains and phases where the corresponding phase/domain boundaries are not uniquely defined. Since there are no structural defects or strain, the interlacing has a minimal effect on electronic properties, but causes a large increase in phonon scattering at the boundaries. The size of domains reaches down to one nanometer, resulting in a high density of the boundaries, making interlaced crystals an attractive candidate for thermoelectric applications. Large-scale molecular dynamics calculations show orders of magnitude increase in the thermal resistivity caused by a high density of boundaries. This is a general effect, arising due to a mass disparity of the cations present in interlaced crystals.

[1]“Interlaced crystals having a perfect Bravais lattices and complex chemical order revealed by real-space crystallography.” X. Shen, et. al, Nature Comm. 10.1038/ncomms6431.

3:18PM Q9.00005 First-principles calculation of phonon-limited mobility in silicon

YUNING WU, XIAOQIANG ZHANG, Department of Physics and Quantum Theory Project, University of Florida, SOKRATES PANTELIDES, Department of Physics and Astronomy, Vanderbilt University — We introduce a new first-principles method to calculate phonon-scattering-limited electron mobilities. The lifetime of a Bloch state due to scattering is represented by an imaginary electron self-energy which is extracted from the complex band structure of a supercell that contains the phonon vibrations within the frozen-phonon approximation. The phonon vibrations are modeled by a set of configurations generated from a Monte Carlo simulation. Mobility contributions are dominated by electrons on the transverse ellipsoids with low effective mass and long lifetime. The results indicate that high-mobility channels form a conduction network above the percolation threshold. As a result the Matthiessen’s rule does not hold for phonon scattering. The overall mobility is evaluated through the configurational average of the percolation-dominant resistor network. The calculated electron mobility agrees with available experimental data.

1This work is supported by the LDRD program at ORNL. Portion of this research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.
3:30PM Q9.00006 Three-dimensional Fully-coupled Electrical and Thermal Transport Model of Oxide Memristors 1

These results show the utility of such measurements in better understanding the material properties of QW’s. Accompanying the spectatorial progress in experimental demonstration of oxide-based memristors, there has been significant modeling effort to aid in understanding of switching physics in memristive devices. However, existing models often simplify the treatment of electronic transport and the interplay of electrically and thermally driven processes. In this work, we present a fully-coupled electrical and thermal numerical model that treats the transport of electrons, holes, and vacancies, together with the Joule heating on an equal footing. Namely, we solve simultaneously the five coupled partial differential equations: the time-dependent drift-diffusion equations for electrons and holes, the time-dependent lattice heat equation, and the Poisson equation for all the charged species in three spatial dimensions. This fully coupled model allows us to investigate the microscopic interplay of field drift, Fickian diffusion, Soret effect, and Joule heating, and to facilitate the understanding of physical mechanisms responsible for the SET and RESET switching processes in tantalum oxide memristors.

1This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy.

3:42PM Q9.00007 Fast response time of electron plasma in high electron mobility transistor channels

These results are important for developing a new generation of terahertz electronic devices and comparing different materials systems for their potential of reaching ultimate switching speed and/or the highest frequency of operation.

3:54PM Q9.00008 Phonon Anharmonicity in Silicon from 100 to 1500 K

Large phonon anharmonicities manifested by phonon energy shifts and broadenings at high temperatures were observed in measured phonon dispersions, and in the phonon density of states. At 1500 K the anharmonicity contributes approximately 80% of the deviation from the harmonic vibrational entropy. These large effects are beyond the predictions of the quasiharmonic model and demonstrate that phonon anharmonicity is a major contributor to both vibrational entropy and phonon lifetimes.

4:00PM Q9.00009 Measurement of the hot electron mean free path in GaN

We present a method for measuring the mean free path (MFP) and relaxation time of hot electrons in GaN using the hot electron transistor (HET). In this device electrons are injected over a high energy emitter barrier into the base, where the carrier density produces a quasiballistic transport well above the conduction band edge. After traversing the base, high energy electrons either surmount the base-collector barrier and become collector current or reflect off the barrier and become base current. We fabricate HETs with various base thicknesses and measure the common emitter transfer ratio (α) for each device. The MFP is extracted by fitting a decaying exponential to a function of base width and the relaxation time is computed using a suitable injection velocity. For current devices with an injection energy of ~1eV, we measure a hot electron MFP of 14nm and calculate a relaxation time of 16fs. These values are in agreement with theoretical calculations where longitudinal optical (LO) phonon scattering is the dominant relaxation mechanism.

4:18PM Q9.00010 Anisotropic lattice thermal conductivity for chain tellurium

Using the ab initio calculations combined with the phonon Boltzmann transport equation we calculate the temperature and pressure dependent lattice thermal conductivity of chain tellurium. The heat transport along and perpendicular to the chain has large anisotropic character, and also for the gruneisen parameter and phonon velocity. The three-phonon scattering rate of the acoustic branches and the phonon mean free path of tellurium are also investigated, which are important for the nanostructure thermoelectric material developing.

4:30PM Q9.00011 Transport Properties of InAs/GaSb Bilayers with a Tunneling Barrier

We have investigated the transport properties of InAs/GaSb bilayers in similarly inverted bands, but with an AlGaSb tunneling barrier placed between InAs and GaSb quantum wells. While the interlayer tunneling are essentially suppressed by increasing the barrier width, we found that the 2D bulk can still be turned into an insulating state that is characterized by a temperature-dependent resistance peak as a function of gate biases. On the other hand, we found no such peak for the 2D bulk in the InAs/GaSb system proposed in Naveh and Lahkim, Phys Rev. Lett. 77, 900 (1996). Work in Rice was supported by DOE DE-FG02-06ER46274.

3:42PM Q9.00012 Estimation of in-plane g-factor and disorder of InSb quantum wells via magnetococonductance mapping

We show the magnetococonductance mapping of an InSb quantum well (QW) and use the mapping to estimate material properties. Measurement and fitting of the suppression of weak antilocalization by an in-plane field oriented along in-plane crystal axes provides estimates of the QW’s g-factor and disorder. By comparing the measurements along different crystal axes, a variation in the estimated parameters is observed. The observed variation is consistent across different hall bars and is dependent on the direction of the applied field with respect to the crystal axes. These results show the utility of such measurements in better understanding the material properties of QW’s.
5:06PM Q9.00014 Ab initio study of complex defects and optical transitions in MgAl₂O₄¹. J.C. GARCIA, P.D. BORGES, Texas State University, USA, F.G. PINTO, J. TRONTO, Universidade Federal de Víncios, Brazil, L. SCOLFRARO, Texas State University, USA — The excellent optical properties of the Magnesium aluminate (MAO) spinel makes it an important material for novel technological applications. Considering that a presence of native defects can promote important changes in these properties, we present in this work a study of the structural, electronic and thermodynamic properties of the MAO. The calculated formation energy for isolated defects, such as the vacancies of manganese, aluminum and oxygen, oxygen interstitial, manganese and aluminum antisites, as well as the complexes in the most stable charge states are shown. In good agreement with experimental data, we obtained that complex centers, such as oxygen vacancies in conjunction with oxygen interstitialal, manganese or aluminum antisites at different charge states are good candidates for the observed optical transitions at 4.75, 5.3, and 6.4 eV. Our findings were obtained from ab initio electronic structure calculations performed within the Density Functional Theory. For the exchange-correlation potential, the generalized gradient approximation was used. Furthermore, a modified Becke-Johnson correction to the exchange potential was applied to obtain a suitable value for the band gap energy, 7.40 eV, in good agreement with the experimental one of 7.8 eV.

¹Support from CNPq and Texas State University

5:18PM Q9.00015 Native point defects and conductivity of ZnRh₂O₄: a GGA + U study¹. PIOTR BOGUSLAWSKI, OKSANA VOLNIAŃSKA, Institute of Physics PAS, Warsaw — ZnRh₂O₄ spinel belongs to the family of transparent conducting oxides, which are promising for applications in optoelectronic technology. To assess essential material properties, we analysed energy levels and formation energies of native point defects, i.e., vacancies (V), interstitials, and cation antisites in ZnRh₂O₄. Calculations were based on generalized gradient approximation (GGA) to the Density Functional Theory supplemented by the +U corrections. The value of U was treated as a free parameter, which allowed for the systematic study of the U-induced changes of the electronic structure. The experimental band gap of ZnRh₂O₄ is reproduced only when the +U term is imposed on both d(Rh) and p(O) orbitals, and the pronounced distortions of the oxygen sublattice are included. Zn:Rh is the dominant acceptor that can be responsible for the observed p-type conductivity in ZnRh₂O₄. The low formation energy of Zn:Rh can make the intentional n-doping difficult. In the O-rich conditions, the second important acceptor is V:Zn. The two dominant donors in Zn-rich and O-rich conditions are V:O and Rh:Zn, respectively. Growth conditions leading to the lowest concentrations of native defects were identified.

¹The work is supported by FNP grant POMOST/2012-5/10 and NCN grant nr 2012/05/B/ST3/03095. Calculations were done at ICM, University of Warsaw.

Wednesday, March 4, 2015 2:30PM - 5:30PM –
Session Q10 DCMP: Emergent Dirac and Weyl Semimetals in Three Dimensions

2:30PM Q10.00001 Building topologic device through emerging robust helical surface states, ZIBO WANG, International Center for Quantum Materials, Peking University, Beijing, China, HUA JIANG, College of Physics, Optoelectronics and Energy, Soochow University, Suzhou, China, XINCHENG XIE, International Center for Quantum Materials, Peking University, Beijing, China — In a 3D Cd₃As₂ ribbon with proper sizes, the system can exhibit a unique finite-size effect. Namely, if magnetic impurities are doped on one side, the surface states on the other side can be altered according to the strengths of these magnetic impurities. As a result, the conductance of the system will also be changed. This finding can be explained by the backscattering between the hybridized surface states due to finite size confinement and the normal surface states. Moreover, this phenomenon can be used to build new topologic devices.

2:42PM Q10.00002 Photoemission studies on the 3D Dirac semiential state in Na₃Bi¹. SUYANG XU, LIU CHANG, SATYA K. KUSHWAHA, Princeton University, RAMAN SANKAR, National Taiwan University, JASON W. KRIZAN², ILYA BELOPOLSKI, MADHAB NEUPANE, GUANG BIAN, NASSER ALIDOUST, Princeton University, TAY-RONG CHANG, HORNG-TAY JENG, National Tsing Hua University, CHENG-YI HUANG, WEI-FENG TSAI, National Sun Yat-Sen University, HSIN LIN, National University of Singapore, PAVEL P. SHIBAYEV, Princeton University, FANGCHENG CHOU, National Taiwan University, ROBERT J. CAVA, M. ZAHID HASAN, Princeton University — A three-dimensional Dirac semimetal is a novel state of matter that has recently attracted interest in condensed matter physics and materials science. We present electronic structure measurements on the (100) surface of a recently discovered Dirac semimetal material Na₃Bi. Our experimental data, for the first time, reveal a Lifshitz transition between the two bulk Dirac cones in the bulk band structure of Na₃Bi. These results identify the first example of a band structure singularity in 3D Dirac materials. This is in contrast to its 2D analogs such as in twisted bilayer graphene or the surface states of topological crystalline insulators, which have been studied extensively. The observation of multiple bulk Dirac nodes along the rotational crystal axis away from the Kramers point also serve as a signature for the symmetry-protected nature of the Dirac semimetal state in Na₃Bi as elaborated in recent theories.

¹The work at Princeton and Princeton-led synchrotron-based ARPES measurements is supported by U.S. DOE DE-FG-02-05ER46200. 
²jkranz@exchange.Princeton.EDU
2:54PM Q10.00003 Linear magnetoresistance caused by mobility fluctuations in a bulk three-dimensional Dirac semi-metal, Cd$_3$As$_2$\textsuperscript{1}, ARJUN NARAYANAN, MATTHEW WATSON, SAMUEL BLAKE, YULIN CHEN, DHARMALINGAM PRABHAKARAN, Oxford University, BINGHAI YAN, Max-Planck-Institut fur Chemische Physik, NICOLAS BRUYANT, Laboratoire National des Champs Magnétiques Intenses, LOIS DRIGO, Laboratoire National des Champs Magn “A”etiques Intenses, IGOR MAZIN, Naval Research Laboratory, CLAUDIA FELSER, Max-Planck-Institut fur Chemische Physik, TAI KONG, PAUL CANFIELD, Ames Laboratory, Iowa State University, AMALIA COLDEÀ, Oxford University — Dirac semimetals and Weyl semimetals are 3D analogues of graphene in which crystalline symmetry protects the nodes against gap formation. Cd$_3$As$_2$ was predicted to be Dirac semimetal \cite{1}, and recently confirmed to be so by photoemission \cite{2,3}. Here we report an interesting property in Cd$_3$As$_2$ that was unpredicted, namely a remarkable protection mechanism that strongly suppresses backscattering in zero H. In single crystals, the protection results in ultrahigh mobility $\mu \sim 9 \times 10^{5} \text{cm}^2\text{V}^{-1}\text{s}^{-1}$ \cite{4} at 5 K. Suppression of backscattering results in a transport lifetime $\tau \sim 10^{9}$ times longer than the quantum lifetime. The lifting of this protection by H leads to a very large magnetoresistance. Quantum oscillations in resistivity, Seebeck and Nernst, show beating effect. We discuss how this may relate to changes to the Fermi surface induced by H. \cite{5} Wang, Z. J. et al., Phys. Rev. B 88, 125427 (2013); \cite{2} Sergey, B. et al., Phys. Rev. Lett. 113, 027603 (2014). \cite{3} Neupane, M. et al., Nature Commun. 5, 3786 (2014). \cite{4} Tian Liang et al., Nature Materials, in press.

\textsuperscript{1}Work supported by EPSRC, UK (EP/1004475/1, EP/I017836/1, EP/L001772/1) Work at Ames Laboratory supported by the U.S. DOE DMSE. Ames Laboratory is operated by the U.S. DOE and Iowa State University under Contract No. DE-AC02-07CH11358

3:06PM Q10.00004 Thermopower and Nernst effect in the Dirac semimetal Cd$_3$As$_2$\textsuperscript{1}, TIAN LIANG, Department of Physics, Princeton University, QUINN GIBSON, MAZHAR ALI, Department of Chemistry, Princeton University, MINHAO LIU, Department of Physics, Princeton University, ROBERT CAVA, Department of Chemistry, Princeton University, NAI PHUAN ONG, Department of Physics, Princeton University — Dirac semimetals and Weyl semimetals are 3D analogues of graphene in which crystalline symmetry protects the nodes against gap formation. Cd$_3$As$_2$ was predicted to be Dirac semimetal \cite{1}, and recently confirmed to be so by photoemission \cite{2,3}. Here we report an interesting property in Cd$_3$As$_2$ that was unpredicted, namely a remarkable protection mechanism that strongly suppresses backscattering in zero H. In single crystals, the protection results in ultrahigh mobility $\mu \sim 9 \times 10^{5} \text{cm}^2\text{V}^{-1}\text{s}^{-1}$ \cite{4} at 5 K. Suppression of backscattering results in a transport lifetime $\tau \sim 10^{9}$ times longer than the quantum lifetime. The lifting of this protection by H leads to a very large magnetoresistance. Quantum oscillations in resistivity, Seebeck and Nernst, show beating effect. We discuss how this may relate to changes to the Fermi surface induced by H. \cite{5} Wang, Z. J. et al., Phys. Rev. B 88, 125427 (2013); \cite{2} Sergey, B. et al., Phys. Rev. Lett. 113, 027603 (2014). \cite{3} Neupane, M. et al., Nature Commun. 5, 3786 (2014). \cite{4} Tian Liang et al., Nature Materials, in press.

\textsuperscript{1}Supported by MURI grant (ARO W911NF-12-1-0461), Army Research Office (ARO W911NF-11- 1-0379) and NSF-MRSEC Grant DMR 0819860.

3:18PM Q10.00005 Optical gyrotropy as a test for dynamic chiral magnetic effect of Weyl semi-metals\textsuperscript{1}, SUMANTA TEWARI, Clemson University, Clemson, SC, USA, PALLAB GOSWAMI, National High Magnetic Field Laboratory and Florida State University, Tallahassee, FL, USA, GIRISH SHARMA, National High Magnetic Field Laboratory and Florida State University, Tallahassee, FL, USA — Dirac semimetals and Weyl semimetals are 3D analogues of graphene in which crystalline symmetry protects the nodes against gap formation. Cd$_3$As$_2$ was predicted to be Dirac semimetal \cite{1}, and recently confirmed to be so by photoemission \cite{2,3}. Here we report an interesting property in Cd$_3$As$_2$ that was unpredicted, namely a remarkable protection mechanism that strongly suppresses backscattering in zero H. In single crystals, the protection results in ultrahigh mobility $\mu \sim 9 \times 10^{5} \text{cm}^2\text{V}^{-1}\text{s}^{-1}$ \cite{4} at 5 K. Suppression of backscattering results in a transport lifetime $\tau \sim 10^{9}$ times longer than the quantum lifetime. The lifting of this protection by H leads to a very large magnetoresistance. Quantum oscillations in resistivity, Seebeck and Nernst, show beating effect. We discuss how this may relate to changes to the Fermi surface induced by H. \cite{5} Wang, Z. J. et al., Phys. Rev. B 88, 125427 (2013); \cite{2} Sergey, B. et al., Phys. Rev. Lett. 113, 027603 (2014). \cite{3} Neupane, M. et al., Nature Commun. 5, 3786 (2014). \cite{4} Tian Liang et al., Nature Materials, in press.

\textsuperscript{1}Work supported by NSF DMR 0654118, AFOSR FA9550-13-1-0045, NSF PHY 1104527

3:30PM Q10.00006 Interacting Dirac liquid in three-dimensional semimetals\textsuperscript{1}, JOHANNES HOFMANN, EDWIN BARNES, Univ of Maryland-College Park, CONDENSED MATTER THEORY CENTER TEAM — We study theoretically the properties of the interacting Dirac liquid, a novel three-dimensional many-body system which was recently experimentally realized and in which the electrons have a chiral linear relativistic dispersion and an axial Coulomb interaction. We find that the “extrinsic” Dirac liquid, where the Fermi energy lies exactly at the nodes of the band dispersion, displays unusual Fermi liquid properties, whereas the “intrinsic” system with finite detuning or doping behaves as a standard Landau Fermi liquid. We present analytical and numerical results for the self-energy and spectral function based on both Hartree-Fock and the random phase approximation (RPA) theories and compute the quasiparticle lifetime, residue, and renormalized Fermi velocity of the extrinsic Dirac liquid. A full numerical calculation of the extrinsic RPA spectral function indicates that the Fermi liquid description breaks down for large-energy excitations. Furthermore, we find an additional plasmon quasiparticle sideband in the spectral function which is discontinuous around the Fermi energy. Our predictions should be observable in ARPES and STM measurements.

\textsuperscript{1}This work is supported by LPS-CMTC.

3:42PM Q10.00007 Axial anomaly and negative longitudinal magnetoresistance: theory vs. experiment, PALLAB GOSWAMI, PED PIXLEY, University of Maryland — Traditionally axial anomaly is associated with quantum mechanical violation of U(1) axial symmetry of relativistic Dirac/Weyl fermions in odd spatial dimensions, in the presence of electromagnetic gauge fields. Recently there has been considerable interest in both condensed matter and high energy physics communities in Nielsen and Ninomiya’s original proposal that the axial anomaly can lead to a negative longitudinal magnetoresistance for condensed matter realization of Weyl fermions. In this talk I will show that the axial anomaly can arise in any generic three dimensional material placed under parallel electric and quantizing magnetic fields. However, the emergence of negative magnetoresistance depends crucially on the forward scattering nature of the underlying relaxation mechanism. Therefore, sufficiently clean and dilute three dimensional materials without magnetism or magnetic impurities can be promising candidates for observing this phenomenon. I will briefly discuss concrete experimental evidence of this enigmatic effect in quasi-2D layered materials.

3:54PM Q10.00008 Molecular beam epitaxial growth of a three-dimensional topological Dirac semimetal Na$_3$Bi, SUNG-KWAN MO, YI ZHANG, YEONGKWAN KIM, ZAHIH HUSSAIN, Advanced Light Source, Lawrence Berkeley National Lab, ZHONGKAI LIU, ZHI-XUN SHEN, SIMES, Stanford University, BO ZHOU, YULIN CHEN, University of Oxford — Three-dimensional topological Dirac semimetals (3D TDS) represent an unusual state of quantum matter that can be viewed as a bulk analogue of graphene. The realization of 3D TDS is recently verified experimentally in Na$_3$Bi and Cd$_3$As$_2$. We report a molecular beam epitaxial growth of Na$_3$Bi on bilayer graphene and Si(111). Our in-situ angle-resolved photoemission data reveal the 3-dimensional Dirac-cone band structure in such thin films even down to 12 unit cell thickness. Our approach of growing Na$_3$Bi thin film provides a potential route for fabrication into practical devices while preserving unique properties of 3D TDS. *Yi Zhang et al. Appl. Phys. Lett. 105, 031901 (2014).
4:06PM Q10.00009 Magnetic Catalysis and Axionic Charge-Density-Wave order in Weyl semimetals, BITAN ROY, JAY DEEP SAU, Condensed Matter Theory Center, University of Maryland — Three-dimensional Weyl and Dirac semimetals are extremely robust against impurity and magnetic correlations. However, when placed in strong magnetic fields, they can support a chiral-symmetry-breaking charge-density-wave order even for sufficiently weak electron-electron repulsion. Such novel phenomena stems from the existence of one-dimensional chiral zero Landau levels which can hybridize for arbitrarily weak interactions. In the former systems, due to the momentum space separation of Weyl nodes the ordered phase lacks translational symmetry and represents a dynamic axionic phase of matter. I will demonstrate the scaling behavior of the spectral gap for a wide range of subcritical (weak) interactions as well as that of diamagnetic susceptibility with magnetic field. I will argue that similar mechanism for charge-density-wave ordering remains operative in double-Weyl semimetals, where dispersion is linear (quadratic) for the $z$ (planar) component(s) of momentum. Role of topological defects, e.g., axion strings, existence of 1-dimensional gapless dispersive modes along the core of such defects, anomaly cancellation through Callan-Hervey mechanism will also be discussed. Pertinence of our study in recently observed Dirac semimetals, such as $Cd_3As_2$, Na$_3$Bi, will be addressed.  


4:18PM Q10.00010 Dirac and Weyl Superconductors in Three Dimensions 1, SHENGYUAN YANG, Singapore, HUI PAN, Beihang University, FAN ZHANG, The University of Texas at Dallas — Inspired by the recent discovery of Dirac and Weyl semimetals, we introduce the concept of 3D Dirac (Weyl) superconductors (SC), which have protected bulk four(two)-fold nodal points and surface Andreev arcs at zero energy. We provide a sufficient criterion for realizing them in centrosymmetric SCs with odd-parity pairing and mirror symmetry. Pairs of Dirac nodes appear in a mirror-invariant plane when the mirror winding number is nontrivial. Breaking mirror symmetry may gap Dirac nodes producing a topological SC. Each Dirac node evolves to a nodal ring when inversion-gauge symmetry is broken, whereas it splits into a pair of Weyl nodes only when time-reversal symmetry is broken. Our physics might be realized in the nodal phase of Cu-doped Bi$_2$Se$_3$ or UPt3.

4:30PM Q10.00011 Magnetization-dynamics-induced current in Weyl semimetals, DAICHI KURE-BAYASHI, KENTARO NOMURA, Institute for Materials Research, Tohoku University — Weyl semimetals recently gather attention because of its novel transport properties, the anomalous Hall effect (AHE) and the chiral magnetic effect (CME), originated from the chiral anomaly. In contrast to the AHE which has been understood after intensive theoretical and experimental studies in condensed matters, the existence of the CME in static cases is still in debate. We propose a magnetically induced current with temporal varying chiral vector potential, which is a new transport phenomenon and essentially different from the CME. We consider the magnetically doped Weyl semimetals, and theoretically study the dynamical effect of the magnetization. As a model, we use the Dirac Hamiltonian coupled to the magnetizations with the exchange interaction. We apply field theoretical methods to derive the expression of the current, and find the magnet-field-driven current induced by the dynamics of magnetic collective excitations. Furthermore, we also conduct the numerical calculation for the lattice model, and obtain the results which agree with the analytical result. Our result, therefore, is not an artifact of taking continuous model, but experimentally observable in solids.

4:42PM Q10.00012 Quantum transport in three-dimensional Weyl electron system — in the presence of charged impurity scattering, YUYA OMINATO, MIKITO KOSHINO, Tohoku Univ — Quantum transport in 3D Weyl electron system with the charged impurity is studied theoretically using a self-consistent Born approximation (SCBA). The scattering strength is characterized by the effective fine structure constant which depends on the dielectric constant and the Fermi velocity of the linear band. The Boltzmann transport theory works well in a condition that the level broadening is much smaller that the Fermi energy, but it fails near the Weyl point. At the Weyl point, the conductivity takes a nearly constant value which is almost independent of the effective fine structure constant, even though the density of states linearly increases with the effective fine structure constant. The qualitative behavior is significantly different from the case of the Gaussian impurities, where the conductivity exhibits exponentially vanishing behavior and vanishes at the Weyl point below a certain critical disorder strength.

4:54PM Q10.00013 Anomalous Conductivity Tensor and Quantum Oscillations in the Dirac Semimetal Na$_3$Bi 1, JUN XIONG, SATYA KUSHWAHA, JASON KRIZAN, TIAN LIANG, ROBERT J. CAVA, NAI PHUAN ONG, Princeton University — Na$_3$Bi is a 3D Dirac semimetal with protected nodes. Angle-resolved photoemission experiments have observed these massless Dirac fermions in the bulk band, but transport experiments have been hampered by the extreme air sensitivity of Na$_3$Bi crystals. Transport experiments can potentially address interesting issues such as charge pumping between the separated Weyl nodes when the time-reversal symmetry is broken by a strong magnetic field. Here we report a transport measurement that reveals robust anomalies in both the conductivity and resistivity tensor. The resistivity $\rho_{xx}$ exhibits a B-lineup up to 317, while the Hall exhibit an unusual profile approaching a step-function. In addition, we have also observed a prominent beating pattern in the Shubnikov de Haas (SdH) oscillations indicating the existence of two nearly equal SdH frequencies when the Fermi energy falls inside the non-trivial gap-inverted regime.

5:06PM Q10.00014 Unconventional localisation transition in high-dimensional semiconductors and Weyl semimetals, SERGEY SYZRANOV, VICTOR GURARIE, LEO RADZIHOVSKY, Univ of Colorado - Boulder — We study a class of non-interacting electron systems with a power-law quasiparticle dispersion $\varepsilon_k \propto k^{\alpha}$ and a random short-correlated potential. We show that, unlike the case of lower dimensions, for $d > 2\alpha$ there exists a critical disorder strength (set by the band width), at which the system exhibits a disorder-driven quantum phase transition at the bottom of the band, that lies in a universality class distinct from the Anderson transition. In contrast to the conventional wisdom, it manifests itself, in e.g., the disorder-averaged density of states. In systems for symmetry classes that permit localisation, the striking signature is a non-analytic behaviour of the mobility edge that is pinned to the bottom of the band for subcritical disorder and grows for disorder exceeding a critical strength. Focusing on the density of states, we calculate the critical behaviour (exponents and scaling functions) at this novel transition, using a renormalisation group, controlled by an $\varepsilon = d - 2\alpha$ expansion. We also apply our analysis to Dirac materials, e.g., Weyl semimetal, where this transition takes place in physically interesting three dimensions.

5:18PM Q10.00015 Density of states scaling at the semimetal to metal transition in three dimensional topological insulators, IGOR HERBUT, Simon Fraser University, KEN IMURA, Hiroshima University, TOMI OHTSU, KOJI KOBAYASHI, Sophia University — The quantum phase transition between the three dimensional Dirac semimetal and the diffusive metal can be induced by increasing disorder. Taking the system of disordered Z2 topological insulator as an important example, we compute the single particle density of states by the kernel polynomial method. We focus on three regions: the Dirac semimetal at the phase boundary between two topologically distinct phases, the tricritical point of the two topological insulator phases and the diffusive metal, and the diffusive metal lying at strong disorder. The density of states obeys a novel single parameter scaling, collapsing onto two branches of a universal scaling function, which correspond to the Dirac semimetal and the diffusive metal. The diverging length scale critical exponent and the dynamical critical exponent are estimated, and found to differ significantly from those for the conventional Anderson transition. Critical behavior of experimentally observable quantities near and at the tricritical point is also discussed. (K. Kobayashi et al, Phys. Rev. Lett. vol. 112, 016402 (2014))
3:20PM Q11.00001 Phonon-driven surface superconductivity in the vicinity of ferroelectric and charge density wave ordering in La(O,F)BiX2 (X=S, Se, O) — TANER YILDIRIM, National Institute of Standards and Technology — Examples of layered superconductors include cuprates, MgB2, CaC2, and recent iron-pnictides. Recently a new family of layered materials containing BiS2 planes was discovered to be superconducting at temperatures up to 10 K. In order to reveal the mechanism of superconductivity, here we present results from first-principles calculations with many surprising findings for La(O,F)BiX2 for X=S, Se, and O. The parent compound LaOBiS2 possesses anharmonic ferroelectric soft phonons at the zone center with a rather large polarization of P ≈ 10 μC/cm². Upon electron doping, new unstable phonon branches appear along the entire line Q=(q,q,0), causing Bi/S atoms to order in a one-dimensional charge density wave (CDW). We find that BiS2 is a strong electron-phonon coupled superconductor in the vicinity of competing ferroelectric and CDW phases. We discuss similar results for X=Se and hypothetical compound X=O. These results will be compared with another interesting system, namely Ba1−xF3BiO3, which exhibits several phases, including CDW, an incommensurate pseudo ferroelectric, and superconductivity at 31 K. Our results suggest new directions to tune the balance between these phases and increase Tc in this new class of materials.

2:42PM Q11.00002 Coexistence of ferromagnetism and superconductivity in CeO3.3F0.7BiS2 — JOOSEP LEE, Oak Ridge National Laboratory, SATOSHI DEMURA, National Institute for Material Science, MATTHEW STONE, Oak Ridge National Laboratory, KAZUKI IIDA, University of Virginia, GEORCH EHLERS, CLARINA DELA CRUZ, MASAAMI MATSUEDA, Oak Ridge National Laboratory, KEITA DEGUCHI, YOSHIHIKO TAKANO, YOSHIKAZU Mizuguchi, National Institute for Material Science, O SUKE MIURA, Tokyo Metropolitan University, DESPINA LOUCA, SEUNG HUN LEE, University of Virginia — Bulk magnetic transport and neutron scattering measurements were performed to investigate the electronic and magnetic properties of a polycrystalline sample of the newly discovered ferromagnetic superconductor, CeO3.3F0.7BiS2. Ferromagnetism develops below Tc( FM ) = 6.54(8) K and superconductivity coexists with the ferromagnetic state below Tc(SC) = 4.5 K. Inelastic neutron scattering measurements reveal a very weakly dispersive magnetic excitation at 1.8 meV that can be explained by an Ising-like spin Hamiltonian. Under application of an external magnetic field, the direction of the magnetic moment changes from the c-axis to the ab-plane and the 1.8 meV excitation splits into two modes. A possible mechanism for the unusual magnetism and its relation to superconductivity is discussed.

2:54PM Q11.00003 Observation of anomalous temperature dependence of spectrum on small Fermi surfaces in a BiS2-based superconductor — L.K. ZENG, X.B. WANG, J. MA, P. RICHARD, S.M. NIE, H.M. WENG, N.L. WANG, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, Z. WANG, Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467, USA, T. QIAN, H. DING, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — We have performed an angle-resolved photoemission spectroscopy study of the BiS2-based superconductor Nd(O,F)BiS2. Two small electron-like Fermi surfaces around (π,π,0) are observed, which enclose 2.4% and 1.1% of the Brillouin zone area, respectively, corresponding to an electron doping of 7% per Bi site. The low-energy spectrum consists of a weakly-dispersing broad hump and a dispersive branch, which follows well the calculated band dispersion. This hump is drastically suppressed with increasing temperature, while the dispersive branch is essentially unaffected. The anomalous thermal effect indicates a highly interacting electronic state, in which the superconducting pairing develops along the entire line Q=(q,q,0), causing Bi/S atoms to order in a one-dimensional charge density wave (CDW). We find that BiS2 is a strong electron-phonon coupled superconductor in the vicinity of competing ferroelectric and CDW phases. We discuss similar results for X=Se and hypothetical compound X=O. These results will be compared with another interesting system, namely Ba1−xF3BiO3, which exhibits several phases, including CDW, an incommensurate pseudo ferroelectric, and superconductivity at 31 K. Our results suggest new directions to tune the balance between these phases and increase Tc in this new class of materials.

3:06PM Q11.00004 Single crystal growth and superconducting properties of the Bi(S,Se)2-based superconductor — TAKUMA YAMAKI, YOSHIHIKO TAKANO, National Institute for Materials Science (NIMS) — Introduction After the discovery of superconductivity in Bi4O4S3 [1], much attention has been paid to synthesizing new superconductors. The BiS2-based compounds have a layered structure similar to those of cuprates or Fe-based superconductors. In these compounds, superconducting layers and blocking layers are stacked alternatively. Many BiS2-based superconductors have been discovered by arranging the blocking layer so far. The modification in superconducting layer is important to clarify the superconducting mechanism of BiS2-based superconductor and the single crystal preparation is necessary to discuss such a intrinsic properties. In this study, we perform the single crystal growth of La(O,F)Bi(S,Se)2 and investigate the substitution effect for the superconducting properties by replacing Se with S. Results and discussion Single crystals of LaO1−xF3BiS2−ySey (0≤y≤2) were synthesized by CsCl flux method. The single crystals were plate-like shape with approximately 1 mm in size, which is sufficient to perform various characteristic measurements, such as single crystal X-ray analysis and electrical resistivity measurement, and so on. We will discuss the crystal structure, electrical resistivity and magnetic properties in detail. [1] Y. Mizuguchi et.al.,Phys. Rev. B 86,220510(2012)

3:18PM Q11.00005 Superconductivity in PdxBi2Se3 by anneal doping — GRACE MCCLINTOCK, J. T. MLACK, NINA MARKOVIC, Johns Hopkins University — We show that superconductivity can be induced in Bi2Se3 by palladium doping via annealing. Thin films of palladium are deposited on prefabricated Bi2Se3 nanodevices and annealed at temperatures in excess of 100 Celsius. We find that Bi2Se3 absorbs Pd under these conditions and that the absorption of Pd results in superconductivity, as evidenced by resistance and magnetoresistance measurements below 1K.

3:30PM Q11.00006 Charge fluctuations in a disordered superconductor, LaO1−xF3BiS2 — ANUSHKA ATHAUDA, SEUNG HUN LEE, DESPINA LOUCA, Univ of Virginia, YOSHIKAZU Mizuguchi, Tokyo Metropolitan University — LaO1−xF3BiS2 is a disordered, non-magnetic superconductor with a transition temperature of 10.8 K at x = 0.5. The parent compound, LaOBiS2, is a band insulator with a layered tetragonal structure. The evolution of the crystal structure and nano-scale atomic fluctuations are investigated as a function of temperature and composition using neutron scattering. Even though the symmetry remains unchanged with doping, lattice strain develops along the c-axis and buckling of the Bi2Se plane changes orientation. In addition, strong local distortions are observed around the Bi ion that are in response to charge fluctuations. Two distinct Bi-S plaquettes are present due to atomic displacement of in-plane sulfur because the Bi ion undergoes a charge disproportionation. The charge fluctuations along with spin-orbit coupling most likely play important roles in the mechanism of superconductivity in this system.

3:42PM Q11.00007 Anisotropic spin-singlet pairings in CuxBi2Se3 and Bi2Te3 — WEI-FENG TSAI, National Sun Yat-sen University, Kaohsiung, Taiwan, LEI HAO, GUI-LING WANG, Southeast University, Nanjing, China, TING-KUO LEE, Institute of Physics, Academia Sinica, Taipei, Taiwan, JUN WANG, YONG-HONG YANG, Southeast University, Nanjing, China — We report possible anisotropic spin-singlet pairings in Bi2X3 (X = Se or Te). Among six pairings compatible with the crystal symmetry, two novel pairings show nontrivial surface Andreev bound states, which form flat bands and could produce zero-bias conductance peak in measurements such as point-contact spectroscopy. By considering purely repulsive short-range Coulomb interaction as the pairing mechanism, the dominant super-exchange terms are all antiferromagnetic, which would usually favor spin-singlet pairing in Bi2X3. Mean-field analyses show that the inter-orbital pairing interaction favors a mixed spatial-parity anisotropic pairing state, and one pairing channel with zero-energy surface states has a sizable component. The results provide important information for future experiments.
3:54PM Q11.00008 Structural role of the pressure-dependent charge-density-wave to superconductor transition in ZrTe$_2$: an inelastic light scattering study$^1$. YEOWN GIM, SAM GLEASON, TAYLOR BYRUM, ASTHA SETHI, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois, Urbana, Illinois 61801, USA. C. PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA. S.L. COOPER, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois, Urbana, Illinois 61801, USA — One of the most exciting areas of condensed matter research involves the study of how superconductivity evolves from magnetic- or charge-ordered phases in strongly correlated systems. We present a Raman scattering study of the temperature- and pressure-induced structural changes leading to the transition between charge-density wave (CDW) and superconducting phase regimes in ZrTe$_2$. We show that the internal deformation modes associated with the Te-Te chains—which support the CDW in this material—exhibit anomalous linewidth changes as a function of temperature, indicating strong electron-phonon coupling associated with these modes. Additionally, the pressure-dependence of these modes suggests that dissociation of the Te-Te chain bonds may be responsible for the suppression of the CDW phase as a function of pressure. These studies provide insight into the structural changes responsible for CDW collapse in this material.

$^1$Work supported by the U. S. Department of Energy, Division of Materials Sciences, under Award No. DE-FG02-07ER46453, and by the National Science Foundation under Grant NSF DMR 08-56321.

4:06PM Q11.00009 A DFT study of electron-phonon coupling in proxy rocksalt CuX (X = S, Se, Te) structures and its relationship to possible manifestation of superconductivity. PAUL GRANT, W2AGZ Technologies, ROBERT HAMMOND, Stanford University — We have previously reported our computational studies on idealized copper monochalcogenide rocksalt structures, both cubic and tetragonal, focusing on their possible antiferromagnetic properties as determined within a Van Vleck-Mott-Anderson-Hubbard framework [1]. For all values of Hubbard U in the range 0-7 eV, only copper monoxide exhibits a Mott-Hubbard electronic structure [2-3], the remainder (S, Se, Te) yielding metallic states characterized by nesting Fermi surfaces arising from Jahn-Teller degenerate s-p overlap. These results suggest exploring possible manifestation of superconductivity via electron-phonon mediated Cooper pairing. We will disclose our results to date applying the Eliashberg-McMillan-Allen-Dynes strong coupling framework to the DFT–derived electronic and vibrational states of CuS, CuSe and CuTe.


4:18PM Q11.00010 Competition between Weak Localization and Superconductivity in Ta$_{1-x}$Pt$_x$Se$_2$ Single Crystal. JINYU LIU, Tulane University, ALI RADMANESH, University of New Orleans, JIN HU, Tulane University, LEONARD SPINU, University of New Orleans, ZHIQIANG MAO, Tulane University — Exotic properties such as superconductivity and charge density wave (CDW) in transition metal dichalcogenides (TMDCs) have attracted a great deal of interest in past decades. Research in this area is focused on understanding the interplay between CDW, structure instability and superconductivity in doped/intercalated TMDCs. We have recently studied the Pt doping effect on electronic properties of 2H – Ta$_2$Se$_2$. With only 2% Pt doping, we observed dramatic changes in its electronic properties. Firstly, Pt doping leads to an evolution from an anisotropic, three-dimensional (3D) metal to a quasi-2D metal. Secondly, while Pt doping suppresses the CDW of Ta$_2$Se$_2$ only to some extent, its superconducting transition temperature is remarkably increased, from 0.2K to 2.1 K. Moreover, Pt doping induces quantum transport behavior prior to the superconducting transition, i.e. weak localization (WL) and strong competition between WL and superconducting pairing was probed in angle-resolved magnetoresistance measurements. We will discuss the origin of the evolution of such exotic phenomena.

4:30PM Q11.00011 STM study on single crystal of noncentrosymmetric superconductor PbTaSe$_2$. RUI WU, ZHIYANG YE, Institute of Physics, Chinese Academy of Sci (CAS) & Department of Physics and Texas Center for Superconductivity, University of Houston., JIHLI WANG, Department of Physics and Texas Center for Superconductivity, University of Houston, XUEJIN LIANG, HANQING MAO, LINGXIAO ZHAO, GENFU CHEN, Institute of Physics, Chinese Academy of Sci (CAS). SHUHENG PAN, Institute of Physics, Chinese Academy of Sci (CAS) & Department of Physics and Texas Center for Superconductivity, University of Houston, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES TEAM, TEXAS CENTER FOR SUPERCONDUCTIVITY TEAM — We use low temperature scanning tunneling microscopy (STM) to study the single crystal of noncentrosymmetric superconductor PbTaSe$_2$. Two types of atomically resolved topographic image have been observed on the surfaces exposed by low temperature in situ cleaving. One of the topographic images clearly displays the noncentrosymmetric crystal structure, which we identify as the Se terminated surface. With the help of lattice symmetry and the step between two terraces, we also identify that the other topographic image belongs to the Pb terminated surface. With the help of lattice symmetry and the step between two terraces, we also identify that the other topographic image belongs to the Pb terminated surface, which is the complementary exposure of the Se terminated. In addition to the lattice symmetry and the surface reconstruction, there is a super modulation with a period of about 10.5 unit cells. This super modulation persists through the superconducting transition (Tc = 3.7K), but is energy dependent, indicating its electronic nature. We will show how this super modulation relates to the normal state tunneling spectrum.

4:42PM Q11.00012 STS study on single crystal of noncentrosymmetric superconductor Pb-TaSe2. ZHIYANG YE, RUI WU, Institute of Physics, Chinese Academy of Sciences, Beijing. Department of Physics and Texas Center for Superconductivity, University of Houston., JIHLI WANG, Department of Physics and Texas Center for Superconductivity, XUEJIN LIANG, HANQING MAO, LINGXIAO ZHAO, GENFU CHEN, Institute of Physics, Chinese Academy of Sciences, SHUHENG PAN, Department of Physics and Texas Center for Superconductivity, University of Houston. Institute of Physics, Chinese Academy of Sciences, Beijing — We report our low temperature scanning tunneling spectroscopic study on single crystals of noncentrosymmetric superconductor PbTaSe$_2$. On the background of the normal state tunneling spectrum, a superconducting energy gap opens at a temperature below the bulk Tc = 3.7K. At $t = 1.4K$, the gap magnitude is estimated to be about 1meV. This energy gap is particle-hole symmetry and is homogeneous in space. Extrapolating the low energy part of the spectrum, we find that the low energy part of the gap spectrum is linear like “V” shape. We will present the results of the numerical fit with various gap functions of proposed possible pairing symmetry. We will also present our preliminary results of the magnetic field dependence measurement and discuss the implications of these observations.

Wednesday, March 4, 2015 2:30PM - 5:30PM – Session Q12 DMP GERA FIAP DCOMP: Focus Session: Theory of Bulk Thermoelectric Materials 007C - David Singh, Oak Ridge National Laboratory
2:30PM Q12.00001 Thermal transport properties of complex oxides from first principles. AQYAN BHATTI, Univ of Texas, Austin, ANKIT JAIN, ALAN MCGAUGHLEY, Carnegie Mellon University, NICOLE BENEDEK, Univ of Texas, Austin — Thermal transport properties of materials are key parameters in the design of many engineering devices. For this reason, it is highly desirable to be able to control or tailor the thermal properties of materials for specific applications. Complex oxides are attractive in this regard, due to their low and potentially highly tunable thermal conductivity. However, the theoretical description of the thermal transport properties of oxides presents a number of challenges compared to conventional semiconductors. For example, oxides tend to have complex crystal structures and the atoms interact through long-range electrostatic forces. In this talk, we use the example of PbTiO$_3$ to discuss some of the challenges and opportunities associated with thermal transport predictions in complex oxides. For example, many oxides contain very low-lying optical branches, which may provide important acoustic-optical scattering channels. In addition, it is often possible to tune the frequencies of such optical modes with epitaxial strain. We also link the observed negative thermal expansion behavior of PbTiO$_3$ to two zone-boundary modes with large, negative Grüneisen parameters and comment on the consequences of this finding for the thermal transport properties of this material.

3:06PM Q12.00004 Part-crystalline part-liquid state and electrical/thermal transport in materials with chemical-bond hierarchy, WENQING ZHANG, Materials Genome Institute, Shanghai University, Shanghai, 200444, China — A concept of part-crystalline part-liquid state (or liquid-like), and even part-crystalline part-glass state (or glass-like), was demonstrated in some materials such as CuSb$_3$S$_3$ with chemical-bond-hierarchy, in which certain constituent species weakly bond to other part of the crystal. Such a material could intrinsically manifest the coexistence of rigid crystalline sublattices and other fluctuating noncrystalline sublattices with thermally induced large amplitude vibrations and even flow of the group of species atoms. The large-amplitude vibrations and movement of atoms can generate unusual severe phonon scattering and thermal damping due to the collective low-frequency vibrations similar to the Boson peak in amorphous or liquid materials. While different phase or state may have large energetic discrepancy, whether the thermally-induced part-crystalline state is undergoing phase transition becomes an interesting issue. In addition, our earlier work reported that second-order phase transition could induce extreme electron and phonon scattering in thermoelectrics. The above work clearly demonstrated that the unusual effect from structural fluctuations on thermal and electrical transport in thermoelectrics should be paid attention to. While materials with these structural changes can retain extremely low lattice thermal conductivity and unusual electron transport and become promising candidates for high-performance thermoelectrics, underlying mechanism is yet to be explored.

3:42PM Q12.00005 Compressed sensing approach for calculating lattice thermal conductivity of complex thermoelectric compounds, VIDVUDS OZOLINS, YI XIA, WESTON NIELSON, Dept of Materials Science and Engineering, University of California, Los Angeles, FEI ZHOU, Lawrence Livermore National Laboratory — Earth-abundant minerals such as tetrahedrite Cu$_{12}$Sb$_3$S$_{13}$ have recently received attention as promising thermoelectrics due to a combination of a relatively high figure of merit (ZT > 1 at T ≈ 700 K in tetrahedrite), good mechanical properties and inexpensive bulk processing methods. Like many large unit-cell thermoelectrics, these compounds often have complex chemical formulas with very large unit cells that pose challenges to our ability to study their lattice dynamical properties theoretically. Here we show that a recently introduced approach, compressive sensing lattice dynamics (CSDL) (F. Zhou et al., Phys. Rev. Lett. 113, 185501 (2014)) provides an accurate and computationally efficient platform for investigating anharmonic lattice dynamics in complex materials. We will discuss the basic ideas and illustrate the performance of CSDL for the lattice thermal conductivity κL of tetrahedrite, collusite, pyrite, and other earth-abundant mineral compounds.

3:54PM Q12.00006 A Robust Approach to Lattice Thermal Conductivity, WESTON NIELSON, Univ of California - Los Angeles, FEI ZHOU TEAM, YI XIA TEAM, VIDVUDS OZOLINS TEAM — Thermal conductivity is a key parameter in designing high performance thermoelectric materials. A multitude of computational methods have been developed to calculate lattice thermal conductivity. Molecular dynamics (MD) based techniques, including equilibrium and non-equilibrium methods, in addition to non MD-based solutions, such as the Boltzmann Transport Equation (BTE), are all capable of calculating thermal conductivity, but each comes with different sets of limitations and difficulties. After extensive use of these different methods, we have developed a robust set of tools for obtaining high-quality lattice thermal conductivity values of crystalline solids. The crux of our method involves a novel compressive sensing (CS) based approach for efficiently calculating high quality force constants for crystalline materials. The result is a technique for building lattice dynamical models that can treat compounds with large, complex unit cells and strong anharmonicity, including those with harmonically unstable phonon modes.

4:06PM Q12.00007 Temperature dependent phonon properties of thermoelectric materials1, OLLE HELLMAN, Department of Applied Physics and Materials Science, California Institute of Technology, Pasadena, California 91125, USA, DAVID BROIDO, Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467, USA, BREN'T FULTZ, Department of Applied Physics and Materials Science, California Institute of Technology, Pasadena, California 91125, USA — We present recent developments using the temperature dependent effective potential technique (TDNP) to model thermoelectric materials. We use an ab initio molecular dynamics method to generate an effective Hamiltonian that reproduce neutron scattering spectra and phonon self energies and heat capacities. Results are presented for (among others) SnSe, Bi$_2$Te$_3$, and Cu$_2$Se proving the necessity of careful modelling of finite temperature properties for strongly anharmonic materials.

1Supported by the Swedish Research Council (VR) project number 637-2013-7296.
4:18PM Q12.00008 Density functional study of silver defects in telluride thermoelectric materials1, BYUNGKI RYU, MIN-WOOK OH, SU-DONG PARK, Korea Electrotech Res Inst — Silver impurity in telluride thermoelectric materials forms various defect and impurity structures, such as AgSb rich nanoregion in Ag-Sb-Pb-Te, Ag2Te and metallic silver in PbTe. To understand the atomic, electronic, energetic, and diffusion properties of silver impurities in telluride systems, we have performed the density functional theory and density functional perturbation theory calculations of silver doped PbTe. Under Te and Ag rich condition, silver telluride impurity phase or Ag-dimer defects are expected to be easily formed. Under Te poor condition, silver point defects are calculated to be easily formed and they are more stable than native point defects of PbTe, implying that silver point defect might be the major dopant responsible for the carrier generation in PbTe. We also calculated the diffusion coefficient and diffusion length of silver point defect in PbTe. Based on the results, we discussed the electrical and thermoelectric properties of silver doped PbTe.

1This work was supported by the National Institute of Supercomputing and Network/Korea Institute of Science and Technology Information with supercomputing resources including technical support (KSC-2014-C1-022).

4:30PM Q12.00009 Quasiparticle structure and thermoelectric transport properties of p-type SnSe, GUANGSHA SHI, EMMANOUIL KIOUPAKIS, Materials Science and Engineering, University of Michigan — We used density functional and many-body perturbation theory to calculate the band structure and electronic transport parameters of p-type SnSe both for the low-temperature Phmnm and high-temperature Cmcm phases. The Phmnm phase has an indirect band gap of 0.829 eV while the Cmcm has a direct band gap of 0.464 eV. Both phases exhibit multiple local band extrema within an energy range comparable to the thermal energy of carriers from the global extrema. We calculated the electronic transport coefficients within the constant relaxation time approximation as a function of doping concentration and temperature for single-crystal and polycrystalline materials to understand experimental measurements. The electronic transport coefficients are highly anisotropic and are strongly affected by bipolar transport effects at low doping and high temperature. Our results indicate that SnSe exhibits optimal thermoelectric performance at high temperature when doped in the 10^13–10^20 cm^{-3} range. This work was supported in part by the National Science Foundation (DMR-1254314) and in part by CSTEM, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science. Computational resources were provided by the DOE NERSC facility.

4:42PM Q12.00010 Thermostrophic properties of higher manganese silicides (HMS) 1, YU-CHIH TSENG, Natural Resources Canada, VIJAY SHANKAR VENKATARAMAN, HAE-YOUNG KEE, University of Toronto — Higher manganese silicides (HMS) are promising thermoelectric materials that may be broadly deployable because of the abundance of the constituent elements and their non-toxic nature. We study the thermostrophic properties of HMS using density functional theory calculations and tight-binding models to fit these calculations. We estimate charge carrier density and mobility, and compare with experimental data. Theoretically obtained thermal and electrical conductivities, and the Seebeck coefficients are presented. Possible scattering mechanisms and relations to figure of merit are also discussed.

1NSERC CREATE - HEATER Program

4:54PM Q12.00011 First-principles Study of Lattice Thermal Conductivity of Cu_{2}SnSe_{2} and Cu_{2}SbSe_{2}, YI XIA, Department of Materials Science and Engineering, University of California, Los Angeles, CA 90095, USA, FEI ZHOU, Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, Livermore, California 94550, USA, WESTON NIELSON, VIDVUDS OZOLINS, Department of Materials Science and Engineering, University of California, Los Angeles, CA 90095, USA — Linearized self-consistent Boltzmann transport equation (BTE), utilizing interatomic force constants (IFCs) obtained via compressive sensing lattice dynamics (CSLD), is used to study the lattice thermal conductivity (κ_{L}) of Cu_{2}SnSe_{2}, Cu_{2}SbSe_{2} and their solid solutions. With these IFCs we obtain bulk lattice thermal conductivity in good agreement with experimental measurements. We also compare Cu_{2}SnSe_{2} and Cu_{2}SbSe_{2} with respect to Grüneisen parameter, group velocity, phonon lifetime, mean free path and cumulative κ_{L}. All the analysis indicates that (1) slightly larger group velocity and lifetime of acoustic modes found in Cu_{2}SnSe_{2} lead to larger κ_{L} compared with Cu_{2}SbSe_{2} over the whole temperature range. Contributions from optical modes to κ_{L} for both compounds are about 25% at temperature higher than 300K. This large portion of κ_{L} can not be neglected if one aims to predict accurate κ_{L}; (2) Nanostructures with length less than 10nm can effectively reduce κ_{L} by about 80% for both of the compounds; (3) solid solution of two compounds can effectively reduce κ_{L} as much as 40% at room temperature.

5:06PM Q12.00012 New insights into thermal conductivity by non-equilibrium molecular dynamics1, PHILIP ALLEN, Stony Brook University, YERONG LI, Nanjing University — Non-equilibrium molecular dynamics (NEMD) is often used to simulate thermal conductivity (κ). A steady state heat current and corresponding temperature gradient are created computationally over a simulation cell of thousands of atoms. We advocate a variation that gives directly the Fourier transform of the non-local (κ(x − x′)) that relates J(z) to 1/V z(x′). The algorithm is tested on the Lennard-Jones liquid and crystal, and is efficient for extraction of the macroscopic κ = −lim_{q→0} q/4πκ_{q} as well as a detailed comparison with simulation. For an isotropic cell (N_x = N_y = N_z), the behavior is κ(q) = κ−A∗q^{1/2}. For the more typical anisotropic cell with one length (N_x) large compared to the others, there is an additional term ∝ q^{−1/2}/N_x N_y. This divergent contribution disappears in the bulk limit. Strategies for extrapolation of simulations are suggested.

1Supported by DOE grant No. DE-FG02-08ER46550

5:18PM Q12.00013 Strain-induced semi-metal to semiconductor transition and strong enhancement in thermopower of TiS_{2}, ATANU SAMANTA, TRIBHUWAN PANDEY, ABHISHEK K. SINGH, Materials Research Centre, Aeronautical Development Agency (ADA) under NPMASS and Department of Science and Technology(DST) nanomission

Indian Institute of Science, Bangalore-560012 — Electronic properties of transition-metal dichalcogenides (TMDs) (MX_{2}, where M = Mo, W and X = S, Se, Te) are very sensitive to the applied pressure/strain, causing a semiconductor to metal transition. Using first principles density functional theory calculations, we demonstrate that bulk TiS_{2} changes from semi-metal to semi-conducting electronic phase upon application of uniform biaxial strain. This phase transition is responsible for the charge transfer from Ti to S and reduces the overlap between Ti-(d)- and S-(p)-orbitals. The transport calculations show a three-fold enhancement in thermopower for both p- and n-type TiS_{2} due to opening of band gap along with changes in dispersion of bands. The electrical conductivity and thermopower shows a large anisotropy due to the difference in the effective masses along the in-plane and out-of-plane directions. We further demonstrate that the enhancement of thermoelectric performance, can also be achieved by doping TiS_{2} with larger iso-electronic elements such as Zr or Hf at the Ti sites.

1Aeronautical Development Agency (ADA) under NPMASS and Department of Science and Technology(DST) nanomission

Wednesday, March 4, 2015 2:30PM - 5:30PM –
Session Q13 DMP: Focus Session: Complex Oxide Interfaces - LaAlO3/SrTiO3 II
007D - Sohrab Ismail-Beigi, Yale University
2:30PM Q13.00001 Combining Mott insulators and ferroelectrics, AGNÈS BARTHELEMY, Unité Mixte de Physique CNRS/Thales — We investigated the properties of high quality heterostructures consisting of a Mott insulator, (Ca,Ce)MnO$_3$ (CCMO) and a ferroelectric, BiFeO$_3$ in the supertetragonal phase (T-BFO) materials. In particular, we studied the electrical response induced by ferroelectric switching in both planar and vertical devices. In the planar geometry, we used thick T-BFO films to explore the possibility to electrically tune the properties of the CCMO compound in a ferroelectric field-effect device with a CCMO channel and a T-BFO gate. Upon polarization reversal of the T-BFO ferroelectric gate, the CMO channel exhibits a nonvolatile resistance switching by a factor of 4 around room temperature, and up to a factor of 10 at 200 K [1]. We also studied Ferroelectric tunnel junctions (FTJs) composed of an ultrathin ferroelectric tunnel barrier of T-BFO sandwiched between a CCMO electrode and a Co/Pt counter-electrode. In these junctions, the tunneling current significantly depends on the orientation of the ferroelectric polarization, resulting in large electroresistance enabling a simple nondestructive readout of the ferroelectric state [2]. FTJs based on ultrathin T-BFO films show fast, stable multistate switching with very high resistance ratios of up to four orders of magnitude [3]. Combined piezoresistance force microscopy (PFM) and electrical measurements give a clear correlation between ferroelectric domain configurations and multiple resistance states. They also provide insights into the switching dynamics in response to trains of nanosecond pulses. Additionally, we demonstrated the very good endurance and retention characteristics of these FTJs [4].


3:06PM Q13.00002 First-principles many-body investigation of δ-doped titanates, FRANK LECHEMANN, MICHAEL OBERMEYER, I. Institute for Theoretical Physics, University of Hamburg — Studying oxide heterostructures provides the possibility for exploring novel composite materials beyond nature’s original conception. In this respect, the doping of Mott-insulating distorted-perovskite titanates such as LaTiO$_3$ and GdTiO$_3$ with a single SrO layer gives rise to a very rich correlated electronic structure [1]. A realistic superlattice by means of the charge self-consistent combination of density functional theory (DFT) with dynamical mean-field theory (DMFT) reveals layer- and temperature-dependent multiorbital metal-insulator transitions. In [001] stacking, an orbital-selective metallic layer at the interface dissolves via an orbital-polarized doped-Mott state into an orbital-selective metallic layer at the interface. We find large differences in the scattering behavior within the latter. Breaking the spin symmetry in δ-doped GdTiO$_3$ results in blocks of ferromagnetic itinerant and ferromagnetic Mott-insulating layers which are coupled antiferromagnetically.


3:18PM Q13.00003 Towards enhancing two-dimensional electron gas quantum confinement effects in perovskite oxide heterostructures, KESONG YANG, SAFDAR NAZIR, MAZIAR BEHTASH, University of California, San Diego — The two-dimensional electron gas (2DEG) in LaAlO$_3$/SrTiO$_3$ perovskite-oxide heterostructure has attracted much attention because of its potential applications in nanoelectronic devices. A 2DEG has two landmark characters: strong charge confinement in the third dimension and high electron conductivity in two dimensions. In an ideal 2DEG system, electrons can move freely along the interface but are tightly confined in the c-axis that is perpendicular to the interface. Nevertheless, the actual electron gas in the SrTiO$_3$-based perovskite heterostructures is extended a few nanometers along the c-axis into the SrTiO$_3$ substrate, and thus they are also called quasi-2DEG. Actually, it is a problem of both fundamental and practical interest to achieve an ideal 2DEG via enhancing the lateral quantum confinement effects. By using first-principles electronic structure calculations, we propose two possible approaches to enhance the quantum charge confinement effects by confining the electron gas within one single atomic layer in the perovskite oxide heterostructure.

3:30PM Q13.00004 Two-dimensional electron gas at the epitaxial alumina/SrTiO$_3$ interface: control of oxygen vacancies, KRISY KORMONDY, AGHAM POSADAS, University of Texas at Austin, THONG NGO, Univ of Texas, Austin, SIRONG LU, Arizona State University, NICHOLAS GOBLE, Case Western Reserve University, JEAN JORDAN-SWEET, IBM T.J. Watson Research Center, XUAN GAO, Case Western Reserve University, MARTHA MCCARTNEY, DAVID SMITH, Arizona State University, JOHN EKERDT, ALEXANDER DEMKOV, University of Texas at Austin — A highly interesting application for SrTiO$_3$ is the formation of a high mobility two-dimensional electron gas (2DEG) at the oxide/oxide interface. We report on the conducting layer formed at the crystalline γ-α alumina/SrTiO$_3$ (STO) interface which is attributed to oxygen vacancies. We describe the structure of thin γ-α alumina layers deposited by molecular beam epitaxy on STO (001), as determined by reflection-high-energy electron diffraction (RHEED), grazing incidence X-ray diffraction, and high-resolution electron microscopy. In-situ x-ray photoelectron spectroscopy was used to confirm the presence of oxygen vacancies at the interface. Electrical characterization indicates a higher sheet resistance for lower deposition temperature. A maximum electron Hall mobility of 3100 cm$^2$/V·s at 3.2 K and room temperature mobility of 22 cm$^2$/V·s are measured.

3:42PM Q13.00005 Optical properties of transition metal oxide quantum wells, ALEXANDER DEMKOV, MIRI CHOI, MATTHEW BUTCHER, The University of Texas, CESAR RODRIGUEZ, New Mexico State University, QIAN HE, Oak Ridge National Laboratory, AGHAM POSADAS, The University of Texas, ALBINA BORISEVICH, Oak Ridge National Laboratory, STEFAN ZOLLNER, New Mexico State University, CHUNGWEE LIN, ELLIOTT ORTMANN, The University of Texas at Austin — We report on the investigation of SrTiO$_3$/LaAlO$_3$ quantum wells (QWs) grown by molecular beam epitaxy (MBE) on LaAlO$_3$ substrate. Structures with different QW thicknesses ranging from two to ten unit cells were grown and characterized using x-ray photoemission spectroscopy, reflection high-energy electron diffraction (RHEED), grazing incidence x-ray diffraction, transmission electron microscopy (TEM), and high-resolution electron microscopy (HREM). Optical properties (complex dielectric function) were measured by spectrophotometric ellipsometry (SE) in the range of 1.0 eV to 6.0 eV at room temperature. We observed that the absorption edge was blue-shifted by approximately 0.39 eV as the STO quantum well thickness was reduced to two unit cells (uc). Density functional theory and tight-binding are used to model the optical response of these heterostructures. Our results demonstrate that the energy level of the first sub-band can be controlled by the QW thickness in a complex oxide material. We acknowledge support from Air Force Office of Scientific Research (FA9550-12-10494).

3:54PM Q13.00006 Polar-nonpolar Oxide heterostructures for photocatalysis, HONGLI GUO, Department of Physics, University of Science and Technology of China, JIN ZHAO, Department of Physics, University of Science and Technology of China, The International Center for Quantum Design of Functional Materials, WISSAM SAID, Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania, 15261, United States — The discovery of two-dimensional electron gas (2DEG) at the interface of polar LaAlO$_3$ (LAO) and non-polar SrTiO$_3$ (STO) opens the research field of layered oxide heterostructures. In this study, we propose new application of oxide heterostructures for photocatalysis. We take a sandwich-like heterostructure STO/LAO/STO as an example and prove it to be a promising photocatalyst which is active for near-infrared light. Because the sandwiched LAO is polarized and generates a build-in electrostatic field, the valance band and conduction band locates on two opposite STO surfaces. First principles calculations prove that the band gap is reduced and the absorption of near-infrared to visible light is improved distinctly. Simultaneously, the build-in electric field in LAO accelerates the electrons and holes into opposite directions, preventing the recombination, and generates an electron doped surface and a hole doped STO surface, which could be used for H$_2$O reduction and oxidation separately. Our study gives a new perspective into the applications of oxide heterostructures in solar energy conversion.

4:06PM Q13.00007

SHIRIN MOZAFFARI, MARK C. MONTI, Department of Physics, The University of Texas at Austin, SAMARESH GUCHHAIT, Microelectronics Research Center, The University of Texas at Austin, JEREMY W. PASTER, DANIEL M. TENNANT, JOHN T. MARKERT, Department of Physics, The University of Texas at Austin — We explored the electronic and magnetic behavior of epitaxial PrAlO$_3$ films on TiO$_2$-terminated SrTiO$_3$ (PAO/STO) substrates grown by pulsed laser deposition at various oxygen pressures. We report structural (x-ray and AFM), electronic (van der Pauw resistivity, magnetoresistance (MR), and Hall effect), and magnetic data for PAO films grown in $10^{-3}$–$10^{-6}$ torr O$_2$. Resistivity data exhibit metallic behavior from 300 K down to 100–150 K (75 K; 40 K) for the interface grown in $10^{-3}$ ($10^{-4}$; $10^{-5}$) torr O$_2$, and semiconducting behavior below that. One $10^{-3}$ torr O$_2$ interface shows typical behavior for current parallel to atomic terraces, and a resistance anomaly in the range 50–100 K for current perpendicular to step edges. MR data for all $10^{-1}$–$10^{-2}$ torr O$_2$ samples show a small ($<0.5\%$) positive MR at low fields, and a larger negative MR (2–30\%) at high fields; for $10^{-2}$ torr O$_2$, the MR is positive up to 9 tesla. Sheet resistivity for the $10^{-3}$ torr O$_2$ interface is anomalously low, suggesting a thick conducting layer. Hall effect data exhibit several variations in the carrier density. We discuss these data considering intrinsic charge transfer, oxygen vacancies and interstitials, and cation interdiffusion.

Orbital order and effective mass enhancement in $t_{2g}$ two-dimensional electron gases

4:18PM Q13.00008

JOHNS TOLMA, University of Texas at Austin, ALESSANDRO PRINCIPI, University of Missouri, MARCO POLINI, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, ALLAN MACDONALD, University of Texas at Austin — It is now possible to prepare d-electron two-dimensional electron gas systems that are formed near oxide heterojunctions and contain $t_{2g}$ electrons with a density much smaller than one electron per metal atom. We will discuss a generic model that captures all qualitative features of electron-electron interaction physics in $t_{2g}$ two-dimensional electron gas systems, and the use of a GW approximation to explore $t_{2g}$ quasiparticle properties in this new context. $t_{2g}$ electron gases contain a high density isotropic light mass $xz$ and low-density $yz$ and $yz$ anisotropic components with light and heavy masses in orthogonal directions. The high density light mass band screens interactions within the heavy bands. As a result the wave vector dependence of the self-energy is reduced and the effective mass is increased. When the density in the heavy bands is low, the difference in anisotropy between the two heavy bands favors orbital order. When orbital order does not occur, interactions still reshape the heavy-band Fermi surfaces. I will discuss these results in the context of recently reported magnetotransport experiments.

4:30PM Q13.00009

ABSTRACT WITHDRAWN

4:42PM Q13.00010 Non-local Signal in Quasi-2DEG of LAO/STO

MI-JIN JIN, Ulsan Natl Inst of Sci & Tech, SEON YOUNG MOON, Korea Institute of Science Technology (KIST), VIJAYAKUMAR MODEPALL, JUNHYEON JO, JUNMINS PARK, Ulsan Natl Inst of Sci & Tech, SEUNG-HYUB BAEK, Korea Institute of Science Technology (KIST), JUNG-WOO YOO, Ulsan Natl Inst of Sci & Tech — Electron gas arizen at the insulating oxide interfaces exhibits high electron mobility, tunable carrier densities and related unique behaviors such as coexistence of superconductivity and ferromagnetism, Kondo resistance, etc. Itinerant electrons at the oxide hetero-interface are predicted to have long spin diffusion length, while they are under the relatively strong Rashba-type spin orbit coupling due to inversion symmetry breaking. We studied non-local spin signal induced by spin orbit coupling with additional gate-controlled Rashba field in quasi-2DEG of LaAlO$_3$/SrTiO$_3$ (LAO/STO) interface. We fabricated simple hall-bar like geometry to measure non-local signal with the variation of channel length ($2 \sim 10 \mu$m). Cleaned sample was patterned using e-beam lithography and reactive ion etching followed by oxygen treatment to anneal out oxygen vacancies. When an electric current flows one line of the hall bar structure, spin orbit coupling will induce the current flow away from the source current channel via spin hall and inverse spin hall effects. The non-local signals were studied under different angles of magnetic field and the variation of applied gate voltage.

3 This work was supported by a grant from (No. 1.140092.01) funded by the Ulsan National Institute of Science and Technology.

4:54PM Q13.00011 Contact resistance tuning at metal / Nb:SrTiO$_3$ interfaces using LaAlO$_3$ interlayers

HISASHI INOUE, ADRIAN SWARTZ, GLAM, Stanford University, TAKASHI TACHIKAWA, Dept. of Adv. Mat. Sci., The Univ. of Tokyo, SIMEIS, SLAC Nat. Accel. Lab., YASUYUKI HIKITA, SIMEIS, SLAC Nat. Accel. Lab., HARALD HWANG, Stanford Univ., SLAC Nat. Accel. Lab. — SrTiO$_3$ (STO) exhibits coexistence of high mobility electrons and possible unconventional superconductivity (SC) [1]. Transition metal (TM) contacts to epitaxial insulator/Nb doped STO (NSTO) structures are prototypically used to probe the electronic structure (ES) of n-type STO in tunneling experiments. However, the field dependent permissivity in STO at low temperatures makes it difficult to probe ES when the barrier height (BH) is large [2]. We show that the contact resistance $R_c$ across TM/NSTO interfaces (IF) can be effectively tuned by inserting a thin LaAlO$_3$ (LAO) interlayer (IL) between the TM and NSTO. Change of IL thickness from 0 to 2 u.c. in Co/LAO/NSTO (100) structures results in systematic reduction of $R_c$ by orders of magnitude, as evidenced by a transition from Schottky-type rectifying to nearly ohmic current-voltage curves. This is because the polar nature of the LAO surface, generating an IF dipole, lowers the Schottky BH. This is a useful method to optimize $R_c$ for tunneling experiments in doped STO with possible applications for SC and spintronics. It is also important that this effect fails for ex-situ deposited TM and we discuss the distinction. [1] Richter et al., Nature 502, 528 (2013) [2] Tsukada et al., Phys. Rev. B 76, 155110 (2007)

5:06PM Q13.00012 Spin injection and spin-charge conversion in LaAlO$_3$/SrTiO$_3$ 1, MANUEL BIBES, EDOUARD LESUE, JUAN CARLOS ROJAS SANCHEZ, CNRS/Thales, SIMON OYARZUN, YU FU, Institut Nanosciences et Cryogénie, CEA & Université Grenoble Alpes, NICOLAS REYREN, CNRS/Thales, MATHIEU JAMET, Institut Nanosciences et Cryogénie, CEA & Université Grenoble Alpes, ERIC JACQUET, AGNES BARTHELEMY, JEAN-MARIE GEORGE, ALBERT FERT, HENRI JAFFRES, CNRS/Thales, LAURENT VILA, Institut Nanosciences et Cryogénie, CEA & Université Grenoble Alpes — The perovskite oxides family provides materials to efficiently generate and control spin polarized currents using respectively half-metallic ferromagnets such as mixed-valence manganites or ferroelectrics and multiferroics. More recently channel materials to transport spin information have also emerged. These include the LaAlO$_3$/SrTiO$_3$ two-dimensional electron system (2DES) which, in addition, possesses a gate-tunable spin-orbit coupling. A limitation of this system is however the minimum LaAlO$_3$ thickness of 4 uc required for 2DES formation. In this presentation we will show that this thickness can be reduced if the LaAlO$_3$ is capped by appropriate metals. We will also present different approaches to inject spins in these engineered LaAlO$_3$/SrTiO$_3$ 2DES and introduce detection schemes taking advantage of efficient spin-charge conversion via interfacial spin-orbit effects.

1 Support by ERC Consolidator grant MINT (no. 615759) is acknowledged.
Therefore, we propose that a moderately Sn-rich condition is optimal when CsSnI$_3$ as hole-transport material in solar cells. In contrast, when Sn becomes richer, the concentration of acceptor defects decreases, so the p-type conductivity may degrade quickly when exposed to heat and moisture. This degradation limits the large scale production of the device. In this work we use molecular dynamics simulations to study CH$_3$NH$_2$PbI$_3$ when exposed to high temperatures (30 – 80°C) and water. The force fields used in the simulations were determined from ab initio calculations on the system. The structural changes that occur in methylammonium lead halide perovskites under conditions of high temperature and humidity will be inferred from the simulations.

In this talk, I will review the developmental milestones in this field and distil the recent findings on the photophysical mechanisms of this remarkable material. I will also highlight some of our latest charge dynamics studies and other investigations on the novel properties of this amazing material system.

The Photophysics of Perovskite Solar Cells . TZE-CHIEN SUM, Nanyang Technological University — Solution processed organic-inorganic lead halide perovskite solar cells, with power conversion efficiencies approaching 20%, are presently the forerunner amongst the next generation photovoltaic technologies. These remarkable performances can be attributed to their large absorption coefficients, long charge carrier diffusion lengths and low non-radiative recombination rates. In addition, these materials also possess excellent light emission and optical gain properties. In this talk, I will review the developmental milestones in this field and distil the recent findings on the photophysical mechanisms of this remarkable material.

The Photovoltaic Properties of Perovskite Solar Cells with Organic-Inorganic Halide Perovskites . PENG XU, Fudan University, SHIYOU CHEN, East China Normal University, HONGJUN XIANG, XIN-GAO GONG, Fudan University, SU-HUAI WEI, National Renewable Energy Laboratory — CsSnI$_3$ is a prototype inorganic halide perovskite that has recently been proposed as a photovoltaic material. Through first-principles calculations, we show that the concentration control of intrinsic defects is critical for optimizing the photovoltaic properties of CsSnI$_3$. Under a Sn-poor condition, high concentration of acceptor defects such as Sn or Cs vacancies can form easily and produce a high p-type conductivity, and deep level defects that can become electron-hole recombination centers, all have high energy. This condition is optimal for growing CsSnI$_3$ as hole-transport material in solar cells. In contrast, when Sn becomes richer, the concentration of acceptor defects decreases, so the p-type conductivity may drop to a moderate level, which can increase the shunt resistance and thus the efficiency of the solar cells with CsSnI$_3$ as the light absorber material (LAM). However, under the Sn-rich condition, the concentration of a deep-level donor defect Sn$_1$ will increase, causing electron trapping and non-radiative electron-hole recombination. Therefore, we propose that a moderately Sn-rich condition is optimal when CsSnI$_3$ is used as LAM.

New GeSi doping strategies based on P(SiH$_3$)$_3$ for next-generation CMOS technologies . ANDREW CHIZMESHYA, CHI XU, Dept of Chem-Biochem, Arizona State University, JAMES GALLAGHER, Dept of Physics, Arizona State University, PATRICK SIMS, Dept of Chem-Biochem, Arizona State University, DAVID SMITH, JOSE MENENDEZ, Dept of Physics, Arizona State University, JOHN KOVETAKIS, Dept of Chem-Biochem, Arizona State University — GeSi n-type films are synthesized using the specially designed hydrides P(SiH$_3$)$_3$, GeH$_4$ and Ge$_2$H$_6$ for applications in next-generation CMOS technologies. The films are grown on Ge-buffered Si(100) at 340 °C using two methods. The first employs a gas-source molecular epitaxy approach and Ge$_2$H$_6$ to yield films with P doping densities up to 3.5 x 10$^{19}$/cm$^3$. The amount of Si incorporated equals or exceeds the 3:1 ratio in the P(SiH$_3$)$_3$ compound. The second approach applies an ultra-high vacuum chemical vapor deposition technique and Ge$_2$H$_6$ in place of Ge$_2$H$_6$ to achieve higher carrier concentrations up to 6 x 10$^{19}$/cm$^3$. The Si:P ratio in this case is well below the 3:1 value expected from the precursor. The electron mobilities for both types of samples are significantly higher than state-of-the-art prototypes, probably due to superior microstructure and dearth of intrinsic donors. The relative stability of P and Ge-P bonds in a Ge matrix is studied with ab initio methods. P − I − N diodes fabricated using P(SiH$_3$)$_3$ show excellent I-V characteristics that are virtually undistinguishable from similar diodes doped with the P(GeH$_3$)$_3$ precursor. These results confirm P(SiH$_3$)$_3$ as a viable doping source that is practical from a process standpoint and therefore attractive for industrial scale-up.

This research is supported by the NSF through grant DMR-1206935.
Theoretical study of defect properties in thermoelectric \((\text{GeTe})_2(\text{AgSbTe}_2)_{1-x}\)  
Hikari Shinya, Akira Masago, Tetsuya Fukushima, Hiroki Funashima, Hiroshi Katayama-Yoshida, Osaka Univ. - We investigate the structural stability of a pseudo-binary alloy \((\text{GeTe})_2(\text{AgSbTe}_2)_{1-x}\) called TAGS by the density functional theory. TAGS shows intermittent reductions of the thermal conductivity without change of the electric conductivity. However, the mechanism of the drastic change of the thermal conductivity has yet to be understood, and even the crystal structures are still under discussion. In this presentation, we will discuss these problems from a viewpoint of the structural stability. To clarify the stable structure, we estimate the formation energies of the point and the complex defects. As a result, a chain structure of Ag-Te-Sb in GeTe host crystal has a lower formation energy compared to the homogeneous distribution. Moreover, the calculated mixing energy shows that the system is favorable to the phase separation. In the phase separation, the grain boundary must play an important role in the large phonon scattering, therefore, it can lead to the thermal conductivity reduction. These calculations were done with Vienna ab initio Simulation Package and MACHIKANEYAMA2002 program package.

A first-principles study of co-doping in lanthanum bromide, Daniel Aberg, Babak Sadigh, Lawrence Livermore Natl Lab, Andre Schleife, University of Illinois at Urbana-Champaign, Paul Erhart, Chalmers University of Technology. - It was recently shown that the energy resolution of Ce-doped LaBr₃ scintillator radiation detectors can be crucially improved by co-doping with Sr, Ca, or Ba. Here we outline a mechanism for this enhancement on the basis of deep electronic structure calculations. We show that Sr dopants create and bind to Br vacancies, resulting in stable neutral complexes. The association with Sr causes the deep vacancy level to move toward the conduction band edge. This is essential for reducing the effective carrier density available for Auger quenching during thermalization of hot carriers. Subsequent de-trapping of electrons from the complexes can activate Ce dopants which have previously captured a hole leading to luminescence. This mechanism implies an overall reduction of Auger quenching of free carriers, which is expected to improve the linearity of the photon light yield with respect to the energy of incident electron or photon. Optical properties of the Ce-Sr-vacancy triple complex are discussed and compared to experiment. Prepared by LLNL under Contract DE-AC52-07NA27344.

Formation and function of vacancies in Si/Ge Clathrates: The importance of broken symmetries, Amrita Bhattacharya, Christian Carbogno, Matthias Scheffler, Fritz Haber Institute of the MPG, Berlin, DE. - One promising material class for improved thermoelectrics are the clathrates, i.e., semiconducting host lattices encapsulating guest atom. Even in simple clathrates such as Si₄₄ and Ge₄₄, the introduction of guests can result in important but not yet understood effects. In Si hosts, the addition of K (or Ba) results in defect-free K₂Si₄₄ (Ba₂Si₄₄) phases. In spite of their structural and electronic similarity, Ge hosts behave fundamentally different upon filling, where the spontaneously formed framework vacancies completely (or partially) balance the electron donated by K (or Ba) guests leading to K₆Ge₄₄ (or Ba₆Ge₄₄) clathrates. In this work, we use density-functional theory, carefully validating the exchange correlation functional, to compute the formation energies of vacancies and vacancy complexes in Si- and Ge-hosts as function of the filling of guests. By taking into account of the structural disorder, geometric relaxations, and vibrational entropies, we verify the experimentally found vacancy concentration and the thermodynamic stabilities of these compounds. We can trace back the contrasting behaviour of Si/Ge clathrates upon filling to a curious, charged vacancy induced break in symmetry that occurs in Si but not in Ge hosts.

Cation-vacancy and electron-hole relaxation in single-walled aluminosilicate nanotubes: a linear-scaling Density Functional Theory study, Emiliano Poli, Gilberto Teobaldi, Univ of Liverpool. - We report a linear-scaling Density Functional Theory (DFT) study of cation-vacancy related defects in single-walled aluminosilicate nanotubes (AlₓSiᵧNTs), based on the structures derived from solid-state Nuclear Magnetic Resonance (NMR). Defect geometry optimization leads to water condensation and modifications to the AlSi NT hydrogen network around the defect sites, leaving no dangling bond. Electronic structure analysis indicates that defect-states are highly localized in real-space and energy, with appearance of shallow and deep occupied defect states above the valence band (VB) edge of the pristine-NT. Electrostatic alignment of the defect states suggests energetically favourable separation of photo-generated electrons and holes on different defects, which may promote defect-centred photochemistry. The peculiar energy alignment of the defect-states is found to be qualitative unaffected by protonation of the defect-sites. These results should be a useful complement to ongoing experimental research in the potential of (alumino)silicate-based nano-porous materials for photocatalysis.

Electronic structure of vitamin B₁₂ within the framework of the Haldane-Anderson impurity model, Zafar Kendemir, Selma Mayda, Nejat Bulut, Izmir Inst of Tech. - We study the electronic structure of vitamin B₁₂ (cyanocobalamin C₈₈H₇₆CoN₁₄O₁₄F₈P) by using the framework of the multi-orbital single-impurity Haldane-Anderson model of a transition-metal impurity in a semiconductor host. Here, our purpose is to understand the many-body effects originating from the transition-metal impurity. In this approach, the cobalt 3d orbitals are treated as the impurity states placed in a semiconductor host which consists of the rest of the molecule. The parameters of the resulting effective Haldane-Anderson model are obtained within the Hartree-Fock approximation for the electronic structure of the molecule. The quantum Monte Carlo technique is then used to calculate the one-electron and magnetic correlation functions of this effective Haldane-Anderson model for vitamin B₁₂. We find that new states form inside the semiconductor gap due to the on-site Coulomb interaction at the impurity 3d orbitals and that these states become the highest occupied molecular orbitals. In addition, we present results on the charge distribution and spin correlations around the Co atom. We compare the results of this approach with those obtained by the density-functional theory calculations.
5:06PM Q14.00012 Characterization of structural defects in GST based nano-PCM devices through resistance drift measurements1, Ibrahim Cinar, Egecan Cogulu, Aisha Gokce, Bogazici University, Barry Stipe, Jordan Katine, HGST, A Western Digital Company, Guleh Akta, Ozhan Ozatay, Bogazici University — Phase change memory (PCM) is a promising nonvolatile data storage technology with its high signal with noise ratio and superior scalability. Resistance drift in amorphous phase of the phase change material poses a crucial reliability problem, especially in multiple-bit-per cell PCM devices. The resistance of the amorphous phase uncontrollably increases with time after a reset operation which alters the read/write conditions of the device. Structural relaxation (SR) through a defect annihilation process is considered to be the underlying physical mechanism for resistance drift. Here, we report on our measurements of the resistance drift in a phase change memory device with a single layer Ge2Sb2Te5 (GST) material not only in the amorphous state but also in the intermediate resistance state in devices with square top contact geometry which enables us to assess the reliability of multiple-bit per cell PCM memory devices. Through an analysis of electrical measurements as a function of time and temperature for increasing annealing times, we estimate a rate of change in trap density for both amorphous and mixed phases of the GST material after a switching operation. Our study allows engineering the phase change materials and optimizing programing conditions for future PCM applications.

1TUBITAK under contract number 113F385, Bogazici University Research Fund, 12B003M1, and European Union FP7 Marie Curie International Reintegration Grant PCM-256281

5:18PM Q14.00013 Bulk photovoltaic effect in CH₃NH₃PbI₃ and CH₃NH₃PbI₃₋ₓClₓ — Nathan Z. Koocher, Fan Zheng, Hiroyuki Takenaka, Fengfeng Wang, Andrew M. Rappe, Univ. of Pennsylvania — The power conversion efficiency of organometal halide perovskites has increased to nearly 20%, fueling interest in understanding the mechanism of its photovoltaic effect. High open-circuit photocurrents and J/V hysteresis curves have been experimentally measured for these materials, which suggest that the bulk photovoltaic effect (BPVE) could be in operation. Shift current is a main mechanism of the BPVE in ferroelectric perovskite oxides, and thus in our work, we calculate the shift current response of MAPbI₃ and MAPbI₃₋ₓClₓ. We find that MAPbI₃ and MAPbI₃₋ₓClₓ have shift current responses about three times larger than that of BiFeO₃. Specifically, the shift current response is enhanced when the molecular dipoles from the methylammonium molecules are aligned in the same direction and when Cl is substituted into the lattice. Because of the large shift current response, the BPVE may play a role in enhancing the performance of the solar cells.

Wednesday, March 4, 2015 2:30PM - 5:30PM — Session Q15 DMP: Focus Session: Energy and Electron Flow at Interfaces in Nanostructures

2:30PM Q15.00001 Schottky barrier formation and reduction at Au/TiO₂ interfaces by dopants from quantum simulations, Yang Jiao, Anders Hellman, Yurui Fang, Applied Physics, Chalmers University of Technology, Shiwu Gao, Beijing Computational Science Research Center, Michael Kall, Applied Physics, Chalmers University of Technology — Excitation of localized surface plasmon resonances (LSPRs) in metallic nanoparticles, especially particles made of noble metals, results in efficient light absorption and strong field enhancement, thereby enabling a multitude of nanooptical applications of high current interest. Recently, the possibility of utilizing LSPRs to generate hot electrons has attracted considerable attention. One method to extract and make use of the hot electrons is by attaching the nanoparticles on a semiconductor surface such that excited electrons with proper energy and momentum can be transferred through the Schottky barrier at the interface. Using ab initio calculations for Au/TiO₂ interfaces, we investigate dopant induced Schottky barrier height reduction effects. We show that dopant induced polarization at the interface is the dominant reason behind the semiconductor band bending and Schottky barrier formation. Calculations for Nb-dopants at different depths (d) below the interface show that the Schottky barrier height reduction depends on the depth and varies from 0.1 eV at d = 4 nm to up to 1.3 eV when the dopant is situated at the interfacial layer. The calculations also indicate that the Schottky barrier can be tuned by up to 1.5 eV by using different transition metal dopants.

2:42PM Q15.00002 Manipulating the charge state and conductance of a single molecule on a semiconductor surface by electrostatic gating1, Jesus Martinez-Blanco, Christophe Nacci, Paul-Drude-Institut fuer Festkörperelektronik, Germany, Steven C. Erwin, Naval Research Laboratory, USA, Kiyoshi Kanisawa, NTT Basic Research Laboratories, Japan, Elina Locane, Martin Thöny, Felix Erwenn, Feit-Brockower, Technische Universität Berlin, Germany, Stefan Foelsch, Paul-Drude-Institut fuer Festkörperelektronik, Germany — We studied the charge state and tunneling conductance of single phthalocyanine molecules adsorbed on InAs(111)A using scanning tunneling microscopy (STM) at 5 K. On the InAs(111)A surface, native +1 charged indium adatoms can be repositioned by the STM tip using atomic manipulation. This allows us to electrostatically gate an individual adsorbed molecule by placing charged adatoms nearby or, alternatively, by repositioning the molecule within the electrostatic potential landscape created by an STM-engineered adatom corral. By stepwise increasing the gating potential, the molecular charge state can be tuned from neutral to -1, as well as to intermediate states. We find that the molecule changes its orientational conformation when the charge state is switched. Scanning tunneling spectroscopy measurements reveal that the conductance gap of the single-molecule tunneling junction can be precisely controlled by the electrostatic gating. We discuss the observed gating-dependent single-molecule tunneling conductance in terms of charge transport through a gated quantum dot.

1Granted by the German Research Foundation (FO 362/4-1; SFB 658).

2:54PM Q15.00003 Self-energy-corrected electronic energy level alignment in molecular junctions and at interfaces with hybrid functionals1, Michele Kotiuga, Physics Department, UC Berkeley & Molecular Foundry, LBNL, David Egger, Leeor Kronik, Department of Materials and Interfaces, Weizmann Institute of Science, Jeffrey B. Neaton, Physics Department, UC Berkeley & Molecular Foundry, LBNL — Accurate calculations of energy level alignment at complex interfaces are imperative for understanding a variety of transport and spectroscopy measurements, as well as for elucidating new interfacial electronic structure phenomena. However, standard approaches to such calculations, based on density functional theory (DFT), are well known to be deficient. In prior work on molecular junctions and physisorbed molecules on surfaces, an approximate GW approach, DFT+Σ, has been successful in describing the conductance and level alignment of amine and pyridine terminated molecules on gold surfaces and in junctions. Here, via the use of hybrid functionals, we perform quantitative studies of the level alignment of thiol- and carbon-terminated phenyls on gold, where the formation of a strong chemical bond and presence of gateway states limit the validity of the DFT+Σ approximation as currently formulated. We contrast these systems to prior work on weakly-coupled molecules, including bipyrindine or phenyl-diamines. Additionally, we compute transmission functions using both DFT-PBE and DFT-HSE starting points and predict conductance and thermopower with these methods, comparing to experiments where possible.

1We acknowledge DOE, DOD, NERSC, ERC, ISF, and FWF.
the contributions arising from inelastic effects. The provided new perspective on interface thermal transport can open new gates towards deeper understanding interfaces and present thermal interface conductance accumulation functions, two-dimensional cross-correlation matrices, and a quantitative determination of and exhibit a high conductance contribution on a per mode basis by strongly coupling to other types of vibrational modes. We apply our formalism to different these new modes, certain classifications emerge, as most modes extend at least partially into the other material. Localized interfacial modes are also present transport across the interface. The new set of vibrational modes is inconsistent with the physical picture described by phonon gas model (PGM), because some of the most important modes are localized and non-propagating and therefore do not have a well-defined velocity nor do they impinge on the interface. Among these new modes, certain classifications emerge, as most modes extend at least partially into the other material. Localized interfacial modes are also present forward the challenge that soft X-rays cannot easily peek into the high-pressure catalytic cells or liquid electrochemical cells. In this presentation a number of examples are given, including the nanocatalysts and the recent experiment performed for studying the hole generation in a specifically designed photothermal chemical cell under operando conditions.

In Situ Soft X-ray Spectroscopy Characterization of Interfacial Phenomena in Energy Materials and Devices. JINGHUA GUO, YI-SHENG LIU, MIKES KAPILASHRAMI, PER-ANDERS GLANS, ALS/LBNL, DEBAJEE BORA, ARTUR BRAUN, EMPA, JUAN JESÚS VELASCO VELÉZ, MIQUEL SALMERON, MSD/LBNL, ALS/LBNL TEAM, EMPA, MSD/LBNL COLLABORATION — Advanced energy technology arises from the understanding in basic science, thus rest in large on in-situ/operando characterization tools for observing the physical and chemical interfacial processes, which has been largely limited in a framework of thermodynamic and kinetic concepts or atomic and nanoscale. In many important energy systems such as energy conversion, energy storage and catalysis, advanced materials and functionality in devices are based on the complexity of material architecture, chemistry and interactions among constituents within. To understand and thus ultimately control the energy conversion and energy storage applications calls for in-situ/operando characterization tools. Soft X-ray spectroscopy offers a number of very unique features. We will present our development of the in-situ/operando soft X-ray spectroscopic tools of catalytic and electrochemical reactions in recent years, and reveal how to overcome the challenge that soft X-rays cannot easily peek into the high-pressure catalytic cells or liquid electrochemical cells. In this presentation a number of examples are given, including the nanocatalysts and the recent experiment performed for studying the hole generation in a specifically designed photothermal chemical cell under operando conditions.

Determining level alignment and coupling strength in single-molecule junctions with chemically-enhanced Raman spectroscopy. PIERRE DARANCET, Center for Nanoscale Materials, Argonne National Laboratory, ALEXEY ZAYAK, Department of Physics, Bowling Green State University — Raman spectroscopy can be used at the nanoscale to probe binding geometries [1], molecule concentrations [2], carrier densities [3], and charging effects [4]. In this talk, we use finite-difference total-energy and energy corrected density functional theory calculations in conjunction with Landauer framework, to study the Raman spectra and transport properties of model nanoscale interfaces, single-molecule junctions – individual molecules contacted with macroscopic metallic electrodes. In the cases of 4,4′-bipyrindine/Gold and polyphenylene vinylene/Gold junctions, we will show how conductance and chemically-enhanced Raman measurement can be used in conjunction to determine the energy scales controlling electron transport i.e. frontier orbital energies and coupling strength.

Nanoscale optical spectroscopy of CdTe photovoltaic devices. NIKOLAI ZHITENEV, CNST/NIST, YOHAN YOON, JUNSEOK CHAE, CNST/NIST and U. Maryland NanoCenter, AARON KATZMENZER, CNST/NIST, HEA YOUNG YOON, CNST/NIST and U. Maryland NanoCenter, ANDREA CENTRONE, CNST/NIST — Thin film solar cells are based on polycrystalline materials such as CdTe and CIGs that are structurally and electronically non-uniform. To further advance the power conversion efficiency it is important to understand the properties of interfaces (p-n junction, contacts) and microstructure (composition, grains) of these inhomogeneous devices. We apply two local optical techniques for spectroscopic characterization of CdTe photovoltaic devices. The samples are cross-sectional lamellas extracted from CdTe cell with sub-micron thickness prepared by focused ion beam. The first tool is variable wavelength infrared interferometry (VWIR) and the second is optical images of the transmitted / absorbed power. The optical wavelength was varied in the range from 400 nm to 900 nm. The contrast of the spatial maps of optical absorption is the strongest at excitation energies close to the band gap of CdTe and it can be associated with the composition variation throughout the device. The second technique uses the photo-thermal effect as a local measurement of absorption and can be used for broader range of wavelengths. Pulsed laser with variable wavelength is used for the excitation, and the local thermal expansion is detected by an atomic force microscope. We compare the resolution and the sensitivity of these two approaches in the range of photon energies close to the band gap where both techniques can be used.

Variable temperature shot noise measurements in mechanically controlled gold break junctions. RUOYU CHEN, LELAND RICHARDSON, DOUGLAS NATELSON, Rice University — Shot noise originates from the discreteness of charge carriers when a finite bias is applied. The noise spectral density reflects the effective charge and the Fano factor. The former may be modified by electron-electron interactions, while the latter can be affected by both interactions and the microscopic nature of transport. The temperature dependence of shot noise is interesting due to the fact that both interactions and the microscopic dynamics and geometries can vary with temperature, as well as length scales associated with scattering. Previous excess noise measurements demonstrate the existence of shot noise in ballistic atomic-scale contacts at room temperature, indicating that the quantum coherence length is at least larger than atomic scale even at 300 K. A detailed temperature dependent study from cryogenic conditions to room temperature is still absent. Here we will present progress on using lithographically patterned gold bowtie junctions on mechanically-bended substrates to study the broadband rf excess noise over different conductance values, electric biases and temperatures.

Dissipation and heating in C$_{60}$ molecular junctions. PAVLO ZOLOTVIN, CHARLOTTE EVANS, DOUGLAS NATELSON, Department of Physics & Astronomy, Rice University — We present a novel experimental approach to study energy dissipation during electron transport through the molecular scale junction containing a C$_{60}$ molecule. One of the pathways for a tunneling electron to dissipate energy in the junction is to excite vibrations of the molecule. Previously, such vibrational heating had been observed by measuring the intensity of anti-Stokes modes in the surface enhanced Raman spectra (SERS). A complimentary electron-focused approach is to use inelastic electron tunneling spectroscopy (IETS) to study the electron-vibronic interactions by tracking the effects of vibrations upon the electronic current. A combination of these two techniques should allow for a quantitative study of the energy dissipation in molecular junctions. The preliminary results of simultaneous IETS and SERS measurements in C$_{60}$ molecular junctions will be presented. We discuss the vibrational heating of C$_{60}$ molecule and future expansion of this work to junctions containing semiconductor nanocrystals. (ARO award W911 NF-13-1-0476)
necessarily on the film thickness. Further, when the conductive filaments in tantalum oxide devices. The effects of Joule heating, chemical species migration and pulsed ionizing radiation from an external source are included in the model. Interface tunneling current is determined via a WKB model, in conjunction with a lattice defect generation scheme. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

4:18PM Q15.00010 Low temperature high bias enhanced noise in atomic-scale Au junctions

1D.N., P.Z., R.C. and L.S. acknowledge support from NSF award DMR-1305879.

4:30PM Q15.00011 Edge-Localised Spin-Polarized State in Nanofacet Formed on SiC(0001)

Surfaces, KEISUKE SAWADA, JUN-ICHI IWATA, ATSUSHI OSHIYAMA, Department of Applied Physics, The University of Tokyo — The nanometer-scale facet (nanofacet) are self-organized on the SiC(0001) surfaces being slightly misoriented toward the (1120) direction[1, 2]. It is known that the nanostructure induces the novel electronic property such as localized states at zigzag graphene edges[3]. In this study, we perform density-functional calculations on the nanofacet formed on the SiC(0001) surface. We find peculiar electron transport in different films without dispersion along the step edges (SEs) near the Fermi level. To explore possibilities of the observation of these peculiar states, we examine the situation that the nanofacet is covered by H atoms and calculate the H absorption energy at the several positions on the nanofacet. We then find that absorbed H atoms energetically prefer terraces to SEs. This leads to a situation in which H atoms at SE C atoms are desorbed. In this case, we find an electronic state distributed along the SE and is spin-polarized. Implication of magnetic transport in such nanofacet will be discussed. [1] H. Nakagawa et al., PRL 91, 226107 (2003). [2] M. Fuji and S. Tanaka, PRL 99, 016102 (2007). [3] M. Fujita et al., JPSJ 65, 1920 (1996).

4:42PM Q15.00012 Thermal conductivity and interfacial thermal conductance of HfN/ScN superlattices

B O SUN, N atl Univ of Singapore, JEREMY SCHROEDER, Linkoping University, YEEKAN KOH, Natl Univ of Singapore — Metal/semiconductor superlattices are known for their potential application as thermionic devices. Understanding thermal properties of such superlattices is essential for the design of new material structures and devices. Here, we measured the cross-plane thermal conductivity of HfN/ScN metal/semiconductor superlattices using time-domain thermoreflectance (TDTR). HfN/ScN superlattices with different period thickness (2nm to 24 nm) were grown on MgO substrate using reactive magnetron sputtering. We found that the minimum thermal conductivity is 4.3 W/m K when the period thickness is 6 nm. By changing the ratio of layer thickness of HfN and ScN (1:4 to 4:1), we studied the contributions electrons and phonons to the thermal conductivity of superlattices. Use a simple thermal resistance calculation, we extract the interfacial thermal conductance between HfN and ScN. The interfacial thermal conductance is 1.8 GW/m2 K, which is 3 times higher than that of AlN/GaN.

4:54PM Q15.00013 Resistivity of thiol-modified Au thin films

, PATRICIO HÄBERLE, JONATHAN CORREA-PUERTA, VALERIA DEL CAMPO, RICARDO HENRIQUEZ, Universidad Técnica Federico Santa María, Chile — Electrical transport in conductors with sizes in the nanoscale range is indeed a surface dependent feature. We report on the modification of electrical transport in thin gold films by the functionalization of alkanethiols, which form a self-assembled monolayer. Theoretical models such as the Fuchs-Sondheimer-Lucas and Namba[1], have been used to describe the electrical conduction, including size effects. Within these models, the resistivity can be attributed to an electron-surface scattering mechanism. Measurements performed in different films display an increased resistivity in the functionalized films. This increment depends mainly of the gold surface topography and not necessarily on the film thickness.


5:06PM Q15.00014 Direct measurement of the intrinsic linewidth of a resonant state

, ZACHARY KOBOS, Department of Electrical Engineering, Yale University, MARK REED, Departments of Electrical Engineering and Applied Physics, Yale University — We have applied inelastic electron tunneling spectroscopy (IETS) techniques to a resonantly-coupled system to determine quantitative differences in resonant versus non-resonant IETS. We use as a model system a set of GaAs-AlGaAs resonant tunneling diodes (RTDs)(footnote: with different barrier widths to tune resonant state linewidths and transmission coefficients. Modulation-broadening studies confirm theoretical predictions; however, the thermal dependence is markedly different than expected from classical IETS theory[1]. An analysis of resonances shut-off reveals that the thermal dependence reflects the thermal broadening of the injector and resonant state density of states. Using this analysis, we show that one can extract both the transmission coefficient and the intrinsic linewidth of the resonant state. This is compared for RTDs of different tunneling barrier widths, and we observe the expected increase in resonance width for thinner barriers.


5:18PM Q15.00015 The Role of Joule Heating and Defect Chemistry in Memristor Modeling

, BRIAN TIERNEY, HAROLD HJALMARSON, MICHAEL MCCLAIN, DENIS MAMALUY, Sandia National Laboratories — Resitive switching in electroformed metal/metal-oxide/metal memristive devices involves the growth and dissolution of conductive filaments within the metal-oxide. These filaments are typically formed/dissolved by applying a voltage pulse of the appropriate polarity across the metal contacts. The induced electric field across the oxide causes Joule heating. This heating is a significant contributor to the migration of lattice defects such as charged oxygen vacancies, which modulate the time-evolution of the conductive filaments, and hence the device resistance. In this talk, continuum calculations are presented that model the temporal evolution of conductive filaments in tantalum oxide devices. The effects of Joule heating, chemical species migration and pulsed ionizing radiation from an external source are included in the model. Interface tunneling current is determined via a WKB model, in conjunction with a lattice defect generation scheme. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

Wednesday, March 4, 2015 2:30PM - 5:18PM

Session Q16 DMP: Focus Session: van der Waals Bonding in Advanced Materials: Nano-Materials 101AB - Alexandre Tkatchenko, Fritz Haber Institute of the Max Planck Society
2:30PM Q16.00001 Beller Lectureship: Van der Waals interactions in adhesion, adsorption and friction experiments1, KARIN JACOBS, Experimental Physics, Saarland University, Saarbrücken, Germany — Van der Waals (vdW) forces are commonly regarded as being weak and of short range and are thus often neglected. However, our experiments give clear evidence that vdW forces significantly contribute to a range of phenomena at interfaces, like thin film stability, protein adsorption, bacterial and gecko adhesion as well as single asperity friction [1-5] and that vdW forces can be of long range. The key for an apt description of vdW and further relevant forces present in these diverse system is a precise knowledge about the interacting objects, for instance their chemical composition from the surface up to roughly 100 nm into the bulk. The effective interface potentials used to describe and understand the different experimental situations can additionally serve as useful descriptions for future simulations of similar systems, which will gain in precision and predictive power when taking vdW interactions into account.

1Financial support of by the German Research Foundation DFG via grants SPP 1164 and SFB 1027 are gratefully acknowledged.

3:06PM Q16.00002 Van der Waals-coupled electronic states in incommensurate double-walled carbon nanotubes, CHENHAO JIN, Department of Physics, UC Berkeley, KAIHUI LIU, Department of Physics, Peking University, XIAOPING HONG, JIHOON KIM, ALEX ZETTLE, Department of Physics, UC Berkeley, ENGE WANG, International Center for Quantum Materials and Collaborative Innovation Center of Quantum Matter, Peking University, FENG WANG, Department of Physics, UC Berkeley — In two-dimensional materials consisting of elements without finite unit cell, such as twisted graphene bilayer or graphene on boron nitride, the incommensurate van der Waals coupling can give rise to emerging physics like Van Hove singularities, pseudospin-mixing potential and Hofstadter butterflies. However, their 1D counterpart, incommensurate double-walled carbon nanotube (DWNT), is conventionally believed to have negligible electron hybridization due to destructive interference. Here we for the first time demonstrate strong and chirality-dependent intertube electronic coupling in DWNTs, which can be well described by a zone folding model of twisted and “stretched” graphene bilayers. Our results demonstrate that incommensurate van der Waals interactions can be important for engineering the electronic structure and optical properties of one-dimensional materials.

3:18PM Q16.00003 Double-walled carbon nanotubes as one-dimensional moiré crystals1, PILKYUNG MOON, NYU Shanghai, MIKITO KOSHINO, Tohoku University, YOUNG-WOO SON, Korea Institute for Advanced Study — Being multi-shell structure, the well-defined atomic periodicity is hardly realizable in double-walled nanotubes because the periodic units of individual tubes therein cannot match well except very few cases, posing a challenge to understand its physical properties. Here we show that moiré patterns generated by superimposing atomic lattices of individual tubes are decisive in determining its electronic structures [1]. By using double-walled carbon nanotubes as an example, we demonstrate that even the combination of semiconducting nanotubes with almost the same physical properties such as diameter and energy gap can end up with very different double-walled nanotubes, of which electronic properties vary from metallic to semiconducting and further to insulating states, depending on the interlayer moiré interference. Our study puts forth a new classification of nanotubes as the first example of one-dimensional moiré crystals and paves a firm ground to utilize superb technological merits of double-walled carbon nanotubes. [1] Mikito Koshino, Pilkyung Moon, and Young-Woo Son, arXiv:1410.7544 (2014).

3:30PM Q16.00004 Dynamical Screening of van der Waals interactions in nanostructures: Sublimation of fullerenes1, ANDREW M. RAPPE, JIANMIN TAO, JING YANG, University of Pennsylvania — Sublimation energy is one of the most important properties of molecular crystals, but it is difficult to study, because the attractive long-range van der Waals (vdW) interaction plays an important role. In this talk, I will discuss our recent work on the calculation of the sublimation of fullerenes, using efficient semilocal density functional theory (DFT), corrected with the dynamically screened vdW interaction (DFT+vdW), the Langreth-Lundqvist nonlocal vdW-DF, and the pairwise-based dispersion-corrected DFT-D2, to study the sublimation of fullerenes. We find that the short-range part, which accounts for the interaction due to the orbital overlap between fullerenes, is negligibly small. Our calculation shows that there exists a strong screening effect on the vdW interaction. On the other hand, higher-order contributions can be as important as the leading-order term. However, these two effects make opposite contributions, leading to significant error cancellation. We demonstrate that, by considering higher-order contributions and the dynamical screening, the DFT+vdW method can yield sublimation energies of fullerenes in good agreement with reference values, followed by vdW-DF and DFT-D2. The insights from this study are important for better understanding of the long-range nature.

1This work was supported by NSF, USAF, and DOE

3:42PM Q16.00005 van der Waals density functional comparison for water monomers, dimers and clusters and the implications on the dynamics of liquid water1, ADRIAN SOTO, MARIVI FERNANDEZ-SERRA, Department of Physics and Astronomy, Stony Brook University, DEyü LU, Center for Functional Nanomaterials, Brookhaven National Laboratory — The appearance of van der Waals (vdW) density functionals has allowed the efficient ab initio molecular dynamics (AIMD) study of systems for which dispersion forces are critical. Despite the great improvement over GGA functionals, the errors in the simulations are still too large for some applications of interest. Furthermore, different vdW functionals can produce qualitatively different results. In particular, for liquid water at ambient conditions there is a discrepancy of approximately 20% in the yielded P(\rho) “equations of state”; the radial distribution functions (RDF) disagree substantially with experiment, giving an overstructured liquid mainly due to an overbinding of the hydrogen bond; the self-diffusion coefficients can vary over 75% [J. Chem Phys. 139, 194502(2013)]. In this study we focus on the role of the electronic polarizabilities, responsible for the vdW dispersion forces using two very different vdW functionals. In particular we study how 1-body, 2-body and 3-body terms modify the molecular polarizabilities and how these effects are linked to the many-body decomposition of the total energy of the systems.

1This work was partially supported by DOE Award No. DE-FG02-09ER16052 and by DOE Early Career Award No. DE-SC0003871.
3:54PM Q16.00006 Van der Waals Coefficients between Clusters or Fullerenes: A Simple but Accurate Model beyond the Atom-Pair Interaction Picture1, JOHN P. PERDEW, ADRIENN RUZSINSZKY, Department of Physics, Temple U., JIANMIN TAO, Department of Chemistry, U. of Pennsylvania — The van der Waals coefficients of all orders between two spherical objects may be computed from the dynamical multipole polarizabilities of the two objects via the Casimir-Polder formula. We present an analytic model [1] for the dynamical polarizabilities that is exact for a classical conducting sphere or spherical shell, exact in the zero- and nearly-exact in the high-frequency limits, and generally accurate. From this model, we compute the low-order van der Waals coefficients for a variety of atom pairs and pairs of clusters or carbon-based fullerenes. We find that the lowest-order coefficient C6 per atom pair may increase or decrease strongly with cluster size, signaling a failure of the simplest version of the atom-pair interaction picture. [1] J. Tao and J.P. Perdew, J. Chem. Phys. 141, 141101 (Commun.) (2014).

4:06PM Q16.00007 Van der Waals’ corrected linear-scaling Density Functional Theory investigation of inner-surface functionalized inorganic nanotubes, JOSHUA ELLIOTT, GILBERTO TEOBALDI, Univ of Liverpool — We report a linear-scaling Density Functional Theory investigation of single-walled open-ended aluminosilicate nanotubes with inner metal functionalization (AlSiMe NTs). In line with the experimental pore-size distribution, optimization of the AlSiMe NT structure with six different semi-local and non-local van der Waals DFT functionals suggests the presence of a shallow energy minimum for NTs with 28 to 32 Al-atoms in the NT circumference, resulting in larger diameter than for aluminosilicate (AlSi) NTs. Analysis of the AlSiMe NTs electronic structure reveals the wall-polarization and real-space separation between Valence Band and Conduction Band, characteristic of AlSi NTs1. Regardless of the functional, the wall of the AlSiMe NTs are however found to be less polarized than AlSi NTs, with NTs of larger diameter being more polarized. We quantify the effect of the AlSiMe NTs wall-polarization and polarizability on the absolute alignment of the states for adsorbed H2O molecules inside and outside the tube-cavity. The simulations indicate shifts as large as 2 eV between the H2O-states for molecules adsorbed inside and outside the NT-cavity.

4:18PM Q16.00008 ABSTRACT WITHDRAWN —

4:30PM Q16.00009 Water Dissociation Mechanism in MOF-741, SEBASTIAN ZULUAGA, Wake Forest University, KUI TAN, University of Texas at Dallas, PIEMANUELE CANEPA, Wake Forest University, YVES CHABAL, University of Texas at Dallas, TIMO THON-HAUSEN, Wake Forest University — Water dissociation represents one of the most important reactions in catalysis, essential to surface and nano sciences. Combining in-situ IR spectroscopy and first-principles calculations, we demonstrate, for the first time, that water starts to dissociate at the metal centers of MOF-74 at temperatures as low as 150 °C. The fingerprint of this reaction is a sharp band in the IR spectrum at 970 cm−1 when D2O is introduced into the MOF. Surprisingly, this fingerprint is not detected with experiments with H2O. To explain this peculiar finding, we perform DFT simulations of the reaction, utilizing vdW-DF to capture the important van der Waals interactions. Our calculations show that, once the D2O molecule is adsorbed at the metal center, the D atom is transferred to the oxygen of the linker (phenolate group), producing the notable O-D absorption band at 970 cm−1, while the OD remains at the open metal sites. Even though we find that H2O undergoes an analogous dissociation reaction, the corresponding O-H mode is strongly coupled to MOF vibrations and cannot easily be detected by experiments. Overall, this work elucidates water interactions with cation-exposed surfaces and aids in the development of more efficient catalysts for water dissociation.

4:42PM Q16.00010 Distortion of a liquid crystal bulk by the Casimir torque, DAVID SOMERS, JEREMY MUNDAY, University of Maryland, College Park — We present an experimental method for measuring the Casimir torque acting on liquid crystals from a birefringent crystal. A liquid crystal bulk that is uniformly aligned at one surface is twisted at the other surface by a crystal such as barium titanate. The liquid crystal is separated from the solid crystal by an isotropic, transparent material such as SiO2. By varying the thickness of the deposited layer, we can observe the effect of retardation on the torque (which differentiates it from the close-range van der Waals torque) and compare experimental results to dispersion data of the materials. We find that a barium titanate slab could cause 5CB liquid crystal to rotate by 10 degrees through its bulk, even when separated by 35 nm of SiO2. The optical technique for measuring this distortion is also outlined.

4:54PM Q16.00011 Casimir-like Forces via Charge Fluctuations1, DAVID DROSDOFF2, University of South Florida, IGOR BONDAREV, North Carolina Central University, LILIA WOODS, University of South Florida — Fluctuations of observables give rise to different forces. Dipolar fluctuations have been studied extensively for a variety of systems as they give rise to Casimir-like forces with particular importance in biological systems. We show that such phenomena are also of relevance to capacitor systems especially when nanostructured materials are involved. We present a theory with a novel view of charge fluctuations induced interactions via the quantum capacitance concept. It is demonstrated that such Casimir-like forces can be important, especially in nanostructures. The theory is applied to nanoscale capacitors involving graphene and other characteristic materials.

5:06PM Q16.00012 Measurement of Casimir forces with nonmonotonic distance dependence between silicon structures with non-conventional shapes, LU TANG, JIE ZOU, HO BUN CHAN, The Hong Kong University of Science and Technology, MILOS NIKOLIC, ALEJANDRO RODRIGUEZ, Princeton University — We measure the Casimir force between silicon components of non-conventional shapes on a silicon-on-insulator wafer. The device consists of a force-sensing micromechanical beam and a comb-drive actuator for controlling the distance. The magneto-motive technique is used to measure the shift in the resonance frequency of the force sensing beam. Each of the interacting surfaces contains an array of T-shaped protusions. Since the protusions on both sides are created by lithography and reactive ion etching, both their shapes and relative positions can be accurately defined. Here, the protusions on the two surfaces are offset by half the period. As the movable electrode is pushed towards the silicon beam by the comb drives, the two sets of protusions inter-penetrates. The lateral Casimir force between the top parts of the T-shaped structures produces in an overall interaction that is either apparently attractive or repulsive depending on the displacement of the comb actuators. The measured non-monotonic dependence of the Casimir force on distance is in qualitative agreement with preliminary calculations using the boundary elements method.
2:30PM Q17.00001 Conductivity noise as a transport-based probe to study the charge-carrier transmission across grain boundaries in polycrystalline graphene

VIDYA KOCHAT, Dept. of Physics, IISc, India, CHANDRA SEKHAR TIWARY, Dept. of Materials Engineering, IISc, India, TATHAGATA BISWAS, Dept. of Physics, IISc, India, GOPALAKRISHNAN RAMALINGAM, Materials Research Centre, IISc, India, SRINIVASAN RAGHAVAN, Materials Research Centre, Centre for Nano Science and Engineering, IISc, India, KAMANIO CHATTOPADHYAY, Dept. of Materials Engineering, IISc, India, MANISH JAIN, ARINDAM GHOSH, Dept. of Physics, IISc, India — Grain boundaries (GBs) form a class of topological defects, intrinsically present in polycrystalline graphene films and inevitably affect the electronic properties of the otherwise perfect honeycomb lattice. In this work, we have studied the charge carrier transmission across individual GBs in graphene having varying levels of disorder. We find that the defect density in the interface region of two adjoining graphene grains is directly related to their misorientation angle. Conductivity noise (low frequency 1/f noise) is a more sensitive probe to identify the microscopic mechanism of carrier scattering and can quantify the disorder levels of various types of GBs. The 1/f noise across wider interfaces were found to be higher by an order of magnitude when compared to the single-crystalline graphene regions, indicating huge amount of disorder at the interface region. We also obtain evidence for enhanced spin-flip scattering at the GBs from the measured conductivity noise at low temperatures suggestive of the fact that the GBs in graphene could sustain local magnetic moments.

2:42PM Q17.00002 Intrinsic carrier mobility of Dirac cones: limitations of the deformation potential theory

ZHENZHU LI, JINYING WANG, ZHIRONG LIU, Peking Univ — An analytic formula for the intrinsic carrier mobility of Dirac cones under acoustic phonon scattering mechanism was obtained for 2D systems such as graphene and graphyne. The influence of both transverse acoustic (TA) and longitudinal acoustic (LA) phonon modes as well as the anisotropy were considered. Some extraordinary characteristics different from the prediction of the deformation potential theory were revealed: the mobility at the neutrality point is proportional to $1/T^3$ where $T$ is the temperature; carrier scattering by TA phonons dominates the mobility of graphene, which explains the overestimated measured deformation potential of graphene in experiments. The theory was combined with first-principles calculation to determine the mobility of graphene and five graphynes with Dirac cones. It was predicted that most graphynes possess much higher mobility than graphene due to the suppression of the scattering by TA phonons.

2:54PM Q17.00003 Dephasing time in graphene due to interaction with flexural phonons

WELIZHAO, KONSTANTIN TIKHONOV, ALEXANDER FINKEL’STEIN, Texas A&M Univ — We investigate decoherence of an electron in graphene caused by electron-flexural phonon interaction. We find out that the flexural phonons can produce dephasing rate comparable to the electron-electron one. The problem appears to be quite special because there is a large interval of temperatures where dephasing rate cannot be obtained using the golden rule. We evaluate this rate for a wide range of density ($n$) and temperature ($T$) and determine several asymptotic regions with temperature dependence crossing over from $\tau_\phi^{-1} \sim T^2$ to $\tau_\phi^{-1} \sim T$ when temperature increases. We also find $\tau_\phi^{-1}$ to be a non-monotonic function of $n$. These distinctive features of the new contribution can provide an effective way to identify flexural phonons in graphene through the electronic transport by measuring the weak localization corrections in magnetoresistance.

3:06PM Q17.00004 ABSTRACT WITHDRAWN

3:18PM Q17.00005 Multi-Band Electron Tunneling Effects in Bilayer and Gapped Graphene

DIPENDRA DAHAL, Hunter College, CUNY, GODFREY GUMBS, Hunter College, CUNY and Donostia International Physics Center (DIPC), ANDRII IUROV, University of New Mexico and Hunter College, CUNY — A detailed study has been made of electron tunneling through a square potential barrier in bilayer, gapped graphene and the relatively new material silicone. The investigation has covered dressed electron states by circularly polarized light of electrons in bilayer graphene for various angles of incidence and through a periodic sequence of potential barriers as well as a quasiperiodic arrangement. The spin degenerate states of silicone may be lifted by a perpendicular electric field. We report spin-dependent tunneling in silicone.

3:30PM Q17.00006 Violation of the Wiedemann-Franz law in clean graphene layers

ALESSANDRO PRINCIPI, GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA — The Wiedemann-Franz law, connecting the electronic thermal conductivity to the electronic conductivity of a disordered metal, is generally found to be well satisfied even when electron-electron ($e-e$) interactions are strong. In ultra-clean conductors, however, large deviations from the standard form of the law are expected, due to the fact that $e-e$ interactions affect the two conductivities in radically different ways. Thus, the standard Wiedemann-Franz ratio between the thermal and the electric conductivity is reduced by a factor $1 + \tau/\tau_{1h}^e$, where $1/\tau$ is the momentum relaxation rate, and $1/\tau_{1h}^e$ is the relaxation time of the thermal current due to $e-e$ collisions. Here we study the density and temperature dependence of $1/\tau_{1h}^e$ in the important case of doped, clean single layers of graphene, which exhibit record-high thermal conductivities. We show that at low temperature $1/\tau_{1h}^e$ is $8/5$ of the quasiparticle decay rate. We also show that the many-body renormalization of the thermal Drude weight coincides with that of the Fermi velocity.

This work was supported in part by DOE grant DE-FG02-05ER46203 and by a Research Board Grant at the University of Missouri.

3:42PM Q17.00007 Dilute fluorinated graphene and bilayer graphene: resonant impurity scattering, anomalous magneto-transport and local spin-orbit coupling

J. ZHU, X. HONG, A. STABILE, C. HERDING, S.-H. CHENG, K. ZOU, B. WANG, J. LI, Penn State University — Graphene is a high-mobility semi-metal with weak spin-orbit coupling (SOC). I will discuss the striking effects of a dilute coverage of chemisorbed fluorine adatoms ($F < 0.1\%$) on charge transport and magneto-transport of graphene and bilayer graphene. We show that electron scattering with the F-adatoms can be quantitatively described by resonant impurity scattering. The $T$-dependence of conductivity reveals strong quantum corrections not yet understood, which differs qualitatively between F-monolayer and F-bilayer. Both F-monolayer and F-bilayer exhibit weak localization in a magnetic field. The dephasing rate $\tau_\phi^{-1}$ is dramatically enhanced in fluorined samples, compared to pristine and defluorinated control samples. It is further tunable by a perpendicular electric field in dual-gated F-bilayer devices. Strikingly, the ratio of $\tau_\phi^{-1}$ over the transport relaxation rate $\tau_\tau^{-1}$ is independent of $n_F$ and scales with the carrier density $n$ as $n^{-1/2}$ in both F-monolayer and F-bilayer. Strong local SOC induced by the F-adatoms, combined with the unusual effect of SOC on the magneto-resistance of WL, is likely to play a key role. Fluorine induced SOC has important implications on spin relaxation and spin Hall current in these engineered materials.
Scattering of two-dimensional massless Dirac electrons in a circular potential barrier. JHJH-JHENG WU, MICHAEL FOGLER, University of California, San Diego — We calculate the differential, total, and transport cross-sections for scattering of two-dimensional massless Dirac electrons in a circular barrier. For scatterer of a small radius, the cross-sections are dominated by quantum effects such as resonant scattering that can be computed using the partial-wave series. Scattering by larger size barriers is better described within the classical picture of reflection and refraction of rays, which leads to phenomena of caustics, rainbow, and critical scattering. Refraction can be negative if the potential of the scatterer is repulsive, so that a p-n junction forms at its boundary. Qualitative differences of this case from the n-N doping case are examined. Quantum interference effects beyond the classical ray picture are also considered, such as normal and anomalous diffraction, and also whispering-gallery resonances. Implications of these results for transport and scanned-probe experiments in graphene and topological insulators are discussed.

Phonon coupling and disorder induce infrared optical transparency in graphene. BRUNO ROUSSEAU, Université de Montréal, FRANÇOIS LAROYONTE, Fritz-Haber-Institut der Max-Planck-Gesellschaft, MICHEL CÔTÉ, RICHARD MARTEL, Université de Montréal — Recent infrared spectroscopy measurements of doped graphene grafted with iodophenyl moieties have revealed fairly narrow transmission windows which vary as a function of the chemical potential, in contrast to the featureless, Drude-like spectrum of pristine graphene in this frequency range. These asymmetric features appear at energies corresponding to phonon modes near the Γ and K points. We propose a model which involves coherent inelastic scattering with defects and phonons, thus relaxing the optical selection rule forbidden access to q ≫ Γ phonons. Numerical simulations based on the model reproduce the features of the experimental observations (number of bands, energies, variation in energy and intensity with respect to chemical potential).

Electron transmission through the stacking domain boundary on multilayer graphene. NAM NGUYEN, MIKITO KOSHINO, Tohoku Univ — We present a theoretical study on the electron transmission through the AB-BA stacking boundary in bilayer trilayer and tetrallyer graphene. Using the Green function method, we calculate the electron transmission probability through the stacking faults as the Fermi energy. In AB-BA bilayer boundary, the system is almost insulating at the low energy, while the transmission sharply rises as the Fermi energy increases to higher energy. This suggests that the stacking fault crucially suppresses the electron transmission in the intrinsic graphene bilayer at the charge neutral. We also study the effect of the perpendicular electric field which opens an energy gap, and find that the gap-opening and the Mexican-hat band deformation significantly enhance the electron transmission at the low-electron density. For the ABA-ABC domain boundary in trilayer graphene, we notice a similar behavior of electron transmission to the bilayer case, but in the tetralayer case (ABAB-ABAC boundary), the low-energy transmission is not much suppressed unlike in bilayer and trilayer cases.

Inelastic carrier lifetime in a coupled graphene electron-phonon system: Role of plasmon-phonon coupling. HONGKI MIN, SEONGJIN AHN, Department of Physics and Astronomy and Center for Theoretical Physics, Seoul National University, E.H. HWANG, SKKU Advanced Institute of Nanotechnology and Department of Physics, Sungkyunkwan University — We calculate the inelastic scattering rates and the hot electron inelastic mean free paths for both monolayer and bilayer graphene on a polar substrate. We study the quasiparticle self-energy by taking into account both electron-electron and electron-surface optical (SO) phonon interactions. In this calculation the leading order dynamic screening approximation (G0W approximation) is used to obtain the quasiparticle self-energy by treating electrons and phonons on an equal footing. We find that the strong coupling between the SO phonon and plasmon leads to a new decay channel for the quasiparticle through the emission of the coupled mode, and gives rise to an abrupt increase in the scattering rate, which is absent in the uncoupled system. In monolayer graphene a single jump in the scattering rate occurs, arising from the emission of the low energy branch of the coupled plasmon-phonon modes. In bilayer graphene the emission of both low and high energy branches of the coupled modes contributes to the scattering rate and gives rise to two abrupt changes in the scattering rate. The jumps in the scattering rate can be potentially used in the hot electron device such as switching devices and oscillators. Ref) Seongjin Ahn, E. H. Hwang, and Hongki Min, arXiv:1409.8394.

Conductivity and thermoelectric power in graphene: Interplay of disorder, Coulomb interaction, and optical phonons. MATTHEW FOSTER, HONG-YI XIE, Rice University — We study the electric and thermoelectric transport of Dirac fermions in graphene using the Boltzmann-equation approach. We consider the effects of quenched disorder, Coulomb interactions, and optical-phonon scattering and analyze the electric conductivity and the thermoelectric power (TEP) as functions of temperature T and chemical potential μ by unbiased numerical solutions to the Boltzmann equation. In the absence of optical phonons, for very clean graphene we observe the crossover from the interaction-limited hydrodynamic regime μ ≪ T to the disorder-limited Fermi liquid regime μ ≫ T. In the hydrodynamic regime, the TEP significantly deviates from Mott’s law and follows the result anticipated by the relativistic hydrodynamic theory. Moreover, we analyze the doping and screening effects upon the quantum minimal conductance, which indicates the dissipation induced by inelastic electron-hole scattering. On the other hand, we find that optical phonons start to contribute at relatively low temperatures, about one order of magnitude less than the phonon excitation energy. Especially, the TEP shows a non-monotonic temperature dependence and a peak appears at about T ≈ 200-300 K for a large variety of doping.

Temperature and bias dependence of barrier heights in graphene / semiconductor Schottky diodes under reverse bias. DUSHYANT TOMER, SHIVANI RAJPUT, LAWRENCE HUDY, LIAN LI, Univ of Wisconsin, Milwaukee — Sensors based on graphene / semiconductor Schottky diodes have shown significant enhancement in sensitivity over field effect devices when operated under reverse bias, where the conductivity has an exponential dependence on the Schottky barrier height. In this work, chemical vapor deposited monolayer graphene is transferred onto Si- and C-face of hexagonal SiC, Si(111), and GaAs001 substrates, as confirmed by scanning tunneling microscopy. Temperature and bias dependence of the barrier height are obtained by current-voltage measurements between 250 and 340 K. For all four junctions, the barrier increases linearly with temperature. However, as a function of reverse bias, it decreases linearly for graphene / SiC, but exhibits a non-linear dependence for graphene / (Si, GaAs) Schottky junctions. These findings and their implication on the performance of sensors based on graphene / semiconductor Schottky diodes will be discussed at the meeting. Supported by U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-07ER46228.
5:18PM Q17.00015 Screening of substrate charged impurities as mechanism of conductance change in graphene gas sensing

Sang-Zi Liang, Pennsylvania State University, Gugang Chen, Avetik Harutyunyan, Honda Research Institute USA Inc., Jorge Sofo, Pennsylvania State University — In graphene sensing of gaseous NO, NO₂, and NH₃, the measured conductance change after the sensor is exposed to the molecules has been traditionally attributed to carrier density change due to charge transfer between the sample and the adsorbed molecule. However, this explanation ignores the effect of the adsorbates on the electron mobility, and analysis of the electron affinity/ionization potential does not favor charge transfer. In this talk, we propose and explore an alternative mechanism. When adsorbed, charged and dipolar functional on the surface of graphene may counteract and screen charged impurities on the substrate. Because scattering of electrons with these charged impurities has been shown to be a limiting factor in graphene conductivity, the screening leads to significant changes in the transport behavior. A model for the conductivity is established using the random phase approximation dielectric function of graphene and the first-order Born approximation for scattering. The model predicts maximal screening magnitudes for the charge and dipole moment. The dipole screening is generally weaker than the charge screening although the former becomes more effective with higher gate voltage.

1This work is supported by Honda Research Institute USA, Inc.

Wednesday, March 4, 2015 2:30PM - 5:30PM

Session Q18 DFD GSOFT: Invited Session: Recent Advances in Field-Responsive Fluids and Suspensions

Mission Room 103A - Rongjia Tao, Temple University

2:30PM Q18.00001 Complex magnetic fields breathe life into fluids. James Martin, Sandia National Laboratories — There are many areas of science and technology where being able to generate vigorous, noncontact flow would be desirable. We have discovered that three dimensional, time-dependent electric or magnetic fields having key symmetries can be used to generate controlled fluid motion by the continuous injection of energy [1-8]. Unlike natural convection, this approach does not require a thermal gradient as an energy source, nor does it require gravity, so space applications are feasible. The result is a highly active material we call a vortex fluid. The homogeneous torque density of this fluid enables it to climb walls, induce ballistic droplet motion, mix vigorously, even in such complex geometries as porous media, and effect highly efficient heat transfer. This vortex fluid can also exhibit a negative viscosity, which can immeasurably extend the control range of the “smart fluids” used in electro- and magnetorheological devices and can thus significantly increase their performance. Because the applied fields are uniform and moderate in strength, vortex fluids of any scale can be created, making applications of any size, from direct microdroplet motion to controlling damping in magneto-rheological dampers that protect bridges and buildings from earthquakes, feasible. Finally, we will demonstrate that such fields can animate fluids in remarkable ways that resemble living systems.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.


3:06PM Q18.00002 Suppressing turbulence and enhancing the liquid suspension flows in pipelines with electrorheology

Rongjia Tao, Temple University — Flows through pipes, such as crude oil through pipeline, are the most common and important transportation of fluids. To enhance the flow output along the pipeline requires reducing viscosity and suppressing turbulence simultaneously and effectively. Unfortunately, no method is currently available to accomplish both goals simultaneously. The talk will show that electrorheology (ER) provides an efficient solution. When a strong electric field is applied along the flow direction in a small section of pipeline, the field polarizes and aggregates the particles suspended inside the base liquid into short chains along the flow direction. Such aggregation breaks the rotational symmetry and makes the fluid viscosity anisotropic. Along the flow direction, the viscosity is significantly reduced; thus the flow along the pipeline is enhanced. In the directions perpendicular to the flow, the viscosity is substantially increased, effectively suppressing the turbulence. Recent field tests with crude oil pipeline have confirmed that this new technology works very well. For untreated crude oil, the flow inside the pipeline is turbulent as the Reynolds number exceeds 2300. However, for ER treated oil, the flow remains laminar even when the Reynolds number reaches 6000. The combination of the viscosity reduction along the flow direction and the turbulence suppression greatly saves the energy required to transport crude oil. In addition, both effects have found lasting more than 11 hours inside the pipeline after one ER treatment. No additive is needed. The process is repeatable. As turbulence is classified as one of the most important unsolved classical physics, this development is not only important for technology applications, but significant for basic physics as well.

1This work is supported in part by STWA and Pipeline Research Council International.
2Dept of Physics, Temple Univ, Philadelphia, PA 19122

3:42PM Q18.00003 ER fluid in microfluidic Systems

Weijia Wen, The Hong Kong University of Science and Technology — Electrorheological (ER) fluid is considered as a kind of smart material which is able to be used for microfluidic systems to achieve active and precise control of fluid by electrical signal. While, microfluidics, especially droplet microfluidic, attracts much attention recently from diverse research fields due to its highly integration, digitalization and computercontrolled characteristics. Here, we will introduce our recent experimental results of ER fluid-based microfluidic droplet generation and manipulation. Two methodologies by employing ER fluid into microfluidic system: digital generation, manipulation of “smart droplets” and droplet manipulation by ER fluid will be presented. Once it is combined with real-time detection, electrorheologically integrated chip with many functions can be realized. Some other applications of using GER fluid in microfluidic chips, such as the microfluidic logic gates, are also introduced. Some potential application of ER fluid for hydraulic system will be also introduced.

4:18PM Q18.00004 Magnetorheological fluids in occupant protection systems

Norman Wereley, University of Maryland — No abstract available.
4:54PM Q18.00005 MR effect enhancement of bidisperse MR fluids containing micron- and nano-sized iron particles, MASAMI NAKANO, Institute of Fluid Science, Tohoku University — Magnetorheological (MR) fluids are suspensions of micron-sized magnetic particles dispersed into carrier oils and behave like a Bingham fluid having magnetic-field responsive yield stress. In this research, bidisperse MR suspensions containing micron- (6.6 mm) and nano- (110nm) sized spherical iron particles into silicone oil were fabricated to enhance the MR effects. The steady and dynamic MR properties have been investigated in close relation to the magnetic-induced particle cluster structure and the visualized shear flow behaviors. The static and dynamic behaviors of the particle cluster structures formed in the MR fluids under applied magnetic fields were directly visualized using an optical microscope. And the steady and dynamic MR properties of the bidisperse MR fluids were measured using a magnetic field applicable parallel-disk rheometer. The MR effects of the bidisperse MR fluids changed significantly as a function of the solid fraction of nano-particles. Interestingly, field-induced shear stress was remarkably enhanced at higher shear rate when the solid fraction of nano-particles was around 25%. The enhancement of the shear stress can be attributed to the formation of distinct and wide particle cluster chains.

Wednesday, March 4, 2015 2:30PM - 5:30PM –
Session Q19 FLAP: Invited Session: Industry Day: Rheology and Processing for Additive Manufacturing Mission Room 103B - Tirtha Chatterjee, The Dow Chemical Company

2:30PM Q19.00001 Polymer Physics as a Key to Advanced Manufacturing at Dow, FLORIAN SCHATTENMANN, The Dow Chemical Company — Dow combines the power of science and technology to passionately innovate what is essential to human progress. The Company is driving innovations that extract value from the intersection of chemistry, physical and biological sciences to help address many of the world’s most challenging problems such as the need for clean water, clean energy generation and conservation, and increasing agricultural productivity. Dow’s integrated, market-driven, industry-leading portfolio of specialty chemical, advanced materials, agrosciences and plastics businesses delivers a broad range of technologies, services and solutions across high-growth sectors such as packaging, electronics, water, coatings and agriculture. In 2013, Dow had annual sales of more than $57 billion with more than 6,000 products manufactured at 201 sites in 36 countries across the globe. Given the large scale of Dow’s manufacturing footprint and broad range of industries, markets and applications Dow serves, a wide range of advanced manufacturing technologies are being developed. The presentation will give an overview of select manufacturing technologies and how polymer physics, modelling, analytical techniques and experimental validation are being employed to drive world leading innovation. We will discuss examples from several product technologies including composites, adhesives and polymers synthesis.

3:06PM Q19.00002 New insights on cellulosic ether hydrogels, ROBERT SAMMILER, The Dow Chemical Company — Aqueous hydroxypropylmethylcellulose materials (HPMC) often have much lower hot gel moduli (<10 Pa) relative to those (3,000 Pa) of aqueous methylcellulose materials (MC) at end-use conditions (<2 wt.%, 90 °C), and these lower moduli limit their use in applications. The origin of their lower moduli is suspected to arise from the order of two thermal transitions when warming. One transition, thought to involve a chain conformation transition, is referred to here as chain collapse. Another, thought to involve the self-assembly of chains into a three-dimensional physical network, is referred to as gelation. Often, chain collapse is thought to proceed gelation when slowly warming aqueous commercial HPMC materials from 5 to 90 °C at 1 °C/min, while the opposite order is thought to occur for many aqueous commercial MC materials. Chain collapse is identified as a sharp drop in the solution viscosity at pre-gel temperatures as T increases. The insensitivity of the chain collapse temperature to HPMC concentration is used to argue that this thermal event is distinct from gelation. These concepts are supported with the preparation of two developmental HPMC materials with similar MW and substitution levels (DS and MS). One HPMC material, prepared by a unique process, is designed to reverse order of the thermal transitions. This HPMC material is found to exhibit high hot gel moduli similar to those of aqueous MC materials; moreover, its gel is able to form syneresis fluid as it contracts in size when warmed. The gel contraction is thought to be a manifestation of chain collapse.

3:42PM Q19.00003 Particle laden interfaces and dispersions: Enabling high performance and multifunctional materials, RAVI SHARMA, Cabot Corporation — Particles at interfaces are finding increasing use in Pickering emulsions due to their superior stability compared to surfactant-stabilized emulsions. In this presentation we present an overview of particle laden interfaces and particle concepts for development of high performance materials, some of which could be used to address current materials problems in additive manufacturing.

4:18PM Q19.00004 Modifying polymer rheology by using nanofillers: applications in additive manufacturing, DILIP GERSAPPE, Stony Brook University — The ability to control the flow properties of polymers is critical to developing materials that can be used for additive manufacturing. The use of nanofillers in polymer matrices can significantly affect the rheological properties of the flow and rheological properties. We use Molecular Dynamics simulations to examine the role nanofillers have on polymer melts and polymer blends. In homopolymer systems, our results indicate that above a critical concentration of filler particles, the network structure formed between the fillers and the polymers strongly affects the dynamics of the nanocomposite under shear. However, we also find that low concentrations of filler particles leads to a large increase in chain orientation (relative to the pure polymer case) when shear is applied. Our results indicate that the ability of fillers to maintain the network during shear in the enhancement of the shear thinning effect at high concentrations of filler particles, while the ability to maintain high degrees of orientation in polymer chains results in shear thinning being present even at lower concentrations of fillers. In particle blends, we show that the nanofillers can reduce the slip at the interface between the two components. We also examine the role of the aspect ratio of the nanofiller on the rheological properties of polymer nanocomposites.

4:54PM Q19.00005 Rheology and Flow-Induced Crystallization of Polyolefins, ANTONIOS DOUFAS, Exxonmobil Chemical Research and Development — This talk will give an overview of melt rheology in shear and extensional flow kinematics as well as flow-induced crystallization (FIC) behavior of polyolefin systems relevant to polymer processing. Examples for both polypropylene (PP) and polyethylene (PE) systems will be discussed. The effect of shear on FIC of several PP resins of various microstructures is studied using parallel-plate and capillary rheometry. Generally, an increase in strain and strain rate to increase of temperature is found to decrease the thermodynamic barrier for crystal formation enhancing the crystallization kinetics at temperatures between the melting and crystallization points. FIC kinetics were enhanced with increased PP molecular weight indicating the importance of the high-end tail of the MWD on FIC. Various dies of different contraction angle and different length-to-diameter (L/D) ratios were used to investigate the effect of flow (mainly extensional kinematics in die entrance) on FIC. Extensional strain is found to be a key parameter influencing FIC. The effect of different molecular structures (from linear to long chain branched) on melt rheology and FIC response of several PE systems will be discussed. The melt rheology and FIC characteristics of thermoplastic materials are important for their processability performance in conventional and advanced fabrication processes such as Additive Manufacturing.

Wednesday, March 4, 2015 2:30PM - 5:30PM –
Session Q20 DMP: Focus Session: Superconductivity in the 2D Limit II Ballroom B - Hanno Wieringa, University of Tennessee, Knoxville
2:30PM Q20.00010 Remarkable effects of disorder on superconductivity of single atomic layers of lead on silicon\(^1\), CHRISTOPHE BRUN, Sorbonne Universit\'es, UPMC Univ Paris 06 et CNRS, UMR 7588, Institut des Nanosciences de Paris, F-75005, Paris, France — It is well known that conventional superconductivity is very robust against non-magnetic disorder \([1]\). Nevertheless for thin and ultrathin films the structural properties play a major role in determining the superconducting properties, through a subtle interplay between disorder and Coulomb interactions \([2]\). Unexpectedly, in 2010 superconductivity was discovered in single atomic layers of lead and indium grown on silicon substrate using scanning tunneling microscopy \([3]\) and confirmed later on by macroscopic transport measurements \([4]\). Such well-controlled and tunable crystalline monolayers are ideal systems for studying the influence of various kinds of structural defects on the superconducting properties at the atomic and mesoscopic scale. In particular, Pb monolayers offer the opportunity of probing new effects of disorder because not only superconductivity is 2D but also the electronic wave functions are 2D. Our study of two Pb monolayers of different crystal structures by very-low temperature STM (300 mK) under magnetic field reveals unexpected results involving new spatial spectroscopic variations \([5]\). Our results show that although the sheet resistance of the Pb monolayers is much below the resistance quantum, strong non-BCS corrections appear leading to peak heights fluctuations in the dI/dV tunneling spectra at a spatial scale much smaller than the superconducting coherence length. Furthermore, strong local evidence of the signature of Rashba effect on the superconductivity of the Pb/Si(111) monolayer is revealed following filling of in gap states and local spatial variations of this filling. Finally the nature of vortices in a monolayer is found to be very sensitive to the properties of step edges areas.

\[\begin{align*}
\text{[1]} & \quad \text{P.W. Anderson, J. Phys. Chem. Solids 11, 26 (1959)} \\
\text{[2]} & \quad \text{M.V. Feigel’man et al. Ann. Phys. 325, 1390 (2010)} \\
\text{[3]} & \quad \text{T. Zhang et al. Nature Materials 6, 104 (2010)} \\
\text{[4]} & \quad \text{Y. Yamada et al. Phys. Rev. Lett. 110, 237001 (2013)} \\
\text{[5]} & \quad \text{C. Brun et al. Nature Physics 44, 10 (2014)}
\end{align*}\]

1This work was supported by University Pierre et Marie Curie UPMC ‘Emergence’ project, French ANR Project ‘ElectroVortex,’ ANR-QuDec and Templeton Foundation (40081), ARO (W911NF-13-1-0431) and CNRS PICS funds. Partial funding by US-DOE grant DE-AC02-07CH1

3:06PM Q20.00002 Josephson Vortex in Indium Monatomic Superconductor on Silicon Terraces\(^1\), TAKUTO KAWAKAMI, International Center for Materials Nanoarchitectonics, National Institute for Materials Science, YUKI NAGAI, CCSE, Japan Atomic Energy Agency, SHUNSUKE YOHIZAWA, International Center for Materials Nanoarchitectonics, National Institute for Materials Science, HOWON KIM, The Institute for Solid State Physics, University of Tokyo, TOMONOBU NAKAYAMA, International Center for Materials Nanoarchitectonics, National Institute for Materials Science, YUKIO HASEGAWA, The Institute for Solid State Physics, University of Tokyo, TAKASHI UCHIHASHI, XIANG HU, International Center for Materials Nanoarchitectonics, National Institute for Materials Science — Superconductivity in Indium monatomic layer on a surface of Silicon substrate is intriguing where the terraces and steps exist. Recently, elliptic vortices trapped at steps have been observed by STM/STS measurement under magnetic field \([1]\). Motivated by this experiment, we clarify the quasiparticle excitation by using Bogoliubov-de Gennes approach \([2]\). The current distribution and zero energy density of states at vortex core show elliptic shape with longer axis parallel to the step. Moreover, the order parameter is restored at the vortex core. By comparing theoretical results with experiments, we conclude that the recent STS measurement has directly detected Josephson vortex. \([1]\) S. Yoshizawa, et al., Phys. Rev. Lett. (in press, arXiv:1405.5953). \([2]\) T. Kawakami, et al., J. Phys.: Conf. Ser. (in press).

1This work is supported by WPI Initiative on Materials Nanoarchitectonics, MEXT, Japan.

3:18PM Q20.00003 High temperature superconductivity in one unit cell FeSe and superconductivity in two-monolayer Ga\(^1\), JIAN WANG, Peking University — By direct transport and magnetic measurements, we provide definitive evidence for high temperature superconductivity in the 1-UC FeSe films on insulating STO substrates with the onset Tc and critical current density much higher than those for bulk FeSe. In addition, by both in situ scanning tunneling microscopy/spectroscopy and ex situ transport and magnetization measurements, we find that the two-atomic-layer Ga film with hexagonal structure on wide band-gap semiconductor GaN is superconducting with Tc up to 5.4 K.

1This work was financially supported by the National Basic Research Program of China

3:30PM Q20.00004 Ballistic superconductivity in high mobility two dimensional electron gas in GaAs heterostructures, ZHONG WANG, ALEKSANDR KAZAKOV, MICHAEL MANFRA, Purdue univ, LOREN PFEIFFER, KEN WEST, Princeton Univ, LEONID ROKHINSON, Purdue.edu — Introduction of a Josephson field effect transistor (JFET) concept sparked active research on proximity effects in semiconductors. Induced superconductivity and electrostatic control of critical current has been demonstrated in two-dimensional gases in InAs, graphene, and top of thical monolayer, but Coulomb repulsion acts as superconductivity friend rather than a foe. Such repulsion-to-attraction transmutation allows to access strong-coupling superconductivity regime even when intrinsic pairing interaction is weak. We analyze pairing interaction in 2DC crystals placed atop a highly polarizable dielectric with dispersive permittivity \(\varepsilon(\omega)\) and predict that by optimizing system parameters a substantial enhancement can be achieved. We also argue that the SCC mechanism can be responsible, at least in part, for 100 K superconductivity recently observed in FeSe monolayers grown on SrTiO\(_3\) substrate, with \(T_c\) more than 10 times larger than in bulk 3D FeSe crystals, arxiv:1406.3435.

4:18PM Q20.00006 Synthetic Superconductivity in Single-Layer Crystals, LEONID LEVITOV, DAN BORG-NIA, PATRICK LEE, Massachusetts Inst of Tech-MIT — Electronic states in atomically thin 2D crystals are fully exposed and can couple to extrinsic degrees of freedom via long-range Coulomb interactions. Novel many-body effects in such systems can be engineered by embedding them in a polar environment. Superconducting pairing interaction induced in this way can enhance the intrinsic electron-phonon pairing mechanism. We take on this notion, which was around since the 60’s ("excitonic superconductivity"), and consider synthetic superconductivity (SSC) induced in 2D crystals by a polar environment. One intriguing aspect of this scenario is that Coulomb repulsion acts as superconductivity friend rather than a foe. Such repulsion-to-attraction transmutation allows to access strong-coupling superconductivity regime even when intrinsic pairing interaction is weak. We analyze pairing interaction in 2DC crystals placed atop a highly polarizable dielectric with dispersive permittivity \(\varepsilon(\omega)\) and predict that by optimizing system parameters a substantial enhancement can be achieved. We also argue that the SCC mechanism can be responsible, at least in part, for 100 K superconductivity recently observed in FeSe monolayers grown on SrTiO\(_3\) substrate, with \(T_c\) more than 10 times larger than in bulk 3D FeSe crystals, arxiv:1406.3435.
4:30PM Q20.00007 The Meissner and Mesoscopic Superconducting States in the Ultrathin FeSe-Films, L. Z. DENG, B. LV, Z. WU, Y. Y. XUE, Texas Center for Superconductivity at the University of Houston, W. H. ZHANG, F. H. LI, Department of Physics, Tsinghua University, Beijing, L. L. WANG, X. C. MA, Institute of Physics, Chinese Academy of Sciences, Beijing, Q. K. XUE, Department of Physics, Tsinghua University, Beijing, C. W. CHU, Texas Center for Superconductivity at the University of Houston; Lawrence Berkeley National Laboratory, Berkeley, California — We carried out a detailed investigation on the superconductivity in eight 1-4 unit-cell FeSe-films on SrTiO3(STO) substrates by measuring their magnetization and resistivity in a field between 5E2 and 7E4 Oe over the last one and half years as a function of temperature and frequency, from 2 to 300 K and 0 to 1.5 kHz, respectively. Systematic aging effect for these samples was also well studied. The results show that samples display a complex superconducting structure, i.e. a Meissner state but populated with weak-links below 20 K, and an unusual superconducting mesostructure up to 45 K. A model is proposed to account for such a superconducting mesoscopic structure, similar to the Andreev reflection between the normal and superconducting carriers. Above 45 K, collective glass-like excitations are evident although their nature is yet to be determined.

4:42PM Q20.00008 ABSTRACT WITHDRAWN

4:54PM Q20.00009 ABSTRACT WITHDRAWN

5:06PM Q20.00010 Superconductivity in a two-dimensional repulsive Rashba gas at low density, LUYANG WANG, HONG YAO, Institute for Advanced Study, Tsinghua University — We study the superconducting instability and the resulting superconducting states in a two-dimensional repulsive Fermi gas with Rashba spin-orbit coupling at low electron density. We find that the superconductivity is enhanced as the Fermi energy $E_F$ decreases, due to two reasons: first, the density of states at $E_F$ increases as $1/\sqrt{E_F}$; second, the particle-hole bubble gains a more significant structure, resulting in an increasing effective attraction. The superconducting state is always in the total angular momentum $j_z = \pm 2$-channel, and breaks time-reversal symmetry. Once a sufficiently large Zeeman coupling is applied to the superconducting state, the spectrum Chern number becomes $\pm 1$, depending on the direction of the Zeeman field, and Majorana zero modes appear in the vortex cores. Collective modes in this superconducting state are also studied.

5:18PM Q20.00011 Metallic ground state in an ion-gated two-dimensional superconductor, YOSHIHOJI IWASA, Quantum-Phase Electronics Center (QPEC) and Department of Applied Physics, The University of Tokyo, Japan, YU SAIITO, QPEC and Department of Applied Physics, The University of Tokyo, Japan, YUICHI KASAHARA, Department of Physics, Kyoto University, Japan, JIANTING YE, Zernike Institute for Advanced Materials, University of Groningen, The Netherlands, TSUTOMU NOJIMA, Institute for Materials Research, Tohoku University, Japan — Ever since a discovery of insulator-superconductor transition in metallic thin films, the ground state of clean two-dimensional (2D) superconductors has been a long standing fundamental question. Recently emerging electric double layer transistors enabled researchers to realize electric-field-induced superconductivity in various substances, which provides us with new opportunities to investigate the ground state of 2D superconductivity. In this presentation, we report that the majority of the field-temperature phase diagram of electric-field-induced superconductivity in ZrNCl including $T = 0$ K is occupied by a metallic state with finite resistance due to the quantum tunneling of isolated vortices and flux flow caused by extreme two-dimensionality and weak pinning potential. These results imply that electric-field-induced superconductivity can be an ideal platform for accessing quantum vortex states in clean 2D superconductors.

Wednesday, March 4, 2015 2:30PM - 5:18PM — Session Q21 DCMP: Metal Insulator Transitions 201 - Dragana Popovic, National High Magnetic Field Laboratory

2:30PM Q21.00001 ABSTRACT WITHDRAWN

2:42PM Q21.00002 An apparent metal insulator transition in high mobility 2D InAs heterostructures, JAYAD SHABANI, CHRIS PALMSTROM, University of California, Santa Barbara — We report on the first experimental observation of an apparent metal insulator transition in a 2D electron gas confined in an InAs quantum well. At high densities we find that the carrier mobility is limited by background charged impurities and the temperature dependence of the resistivity shows a metallic behavior with resistivity increasing with increasing temperature. At low densities we find an insulating behavior below a critical density of $n_c = 5 \times 10^{15}$ cm$^{-2}$ with the resistivity decreasing with increasing temperature. We analyze this transition using a percolation model arising from the failure of screening in random background charged impurities [1]. We also examine the percolation transition experimentally by introducing remote ionized impurities at the surface. Using a bias during cool-down, we modify the screening charge at the surface which strongly affects the critical density. Our study shows that transition from a metallic to an insulating phase in our system is due to percolation transition.


2:54PM Q21.00003 Electrically induced Metal-Insulator Transition in Nb/NbO$_2$/TiN Devices, YUHAN WANG, STUART A WOLF, JIWEI LU, Univ of Virginia — Niobium dioxide (NbO$_2$) exhibits a metal insulator transition (MIT) as well as a structural transition at 1081 K. It has also been observed that an MIT could be induced by applied electrical field, which makes it attractive as potential electric and optical switch applications. A reactive bias target ion beam deposition (RBTIBD) technique was employed to synthesize Nb/NbO$_2$ thin films on TiN/Si substrates, in which the Nb top layer was used as the top electrodes. Electrically induced MIT was observed in the Nb/NbO$_2$/TiN devices, showing threshold characteristics. The electrically induced MIT was uni-polar with very minimal hysteresis behavior and good reproducibility. Such transitions were observed up to 200 $^\circ$C without obvious phase changes of NbO$_2$, indicating good thermal stability. We will discuss the evolution of electrical fields, current densities and input power at switching with the number of switches, as well as their dependence on the size of contacts. To study the possible effects from the interfaces between NbO$_2$ films and contacts, annealing processing in forming gas was conducted and transition behaviors were compared before and after annealing. The possible mechanisms for this induced MIT will be discussed.
3:06PM Q21.00004 Electrical transport properties of CaB₆₁

JOLANTA STANKIEWICZ, Instituto de Ciencia de Materiales de Aragón and Departamento de Física de la Materia Condensada, CSIC–Universidad de Zaragoza, 50009-Zaragoza, JAVIER SESE, Instituto de Nanociencia de Aragon and Departamento de Física de la Materia Condensada, Universidad de Zaragoza, 50018-Zaragoza, Spain, GEETHA BALAKRISHNAN, Department of Physics, University of Warwick, Gibbet Hill Road, Coventry CV4 7AL, UK, ZACHARY FISK, Department of Physics and Astronomy, University of California, Irvine, CA 92697, USA — We report results from a systematic electron-transport study in a broad temperature range on twelve CaB₆ single crystals. None of the crystals were intentionally doped. The different carrier densities observed presumably arise from slight variations in the Ca:B stoichiometry. In these crystals, the variation of the electrical resistivity and of the Hall effect with temperature can be consistently explained by a variable charge state of intrinsic defects, most likely B-antisites (B atom replacing Ca atom). Our model is also consistent with the presence of a narrow, defect related, impurity band close to the Fermi level. Thus it may indicate the validity of defect-driven intrinsic ferromagnetism in alkaline-earth hexaborides. The magnetotransport measurements reveal that most of the samples we have studied are close to a metal-insulator transition at low temperatures. The magnetoresistance changes smoothly from negative—for weakly metallic samples—to positive values—for samples in a localized regime.

1We acknowledge support from grant MAT2012-38213-C02-01 of MEC, Spain and EP/1007210/1 from EPSRC, UK.

3:18PM Q21.00005 Metallic Hydrogen

ISAAC SILVERA, MOHAMED ZAGHO, ASHRAN SALAMAT, Lyman Laboratory of Physics, Harvard University — Hydrogen is the simplest and most abundant element in the Universe. At high pressure it is predicted to transform to a metal with remarkable properties: room temperature superconductivity, a metastable metal at ambient conditions, and a revolutionary rocket propellant. Both theory and experiment have been challenged for almost 80 years to determine its condensed matter phase diagram, in particular the insulator-metal transition. Hydrogen is predicted to dissociate to a liquid atomic metal at multi-megabar pressures and T = 1.1-1.7 Mbar and up to 2200 K. We observe a first-order phase transition in the liquid phase, as well as sharp changes in optical transmission and reflectivity when this phase is entered. The optical signature is that of a metal. The mapping of the phase line of this transition is in excellent agreement with recent theoretical predictions for the long-sought plasma phase transition to metallic hydrogen.

2Research supported by the NSF, grant DMR-1308641, the DOE Stockpile Stewardship Academic Alliance Program, grant DE-FG52-10NA29656, and NASA Earth and Space Science Fellowship Program, Award NNX14AP17H.

3:30PM Q21.00006 Nanoscale Electrical Imaging of Metal-Insulator Transition in Ion-Gel Gated ZnO Field Effect Transistors

YUAN REN, Department of Physics, University of Texas at Austin, HONGTAO YUAN, Geballe Laboratory for Advanced Materials, Stanford University, XIAOYU WU, Department of Physics, University of Texas at Austin, YOSHIHIRO IWASA, Quantum Phase Electronics Center and Department of Applied Physics, University of Tokyo, YI CUI, HAROLD HWANG, Geballe Laboratory for Advanced Materials, Stanford University, KEJI LAI, Department of Physics, University of Texas at Austin — Electric double-layer transistors (EDLTs) using ionic liquid as the gate dielectric have demonstrated a remarkably wide range of density modulation, a condition crucial for the study of novel electronic phases in complex quantum materials. Yet little is known microscopically when carriers are modulated in the EDLT structure because of the technical challenge to image the buried electrolyte-semiconductor interface. With a novel nanoscale resistive microscope, we demonstrate the real-space conductance imaging and mapping in ZnO EDLTs with a spatial resolution of 100nm. A thin layer of ion gel, which solidifies below the glass transition temperature of 200K, was spin-coated on the ZnO surface to induce the metal-insulator transition. The microscope images acquired at different channel conductance clearly showed the spatial evolution of local conductivity through the transition. In addition, by applying a large source-drain bias, electrical inhomogeneity was also observed across the source and drain electrodes.

3:42PM Q21.00007 Metal-insulator transition in 2D quantum walks

JONATHAN EDGE, Nordita, JANOS ASBOTH, MTA Wigner FK SZFKI — We investigate the localisation properties due to disorder of several different two-dimensional quantum walks. We find that, contrary to claims in the literature, the Hadamard quantum walk does not localise. In a different quantum walk system we find a way to induce localisation. By tuning the parameters of the system we further manage to drive the quantum walk through a metal-insulator transition and show that the transition is related to the plateau transition of the integer quantum Hall effect.

3:54PM Q21.00008 Compression-Driven Enhancement of Electronic Correlations in Simple Alkali Metals

GILBERTO FABBRI, Argonne National Lab./Washington University in St. Louis, JINHYUK LIM, Washington University in St. Louis, LARISSA VEIGA, Argonne National Lab./Brazilian Synchrotron Light Lab., DANIEL HASKEL, Argonne National Lab., JAMES SCHILLING, Washington University in St. Louis — Alkali metals are the best realization of the nearly free electron model. This scenario appears to change dramatically as the alkalis are subjected to extreme pressure, leading to unexpected properties such as the departure from metallic behavior in Li and Na, and the occurrence of remarkable low-symmetry crystal structures in all alkalis. Although the mechanism behind these phase transitions is currently under debate, these are believed to be driven by electronic quantum melting. In this study the high-pressure electronic and structural ground state of Rb and Cs was investigated through low temperature XANES and XRD measurements combined with ab initio calculations. The results indicate that the pressure-induced localization of the conduction band triggers a Peierls-like mechanism, inducing the low symmetry phases. This localization process is evident by the pressure-driven increase in the number of d electrons, which takes place through strong spd hybridization. These experimental results indicate that compression turns the heavy alkali metals into strongly correlated electron systems.

1Hungarian National Office for Research

Work at Argonne was supported by DOE No. DE-AC02-06CH11357. Research at Washington University was supported by NSF DMR-1104742 and CDAC/DOE/NNSA DE-FG52-08NA28554.

4:06PM Q21.00009 From Coulomb Fluid to Self-Generated Charge Glass due to Long-Range Interactions and Geometric Frustration

SAMIYEH MAHMOUDIAN, National High Magnetic Field Laboratory and Florida State University, LOUK RADEMAKER, Kavli Institute for Theoretical Physics, University of California Santa Barbara, ARNAUD RALKO, SIMONE FRATINI, Institut Néel-CNRS and Université Joseph Fourier, VLADIMIR DOBROSAVLJEVIĆ, National High Magnetic Field Laboratory and Florida State University — We show that introducing long-range Coulomb interactions immediately lifts the massive ground state degeneracy induced by geometric frustration for electrons on quarter-filled triangular lattices in the semi-classical regime. This products not only a stripe-ordered (global) crystalline ground state, but also very many low-lying metastable states with amorphous “stripe-glass” spatial structure. At intermediate temperatures, such a frustrated Coulomb liquid shows remarkably slow (viscous) dynamics, with very long relaxation times growing in Arhenius fashion upon cooling, as typical of “strong glass formers.” On shorter time scales, the system falls out of equilibrium and displays the “aging” phenomena characteristic of supercooled liquids around the glass transition. Our results, which are obtained using mean field theory, classical Monte Carlo simulations and exact diagonalization, show remarkable similarity with the recent observations of charge-glass behavior in ultra-clean triangular organic materials Ω-RbZn and Ω-CsZn.

1F. Kagawa et al., Nat. Phys. 9, 419-422, (2013)
4:18PM Q21.00010 Strong-disorder renormalization group study of the Anderson localization transition in three and higher dimensions, HOSSEIN JAVAN MARD, VLADIMIR DOBROSAVLJEVIĆ, National High Magnetic Field Laboratory, Florida State University, JOSE A. HOYOS, Instituto de Física de São Carlos, Universidade de São Paulo, EDUARDO MIRANDA, Universidade Estadual de Campinas(Unicamp), SP, Brazil — We implement an efficient strong-disorder renormalization group (SDRG) procedure for disordered tight-binding models in dimension $D > 3$, including the localization properties on Erdős-Rényi random graphs, which represent an appropriate infinite dimensional limit. Our dramatically improved SDRG algorithm is based on a judicious elimination of most (irrelevant) new bonds generated under RG. It yields excellent agreement with exact numerical results for universal properties at the critical point, without significant increase of the required computer time, even as the spatial dimension is increased beyond $D = 3$. This opens an efficient avenue to explore the critical properties of Anderson transition in the strong-coupling limit of high spatial dimensions.  


4:30PM Q21.00011 Unstable Domain-Wall Solution in the Metal-Mott Insulator Coexisting Regime, TSUNG-HAN LEE, VLADIMIR DOBROSAVLJEVIC, Florida State University and National High Magnetic Field Laboratory, JAKSA VUCICEVIC, DARKO TANASKOVIC, Institute of Physics Belgrade, Serbia, EDUARDO MIRANDA, Campinas State University, Brazil — We employ Dynamical Mean Field Theory (DMFT) with multiphysical optimization (Conjugate Gradient and Broyd method) to investigate the transport properties of the unstable solution in the Mott metal-insulator coexisting regime. Physically, this solution is expected to describe the properties of the domain wall separating the metallic and the Mott-insulating regions in a spatially inhomogeneous case. We show that the multidimensional optimization can efficiently converge not only to the local minima of the free energy, describing the two coexisting phases, but also to the saddle-point describing the unstable solution. This unstable solution represents a new phase of matter: its low temperature transport properties differ qualitatively from both the metal and the insulator, displaying incoherent metallic behavior down to lowest temperatures.

4:42PM Q21.00012 ABSTRACT WITHDRAWN —

5:04PM Q21.00013 Large Disorder Renormalization Group Study of the Anderson Model of Localization1, SONIKA JOHRI, R. N. BHATT, Princeton University — We describe a large disorder renormalization group (LDRG) scheme for the Anderson model of localization in one dimension which eliminates eigenstates based on the size of their wavefunctions rather than their energy[1] (as done in RG models to date). We show that our LDRG scheme flows to infinite disorder, and thus becomes asymptotically exact. We use it to obtain the disorder-averaged inverse participation ratio and density of states and compare these with results obtained by exact numerical diagonalization for the entire spectrum. A modified method is formulated for higher dimensions, which is found to be less efficient, but capable of improvement. The possibility of extending this scheme to many-body localized states will be discussed.

1This work was supported by Department of Energy Grant No. DE-SC0002140.

5:06PM Q21.00014 Quantum phase transitions of a boson Hubbard model in one and two dimensions: a modified Time-Evolving Block Decimation study1, J-WOO LEE, SONG MOON KIM, HWAN BIN CHOI, Myongji University — We study quantum phase transitions of a boson Hubbard model in one and two dimensions at zero temperature. The model has a repulsive energy term ($U$) between the bosons located at the same site and a hopping energy term ($t$) to nearest neighboring sites. We construct matrix product states for one dimension and projected entangled pair states for two dimensions to represent ground states by a modified Time-Evolving Block Decimation. By exploring the energies and correlation functions, we obtain a phase diagram for this model as a function of chemical potential ($\mu$) and hopping energy ($t$) as we fix $U = 1$. Our results are compared with other methods, such as strong-coupling perturbation results and Monte Carlo results. Our method can be useful in calculating ground-state properties since we can control the accuracy of the ground state and the number of parameters for quantum entanglement.

1This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (NRF-2012R1A1A2006113).

Wednesday, March 4, 2015 2:30PM - 5:06PM —
Session Q22 DCMP: Heavy Fermions: Ce-based Compounds: Experiment 202A - Sergey Bud’ko, Ames Laboratory/Iowa State University

2:30PM Q22.00001 Surface bulk differences in a Kondo lattice system, KALOBARAN MAITI, Tata Inst of Fundamental Res, Thomas PRUSCHKE, University of Goettingen, KHADIZA ALI, DEEPNARAYAN BISWAS, SANGEETA THAKUR, SWAPNIL PATIL, NISHAINA SAHADEV, GANESH ADHIKARY, Tata Inst of Fundamental Res, G. BALAKRISHNAN, University of Warwick — Antiparallel coupling between the magnetic moment and conduction electrons leads to a non-magnetic Fermi liquid phase in a magnetic material - this is known as Kondo effect. Such coupled electronic states appear as a sharp feature at the chemical potential at low temperatures, called Kondo resonance feature. Photoemission spectra of Kondo systems often exhibit growth of multiple Kondo resonance features with large intensity at temperatures much higher than the Kondo temperature. We studied the evolution of the Kondo resonance feature in CeB6 employing high resolution photoemission spectroscopy and state of the art calculations based on dynamical mean field theory. We observe multiple Kondo resonance features with anomalies in their temperature evolution. It appears that the surface of these systems possess high Kondo temperature compared the bulk that causes unusual temperature evolution in these materials.

4:24PM Q22.00002 Spin fluctuations in the Kondo Semimetal CeRu4Sn6,1 WESLEY FUHRMAN, IQM, Johns Hopkins University, J. HAENEL, A. PROKOFIEV, S. PASCHEN, Vienna University of Technology, D.T. ADROJA, ISIS, J.A. RODRIGUEZ, NIST, C.L. BROHOLM, IQM, NIST, Johns Hopkins University — We present neutron scattering results for CeRu4Sn6. Tentatively classified as one of the few non-cubic Kondo insulators, CeRu4Sn6 has highly anisotropic physical properties. Using cold neutron inelastic neutron scattering, we have identified a magnetic signal for $h\nu < 1$ meV with a $4\pi$ like form factor and Q-dependence that is indicative of anisotropic antiferromagnetic spin correlations. The implications for the classification and understanding of CeRu4Sn6 are discussed.

1The work at IQM was supported by the US Department of Energy, office of Basic Energy Sciences, Division of Material Sciences and Engineering under grant DE-FG02-08ER46544.
2:54PM Q22.00003 Quantum Criticality in Kondo Compound CeAgBi2, SEAN THOMAS, PRISCILA ROSA, ZACHARY FISK, JING XIA. Univ of California - Irvine — We report a systematic study of the dense Kondo compound CeAgBi2 by means of electrical resistivity, heat capacity, and magnetic measurements, including torque magnetometry and Sagnac interferometry. By comparing our results with previous reports, we observe at zero field a slightly larger antiferromagnetic ordering temperature than $T_N = 0.4$ K. Moreover, five field-induced metamagnetic transitions are observed in magnetic fields up to 12 T applied parallel to the $c$-axis, including a remarkable signature for a first order transition at $H_c$. The low temperature specific heat coefficient $\gamma$ and the $T^2$ resistivity coefficient also show a divergence at the same $H_c$, indicating a putative quantum critical point. This work is supported by NSF grant DMR-1350122. The development of Sagnac interferometer is supported by NSF grant ECCS-1346603.

3:06PM Q22.00004 Doping Dependence of the Structural and Magnetic Properties of CeCu$_{6-x}$T$_x$ ($T$ = Ag, Pd). L. POUDDEL, Univ of Tennessee, Knoxville and Oak Ridge National Laboratory, M.A. MCGUIRE, C. DE LA CRUZ, S. CALDER, A.F. MAY, W. TIAN, M. MATSUDA, H.B. CAO, T. HONG, A.E. PAYZANT, Oak Ridge National Laboratory, H. JEEN, Oak Ridge National Laboratory and Pusan National University, S. Korea, H.N. LEE, Oak Ridge National Laboratory, M. KOEHLER, H. ZHOU, V. KEPPENS, Univ. of Tennessee, Knoxville, D. MANDRUS, A.D. CHRISTIANSON, Univ. of Tennessee, Knoxville and Oak Ridge National Laboratory — CeCu$_{6-x}$Au$_x$ is a well-known heavy fermion system that exhibits an antiferromagnetic quantum critical point (QCP) at $x \sim 0.1$. The end-member, CeCu$_6$ undergoes a structural transition, which is suppressed as Cu is partially substituted by Au in CeCu$_{6-x}$Au$_x$: the critical concentration being at $x \sim 0.1$. This critical point occurs in close proximity to the antiferromagnetic QCP. Here, we study related systems, CeCu$_{6-x}$Ag$_x$ and CeCu$_{6-x}$Pd$_x$, to determine more globally the role of structural degrees of freedom in the observed critical behavior. For magnetically ordered compositions of CeCu$_{6-x}$Ag$_x$ and CeCu$_{6-x}$Pd$_x$, we find a long-range order with the wave-vector similar to that observed in CeCu$_{6-x}$Au$_x$. The structural transition temperature of CeCu$_{6-x}$Ag$_x$ decreases linearly with Ag concentration until the transition is completely suppressed at $x \sim 0.1$. In contrast, moderate Pd-doping does not affect the structural transition, which is observed in CeCu$_{6-x}$Pd$_x$ with $x \lesssim 0.4$.

3:18PM Q22.00005 High Magnetic Field Properties of Ce$_3$Rh$_3$Ge$_5$, MARK WARTENBE, NHML, FSU, LANL, FERMILOGY OF Ce2Rh3Ge5 TEAM$^1$ — The competition between localized and delocalized f electrons in heavy fermion materials produces a wide variety of interesting physical phenomena. Among these compounds is Ce$_2$Rh$_3$Ge$_5$. This heavy-fermion system undergoes an antiferromagnetic transition below 4K and exhibits an angle dependent magnetic phase transition around 25 K. In addition, we conduct inelastic neutron measurements in pulsed field (65T) that reveal quantum oscillations. Temperature dependence at fixed angle indicates relatively high effective masses of values ranging from around 3m to 10m. This indicates that the narrow f-electron density of states is partially hybridized close to the Fermi energy, but also places strict cryogenic constraints upon the measurement ($^3$He temperatures are required). Fermi surface calculations have produced complex figures which lend validation to such rich behavior.

$^1$Ryan Baumbach, Andrew Gallagher, Eric Bauer, Ross McDonald, Kuan-Wen Chen, David Graf

3:30PM Q22.00006 $^{119}$Sn NMR studies on the heavy fermion compound CeSn$_3$, JOHN CROCKER, ANDREW KIM, PETER KLAVINS, NICHOLAS CURRO, UC Davis — CeSn$_3$ does not exhibit long-range order at low temperatures, thus it provides an interesting baseline for NMR studies of the Knight shift. We report the synthesis and characterization of single crystals of CeSn$_3$, as well as $^{119}$Sn nuclear magnetic resonance (NMR) measurements from 4.5K to room temperature. Our data reveal a broad peak in the knight shift ($K$) at $T_{\text{max}} \approx 135$ K, and a knight shift anomaly at $T^* \approx 85$K.

3:42PM Q22.00007 Magnetic structure and CEF levels in CeNiAsO$^1$, S. WU, C. BROHOLM, W.A. PHELAN, T.M. MCQUEEN, Johns Hopkins University, J.C. NEUFELD, M.B. STONE, Oak Ridge National Laboratory — Some HF materials like CeCu$_x$-xAux and YbRh$_2$Si$_2$ have been interpreted as exhibiting unconventional local criticality, rather than a conventional magnetic instability. However, the situation is far from settled so there is great interest in exploring new HF systems in the proximity of magnetic instabilities. Recent reports on CeNiAsO indicate this is a good candidate for such studies. CeNiAsO is isomorphous with the 1111 Fe-based superconductors but exhibits a different type of itinerant magnetism associated with the rare earth site. CeNiAsO has two successive phase transitions at 9.3K and 7.3K that were tentatively associated with antiferromagnetism. To understand these transitions, we carried out magnetic neutron diffraction experiments at the Spallation Neutron Source. We have identified the long range magnetic order and associated the lower transition with a reorientation of the magnetic moment. We also report inelastic neutron powder experiments that determine the crystal field level scheme, which differs from that reported for CeFeAsO and corroborate our analysis of the magnetic structure.

$^1$This research was supported by the U.S. Department of Energy, office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-08ER46544.

3:54PM Q22.00008 Momentum space of quasielectronic spin fluctuations in Ce$_3$Pd$_{20}$Si$_5$, ALISTAIR CAMERON, PAULO PORTNICHENKO, MAKSYM SURMACH, Institut für Festkörperphysik, TU Dresden, PASCALE DEEN, European Spallation Source, SILKE PANZEN, ANDREY PROKOFIEV, Institute of Solid State Physics, Vienna University of Technology, JEAN-MICHEL MIGNOT, Laboratoire Léon Brillouin, ANDRE STRYDOM, Physics Department, University of Johannesburg, MARK TELLING, ISIS Facility, Rutherford Appleton Laboratory, ANDREY PODLESNYAK, Quantum Condensed Matter Division, Oak Ridge National Laboratory, DIMYTO INOSOV, Institut für Festkörperphysik, TU Dresden — Ce$_3$Pd$_{20}$Si$_5$ is one of the heaviest electron systems amongst the heavy-Fermion metals. We have used high-resolution neutron spectroscopy to observe the low-energy region of magnetic scattering from the paramagnetic state, finding that at low temperatures the quasielastic magnetic response is present throughout the Brillouin zone. It forms a broad hump, centred at the (111) scattering vector, surrounded by minima of intensity at (002), (220) and the equivalent wavevectors. This momentum space structure distinguishes it from a simple crystal-field excitation, as proposed previously, and suggests it results from short-range dynamical correlations between the Ce ions, mediated by itinerant $f$-electrons via the RKKY interaction. The momentum-space symmetry of the quasielastic response suggests that it stems from the cubic Ce sub-lattice occupying the 8c Wyckoff site, which is responsible for hosting static AFM order below $T_N$, in contrast to the crystallographically inequivalent 4a site which does not appear to contribute magnetically.

4:06PM Q22.00009 Complex T-H phase diagram in Ce$_3$TiSb$_5$, D.E. JACKSON, T. STEVENSON$^2$, D. VANGENNEP, B. JONES, J.J. HAMLIN, University of Florida - Gainesville, Florida 32611 — We have carried out a detailed characterization of single crystals of the hexagonal compound Ce$_3$TiSb$_5$, via electrical resistivity, magnetization, and specific heat. These results are consistent with Kondo lattice behavior and an antiferromagnetic ordering temperature of 5.5 K. For magnetic fields applied along specific crystallographic orientations, metamagnetic transitions appear and are accompanied by a large negative magnetoresistance. As the temperature is progressively lowered, the metamagnetic transitions bifurcate.

$^1$A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by Nationa Science Foundation Cooperative Agreement No. DMR-1157490, the State of Florida, and the U.S. Department of Energy

$^2$TS supported by UF REU program NSF DMR-1156737.
Shubnikov-de Haas Oscillations of filled skutterudite compounds CeOs$_4$Sb$_{12}$ and NdOs$_4$Sb$_{12}$: P.-C. HO, Physics/CSU-Fresno, J. SINGLETON, F. F., BALAKIREV, NHMFL/LANL, M. B. MAPLE, Physics/UC San Diego, T. YANGASGAWA, Hokkaido U, Japan — The filled skutterudite compounds CeOs$_4$Sb$_{12}$, PrOs$_4$Sb$_{12}$, and NdOs$_4$Sb$_{12}$ are respectively a 1 K antiferromagnetic (AFM) Kondo insulator, a 1.85 K unconventional superconductor (SC), and a 1 K mean-field type ferromagnet (FM). Since SC in PrOs$_4$Sb$_{12}$ exhibits non-BCS properties, it may originate from proximity to AFM and FM quantum-critical points. Therefore, Fermi-surface measurements of NdOs$_4$Sb$_{12}$ and CeOs$_4$Sb$_{12}$ become crucial in understanding the SC pairing mechanism in PrOs$_4$Sb$_{12}$. MHz skin-depth measurements of single crystals of CeOs$_4$Sb$_{12}$ and NdOs$_4$Sb$_{12}$ were performed for temperatures down to 1.3 K and magnetic fields of up to 60 tesla in the Pulsed Field Facility at NHMFL/LANL. Proximity detection oscillator (PDO) data are taken in the 60 tesla generator-driven magnet (∼1 s) using a rotational probe. Shubnikov-de Haas oscillations were detected for various direction of the magnetic field with respect to the crystalline orientations. The results indicate that NdOs$_4$Sb$_{12}$ has similar Fermi surfaces to those of PrOs$_4$Sb$_{12}$ and LaOs$_4$Sb$_{12}$ but that the Fermi surface of CeOs$_4$Sb$_{12}$ is much different from those of the other three compounds.

3Research at CSU-Fresno is supported by NSF DMR-1104544; at UCSD by NSF DMR-1206553 and US DOE DE-FG02-04ER46105; at NHMFL by DOE, NSF, and FL; at Hokkaido U by MEXT, Jpn.

Magnetic Structure of the Heavy-fermion Compound CeAuSb$_2$ in Zero-field: GUY G. MARCUS, Institute for Quantum Matter and Johns Hopkins University, DAE-JEONG KIM, HANNOH LEE, ZACHARY FISK, University of California at Irvine, JOSE A. RODRIGUEZ-RIVERA, NIST Center for Neutron Research, COLLIN L. BROHOLM, Institute for Quantum Matter, Johns Hopkins University, and NIST Center for Neutron Research — We have used neutron diffraction to determine the zero-field magnetic structure of the heavy-fermion compound CeAuSb$_2$. Below $T_N \approx 0.2 K$, we observe the development of antiferromagnetic Bragg diffraction consistent with previous transport and magnetization measurements. The intensities observed at 7 magnetic satellite locations indicate the staggered magnetization is predominantly along the $c$-axis. The maximum moment size is $1.15 \pm 0.08 \mu_B$ which is large compared with the $0.4 \mu_B$ moment in the isostructural heavy fermion ferromagnet CeAgSb$_2$. This suggests that the antiferromagnetic CeAuSb$_2$ is deeper into a magnetic phase. The spin structure, due mainly to the Ce-4f sites, is described as a transverse polarized spin density wave with an incommensurate component of the wave vector in the basal plane. We will discuss these results and bulk measurements in terms of an ANNNI model and effective near neighbor exchange interactions.

1The work at IQM was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences and Engineering under Grant No. DE-FG02-08ER46544. GGMM also acknowledges support from the NSF-GRFP Grant No. DGE-1232825.

Structural and physical properties of new Ce-based silicides CeMAL4Si2 (M= Rh, Ir, Pt) and germanides: NIRMAL GHIMIRE, FILIP RONNING, DARRICK WILLIAMS, BRIAN SCOTT, YONGKANG LUO, Los Alamos Natl Lab, SAMANTHA CARY, THOMAS ALBRECHT-SCHMITT, Florida State University, JOE THOMPSON, ERIC BAUER, Los Alamos Natl Lab — There is a great deal of interest in the Ce-based intermetallic compounds because of the wide variety of strongly correlated electron behavior they exhibit including heavy Fermanion behavior, quantum criticality, unconventional superconductivity and complex magnetic order. Recently we have synthesized new Ce-based tetragonal layered silicides - CeMAL$_4$Si$_2$ (M= Rh, Ir, Pt) that show anisotropic behavior in magnetic susceptibility and electrical resistivity. Furthermore, electronic structure calculations reveal a quasi 2D-character of the Fermi surface. We will discuss the importance of these observations and relevance of these and the related compounds in search of new heavy fermion superconductors. We will also present the structural and physical properties of the related Ce-based tetragonal/hexagonal germanides.

4:42PM Q22.00002 Converged Nuclear Quantum Statistics from Semi-Classical Path Integrals, IGOR POLTAVSKY, ALEXANDRE TKATCHENKO, Dr. — The quantum nature of nuclear motions plays a vital role in the structure, stability, and thermodynamics of molecular systems. The standard approach to take nuclear quantum effects (NQE) into account is the Feynman-Kac imaginary-time-path integral molecular dynamics (PIMD). Conventional PIMD simulations require exceedingly large number of classical subsystems (beads) to accurately capture NQE, resulting in considerable computational cost even at room temperature due to the rather high internal vibrational frequencies of many molecules of interest. We propose a novel parameter-free form for the PI partition function and estimators to calculate converged thermodynamic averages. Our approach requires the same ingredients as the conventional PIMD simulations, but decreases the number of required beads by roughly an order of magnitude. This greatly extends the applicability of ab initio PIMD for realistic molecular systems. The developed method has been applied to study the thermodynamics of N$_2$, H$_2$O, CO$_2$, and C$_2$H$_4$ molecules. For all of the considered systems at room temperature, 4 to 8 beads are enough to recover the NQE contribution to the total energy within 2% of the fully converged quantum result.

2:30PM Q22.00010 Converged Nuclear Quantum Statistics from Semi-Classical Path Integrals, IGOR POLTAVSKY, ALEXANDRE TKATCHENKO, Dr. — The quantum nature of nuclear motions plays a vital role in the structure, stability, and thermodynamics of molecular systems. The standard approach to take nuclear quantum effects (NQE) into account is the Feynman-Kac imaginary-time-path integral molecular dynamics (PIMD). Conventional PIMD simulations require exceedingly large number of classical subsystems (beads) to accurately capture NQE, resulting in considerable computational cost even at room temperature due to the rather high internal vibrational frequencies of many molecules of interest. We propose a novel parameter-free form for the PI partition function and estimators to calculate converged thermodynamic averages. Our approach requires the same ingredients as the conventional PIMD simulations, but decreases the number of required beads by roughly an order of magnitude. This greatly extends the applicability of ab initio PIMD for realistic molecular systems. The developed method has been applied to study the thermodynamics of N$_2$, H$_2$O, CO$_2$, and C$_2$H$_4$ molecules. For all of the considered systems at room temperature, 4 to 8 beads are enough to recover the NQE contribution to the total energy within 2% of the fully converged quantum result.
This work was partially financially supported by NSF DMR-1056536.
4:42PM Q24.00012 Overcoming the fermion sign problem in homogeneous systems, ETH Zürich, JONATHAN DUBOIS, BERNI ALDER, Lawrence Livermore National Laboratory — Explicit treatment of many-body Fermi statistics in path integral Monte Carlo results in exponentially scaling computational cost due to the near cancellation of contributions to observables from even and odd permutations. Through direct analysis of exchange statistics we find that individual exchange probabilities in homogeneous systems are, barring known combinatorial factors, independent of the configuration of other permutations present. For two representative systems, 3-He and the homogeneous electron gas, we find that this allows the entire antisymmetrized density matrix to be generated from a simple model depending only on a few parameters obtainable directly from a standard PIMC simulation. Finally, we show this model may be extended to arbitrary order, resulting in a polynomial scaling algorithm for measuring fermionic observables.

4:54PM Q24.00013 Infinite Variance in Fermion Quantum Monte Carlo Calculations Without the Sign Problem1, SHIWEI ZHANG, HAO SHI, William & Mary Coll — For several important classes of fermion problems, for example the half-filled repulsive Hubbard model and the spin-balanced attractive Hubbard model, quantum Monte Carlo methods using auxiliary-fields allow exact calculations without the sign problem. We show, however, that in most commonly employed algorithms the variance diverges, leading to unreliable estimates of the Monte Carlo statistical error. An approach is proposed to solve the problem. Illustrative results in Hubbard model will be presented.

5:06PM Q24.00014 Spin-Liquid Behavior of a Simple Spin Model on the Triangular Lattice1, RIBHU KAUL, University of Kentucky — I will report on numerical studies of phase transition between competing magnetic (M) and valence bond solid states (VBS) using unbiased quantum Monte Carlo methods in sign-problem free models on non-bipartite lattices in two dimensions. On bipartite lattices the transition between these two phases is a direct second order critical point - consistent with various aspects of the “deconfined” criticality scenario. In contrast, on non-bipartite lattices an intermediate phase appears between M and VBS. We present evidence that this new phase is a quantum spin liquid.

1Supported by NSF and DOE.

Wednesday, March 4, 2015 2:30PM - 5:30PM — Session Q25 DMP: Focus Session: Cooperative Phenomena in Plasticity II — Georgios Tsekenis, Harvard University

2:30PM Q25.00001 Satisfying Detailed Balance in Mesoscale Lattice Models of Amorphous Plastic Deformation, MICHAEL FALK, Johns Hopkins Univ — A number of lattice and finite element models have been proposed to model the correlations and localization transitions that occur during driven plastic flow in glasses and granular media. Green’s function formulations are used to redistribute stress from local shear transformation events. However the ad hoc kinetic assumptions used in such models often lead to violations of detailed balance. These violations preclude the association of a given configuration of the model with a well-defined energy. In this way these models are very different from atomistic models of deformation, where energy is explicitly defined and forces are derived from the underlying energy description. Here we discuss the origin of these violations of detailed balance, and discuss how mesoscale lattice models of shear transformation activity that satisfy detailed balance can, in principle, be constructed.

2:42PM Q25.00002 Modeling the toughness of metallic glasses, CHRIS RYCORFT, Harvard University, ERAN BOUCHBINDER, Weizmann Institute of Science — Metallic glasses are a new type of alloy whose atoms form an amorphous structure in contrast to most metals. They have many favorable properties such as excellent wear resistance and high tensile strength, but are prone to breakage in some circumstances, depending on their method of preparation. This talk will describe the development of a quasi-static projection method in an Eulerian finite-difference framework, for simulating a physical model of a metallic glass based on the shear transformation zone theory. The simulations are capable of resolving the multiple timescales that are involved, and provide an explanation of the experimentally observed differences in breakage strength.

2:54PM Q25.00003 Statistical modeling of athermal micromechanical yielding in amorphous solids and mean-field approaches, STEFANOS PAPANIKOLAOU, Johns Hopkins University — We investigate the micromechanical properties of non-equilibrium yielding under stress of an amorphous solid, modeled in terms of shear-transformation zones. First, we investigate in detail the possible mean-field limits of such models and their capacity to capture the character of the original micromechanical model. For this purpose, we utilize exact as well as numerical solutions. Second, we study the dynamical features of such models when short-time relaxation effects (induced by beta-relaxation modes) are incorporated in simple ways: we demonstrate that shear-banding and stick-slip serrated plastic flow are generic outcomes of such features. Finally, we discuss the relation of this mechanism with the self-induced stochastic resonance effects in non-linear dynamical systems.

3:06PM Q25.00004 Reversible Avalanches and Criticality in Amorphous Solids, CHARLES REICH-HARDT, Los Alamos National Laboratory — Despite its importance for basic science and industry, the physical process that causes a solid to change its shape permanently under external deformation is still not well understood. In this paper we use molecular dynamics simulations of amorphous solids under oscillatory shear to study this phenomenon, and show that at a critical strain amplitude, the size of the cooperative atomic motion that allows for a permanent deformation diverges. We compare this non-equilibrium critical behavior to that of a “front depinning” transition. This viewpoint, based on fluctuations and statistics, is complementary to the dynamical “transition to chaos” which was previously identified at the same strain amplitude. Below this irreversible-depinning transition, we observe large avalanches which are completely repetitive with each shear strain cycle. This suggests that while avalanches on their own do not cause irreversible deformation, it is likely that the irreversibility transition and the “depinning-like” transition are two aspects of the same phenomena. One implication is that the transition could be detected before the onset of irreversible flow by an analysis of the power spectra of avalanches.

Experimental evidence for both progressive and simultaneous shear during quasistatic compression of a bulk metallic glass, YI CUI, HAROLD HWANG, WENDY MAO, Stanford University; QIAOSHI ZENG, ZHENXIAN LIU, Geophysical Laboratory, Carnegie Institution of Washington; KIRIT PATEL, GUNVANT SOLANKI, Sardar Patel University.

Layered transition-metal dichalcogenides 2H-MX2, Jonathann Uhl, Private, Karin Dahmen, Department of Physics, University of Illinois at Urbana Champaign.

Atomic signatures of beta relaxations in metallic glasses will be addressed based on recent computer simulations. Understanding of chemical influence to get desirable properties [1]. Atomic signatures of beta relaxations in metallic glasses will be addressed based on recent computer simulations. Understanding of chemical influence to get desirable properties [1].

A model for flash heating in sheared fault gouge, Jean Carlson, University of Illinois Urbana Champaign; Ahmed Elbanna, University of California Santa Barbara.

We develop a model for sheared gouge layers that accounts for the local increase in temperature at the grain contacts during sliding. We use the shear transformation zone (STZ) theory, a statistical thermodynamic theory, to describe irreversible macroscopic plastic deformations due to local rearrangements of the gouge particles. We track the temperature evolution at the grain contacts using a one dimensional heat diffusion equation. Our model predicts a logarithmic rate dependence of the steady state shear stress in the quasi-static regime.

A simple model for flash heating in sheared fault gouge was performed under the auspices of the U.S. Dept. of Energy under contract DE-AC52-06NA25396. The support of the LANL ASC-PEM program is gratefully acknowledged.

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In contrast to MoS2, the crystal structure of MoS2 does not exhibit a two-dimensional layered structure. Instead, the transition to MoS2 results from a reorganization of the constituent atoms into a more stable configuration. The initial grain structure evolves to a complex dynamic steady state grain morphology that is very different from the initial grain structure and is characterized by large plastic strains and strain rates in a deformation region of thickness 150 nm at the interface in the normal direction. The steady state shows a sequence of grain growth and refinement and a highly strained graded microstructure. This behavior is similar to that seen in simulations for 13 and 20 nm grains and a mesoscale model that takes into account the large plastic strains and strain rates, and the size of the deformation region is able to reproduce the values of the frictional force per unit area.

Metaheuristic optimization algorithms for the simulation of slip and flow in sheared gouge, John Houghton, Los Alamos National Laboratory; R.J. Ravelo, University of Texas, El Paso; T.C. Germain, Los Alamos National Laboratory.

Amorphous metallic glasses are fascinating materials with unique properties that are not found in crystalline counterparts. These materials possess highly tunable optical and electrical transport properties as a function of pressure, which is essentially determined by the narrowing of its band gap followed by closure at around 40 GPa. Our ab-initio calculations further support the semiconductor to metal transition.

5:06PM Q25.00010 Frictional sliding at a compressed polycrystalline 50 nm grain size Al-Al interface, J.E. Hammerberg, Los Alamos National Laboratory; R.J. Ravelo, University of Texas, El Paso.
of the 1.4-MHz peak. The T dependences of this 3-Lor set and their B-field dependences at 17°C are reported and discussed, and their relation to precursor earthquake-like O-valency effects. Research supported by RSAC-SJSU, SETI, WISE-SJSU and AFC San Jose.


Wednesday, March 4, 2015 2:30PM - 4:42PM —
Session Q26 DCP: Focus Session: Non-Adiabatic Dynamics: New Insights from Experiment and Theory IV

2:30PM Q26.00001 Multi-reference vs. single-reference quantum chemical methods in surface hopping dynamics, HANS LISCHKA, Texas Tech University — The reliability of quantum chemical methods plays a critical role in performing reliable nonadiabatic dynamics simulations. Unfortunately, the methods for computing excited states including larger regions of the energy surfaces are still computationally expensive or need support from higher level methods. In this talk the capabilities of multireference (MR) versus single reference (SR) methods will be discussed. In terms of SR approaches we focus our attention on the second-order algebraic diagrammatic construction method (ADC(2)). In addition to the direct calculation of nonadiabatic coupling vectors also the method of computing wavefunction overlaps between consecutive time steps is used. Several interesting examples are discussed such as the charge transfer between systems and the photodecatavation of adenine. The in latter example an extensive comparison of the results concerning deactivation pathways and decay times is given for different methods including multireference configuration interaction, ADC(2) and time-dependent density functional theory (TDDFT) using various functionals. The surface hopping dynamics simulations are performed on the basis of the public domain program system NEWTON-X [M. Barbatti, M. Ruckenbauer, F. Plasser, G. Granucci, M. Persico, and H. Lischka, WIREs:CMS 2014, 4, 26-33].

3:06PM Q26.00002 Unravelling Two State Reactivity: New Insights Combining Experimental, Ab Initio, and Statistical Modelling Techniques, SHAUN ARD, AFRL, JOSHUA MELKO, University of North Florida, OSCAR MARTINEZ, AFRL, VLADIMIR USHAKOV, Max Plank Institute, ANYANG LI, RYAN JOHNSON, University of New Mexico, NICHOLAS SHUMAN, AFRL, HUA GUO, University of New Mexico, JURGEN TROE, Max Plank Institute, ALBERT VIGGIANO, AFRL — Non-Adiabatic dynamics have long played a role in understanding numerous ion molecule reactions. As calculation techniques have improved, even spin-allowed reactions have been found to be significantly impacted by low lying excited spin states, so-called Two-State reactivity. This talk will focus on recent studies of several canonical examples, FeO+ + H2FeO+ + CH4, and Fe2+ + N2O. Experimentally, the kinetics of these reactions are studied from 100 to 700K. Combined with computations of the reaction surface, statistical modelling employing the Statistical Adiabatic Channel Model (SACM) of this near thermal energy range gives unique insight into kinetic details of these systems. Implications of this combined approach, specifically towards better quantifying Two-State reactivity in ion-molecule reactions, will be discussed.

3:18PM Q26.00003 New insights into the nonadiabatic dynamics of proton-coupled electron transfer reactions from the mixed quantum-classical Liouville approach, GABRIEL HANNA, FARNAZ SHAKIB, University of Alberta — The nonadiabatic dynamics of model proton-coupled electron transfer (PCET) reactions is studied for the first time using a surface-hopping solution of the mixed quantum-classical Liouville (MQCL) equation. In contrast to Fewest Switches Surface-Hopping (FSSH), which is commonly used in the simulation of PCET, the MQCL approach provides a rigorous treatment of decoherence in dynamics simulations of MQC systems. The studied model consists of a proton and an electron in a donor-acceptor complex (i.e. quantum subsystem) and a collective solvent coordinate (i.e. classical environment). Using this model, both concerted and sequential PCETs are studied under different proton/electron-solvent coupling conditions, and insights into the dynamical principles underlying these reactions are gained. Notably, an analysis of the trajectories reveals that the solvent coordinate spends a large fraction of its time on the mean of two coherently coupled potential energy surfaces (PESs), as opposed to on single PESs as in the FSSH approach. The results of this study not only demonstrate the applicability of the MQCL approach for PCET simulations, but also emphasize the importance of incorporating decoherence effects through mean surface evolution into calculations of PCET rate constants.

3:30PM Q26.00004 Variational state specific solvent models for excited states from time dependent self-consistent field methods, JOSIAH BJORGAARD, KIRILL VEZIZHANIN, SERGEI TRETIAK, Los Alamos National Laboratory — The effect of a dielectric environment on a molecule can be profound, causing changes in nuclear configuration and electronic structure. Quantum chemical simulation of a solute-solvent system can be prohibitively expensive due to the large number of degrees of freedom attributed to the solvent. To remedy this, the solvent can be treated as a dielectric cavity. Mutual polarization of the solute and solvent must be considered for accurate treatment of an optically excited state (ES) with a state-specific solvent model (SSM). In vacuum, time dependent self-consistent field (TD-SCF) methods (e.g. TD-HF, TD-DFT) give variational excitation energies. With the well known Z-vector equation, a variational ES energy is used to explore the ES potential energy surface (PES) with analytical gradients. Modification of the standard TD-SCF eigensystem to accommodate a SSM creates a nonlinear TD-SCF equation with non-variational excitation energies. This prevents analytical gradients from being formulated so that the ES PES cannot be explored. Here, we show how a variational formulation of existing SSMs can be derived from a Lagrangian formalism and give numerical results for the variability of calculated quantities. Model dynamics using SSMs are showcased.
3:42PM Q26.00005 Electronic Structure and Potential Fitting Methods Suitable For Multi-state Reactive Surfaces. RICHARD DAWES, Missouri University of Science and Technology — Part of this talk describes the development of a ab initio data software that can be used to geometric problems on High-Performance Computing (HPC) clusters to construct PESs automatically. The electronic structure of molecules is described to be difficult to describe continuously across global reactive PESs since it changes qualitatively as bonds are formed and broken along reaction coordinates. I will discuss a high-level ab initio method (GDW-SA-CASSCF/MRCI) designed to allow the electronic wavefunction to smoothly evolve across the PES and provide an accurate and balanced description of the entire region. These methods are combined to study a number of small gas-phased molecules from the areas of atmospheric, combustion and interstellar chemistry including a large variational calculation of all of the vibration states of ozone and the photodissociation dynamics of the simplest Criegee intermediate (CH$_2$OO).

4:18PM Q26.00006 Phase-space formulation of Nonadiabatic Quantum Processes. ANDRES ESTRADA-GUERRA, LEONARDO PACHON, Univ de Antioquia — Based on Schwinger’s exact mapping of the discrete quantum variables onto continuous degrees of freedom and the phase-space path-integral representation of quantum dynamics by Marínov, a phase-space approach is developed here to analyze the quantum features of non-adiabatic processes. Being a phase-space formulation, the associated semiclassical description is by construction an initial value representation and allows for clearly analyzing classical and quantum contributions to the dynamics. The formulated theory is applied to the context of light-harvesting systems in photosynthetic complexes to understand the extent to which quantum effects are determinant in this nonadiabatic process.

4:30PM Q26.00007 Coherent Dynamics Following Strong Field Ionization of Polyatomic Molecules. ARKAPRABHA KONAR, YINAN SHU, VADIM LOZOVoy, JAMES JACKSON, BENJAMIN LEVINE, MARCOS DANTUS, Michigan State University — Molecules, as opposed to atoms, present confounding possibilities of nuclear and electronic motion upon strong field ionization. The dynamics and fragmentation patterns in responses to the laser field are structure sensitive: therefore, a molecule cannot be treated as a “bag of atoms” during field induced ionization. We consider here to what extent molecules retain their molecular identity and properties under strong laser fields. Using time-of-flight mass spectrometry in conjunction with pump-probe techniques we study the dynamical behavior of these molecules, monitoring ion yield modulation caused by intramolecular motions post ionization. The delay scans show that among positional isomers the variations in relative energies, amounting to only a few hundred meVs, influence the dynamical behavior of the molecules despite their having experienced such high fields (V/A). Ab initio calculations were performed to predict dynamics along with single and multiphoton resonances in the neutral and ionic states. We propose that single electron ionization occurs within an optical cycle with the electron carrying away essentially all of the energy, leaving behind little internal energy in the cation. Evidence for this observation comes from coherent vibrational motion governed by the potential energy surface of the ground state of the cation. Subsequent fragmentation of the cation takes place as a result of further photon absorption modulated by one- and two-photon resonances, which provide sufficient energy to overcome the dissociation energy.

Wednesday, March 4, 2015 2:30PM - 4:54PM — Session Q27 DCP: Focus Session: Chemical Physics of Clusters: Bridging from Angstrom-scale Clusters to Micron-scale Aerosol Particles IV

2:30PM Q27.00001 Stability of Phosphine-Ligated Gold Cluster Ions toward Dissociation: Effect of Ligand and Cluster Size. JULIA LASKIN, Pacific Northwest National Laboratory — Precise control of the composition of phosphine-ligated gold clusters is of interest to their applications in catalysis, sensing, and drug delivery. Reduction synthesis in solution typically generates a distribution of ligated clusters containing different number of gold atoms and capping ligands. Ligand binding energy is an important factor determining the kinetics of cluster nucleation and growth in solution and hence the resulting cluster distribution. Phosphines are popular capping ligands with tunable electronic and steric properties that affect their binding to the gold core. We examined the effect of the number of gold atoms in the cluster and the properties of the phosphine ligand on the ligand binding energy to the gold core using surface-induced dissociation (SID) of mass selected cluster cations produced through electrospray ionization. SID of vibrationally excited ions is ideally suited for studying gas-phase fragmentation of complex ions such as ligated gold clusters. The energetics, dynamics, and mechanisms of cluster ion fragmentation in the absence of solvent are determined through RRKM modeling of time and kinetic energy dependent SID spectra. This novel method provides quantitative information on the ligand binding energies in phosphine-ligated gold clusters important for understanding their formation in solution. Furthermore, ligand binding energies derived from SID data provide the first benchmark values for comparison with electronic structure calculations.

3:06PM Q27.00002 Novel Electro catalysts Prepared by Soft Landing of Mass-Selected Cluster Ions. GRANT JOHNSON, TREVOR MOSEr, NIGEL BROWNING, MARK ENGELHARD, JULIA LASKIN, Pacific Northwest National Laboratory — Metal clusters, which possess size and composition dependent properties, are promising materials for use as catalysts to promote electrochemical reactions in fuel cells. A physical synthesis technique, magnetron sputtering combined with gas-aggregation, has been employed to produce anionic metal clusters in the gas-phase across a range of sizes, shapes, and compositions for mass-selection and deposition onto glassy carbon electrodes. Sputtering of multiple targets in the same region of gas aggregation is demonstrated to produce uncapped binary and ternary alloy clusters with defined composition and morphology that are not accessible through synthesis in solution. Introduction of reactive gases including acids, alkanes, and amines into the sputtering region is shown to result in the formation of complex cluster morphologies containing carbon, nitrogen, and oxygen. A suite of cutting-edge characterization techniques is utilized to demonstrate how the size, shape, elemental composition, and surface density of clusters may be tuned through variations in source parameters such as the sputtering power, gas flow rates, and aggregation distance. The catalytic activity of the soft landed clusters towards the oxygen reduction reaction, a critical process occurring in hydrogen fuel cells, is measured using cyclic voltammetry. Alloy clusters containing reduced quantities of precious metals are shown to exhibit promising catalytic activity.

3:18PM Q27.00003 Quantum Monte Carlo study of charged transition-metal organometallic cluster systems. KAMIL TOKAR, RENE DERIaN, IVAN STICH, Inst. of Physics, Slovak Academy of Sciences — Using accurate fixed-node quantum Monte Carlo (QMC) methods we study 1D clusters formed by transition metal atoms separated by benzene molecules (TMBz), both positively and negatively charged. TMBz are among the most important π-bonded organometallics, which, however, often require charged states for experimental studies. We have performed a systematic study of ground-state spin multiplet, ionization potentials, electron affinities, and dissociation energies of vanadium-benzene cationic and anionic half- and full-sandwiches. By comparison of QMC and DFT results, we find a very strong impact of electronic correlation on properties of these systems, such as dissociation energies, where ≈1 eV energy corrections are found. In particular, the anions are unstable at the DFT level and are stabilized only at the QMC level after sophisticated optimization of the trial wavefunction.

1Supported by APVV-0207-11 and VEGA (2/0007/12) projects
3:30PM Q27.00004 Isolation and structural characterization of a silver-platinum nanocluster, Ag₄Pt₂(DMSA)₄. ANTHONY PEDICINI, ARTHUR REBER, Virginia Commonwealth University, SCOTT BILTEK, AYUSMAN SEN, Pennsylvania State University, SHIV KHANNA, Virginia Commonwealth University — Cluster assembled materials offer an attractive prospect of making nanoscale materials with tunable characteristics. Here, we report the synthesis, isolation, and characterization of the ligand-protected bimetallic cluster, Ag₄Pt₂(DMSA)₄ (DMSA=meso-2,3-dimercaptosuccinic acid) and its analogue, Ag₄Pd₂(DMSA)₄. The procedure is similar to the one employed previously for the synthesis of Ag₄Ni₂(DMSA)₄. Theoretical studies show that the Pt and Ni atoms are square planar in configuration. Furthermore, the dependence on the optical spectrum due to congener replacement of the transition metal is highlighted. Since the crystal field splitting of 5d orbitals is typically larger than that for 3d orbitals, we show the Pt-based cluster has an optical spectrum that is significantly blue shifted as compared to the Ni-based cluster.

This work was supported by an Air Force Office of Scientific Research (AFOSR) Basic Research Initiative Grant FA9550-12-1-0481.

3:42PM Q27.00005 Cluster size matters: Size-driven performance of subnanometer clusters in catalysis, electrocatalysis and Li-air batteries, STEFAN VAJDA, Argonne National Laboratory — This paper discusses the strongly size-dependent performance of subnanometer cluster based catalysts in 1) heterogeneous catalysis, 2) electrocatalysis and 3) Li-air batteries. The experimental studies are based on I. fabrication of ultrasmall clusters with atomic precision control of particle size and their deposition on oxide and carbon based supports; II. test of performance, III. in situ and ex situ X-ray characterization of cluster size, shape and oxidation state; and IV. electron microscopies. Heterogeneous catalysis. The pronounced effect of cluster size and support on the performance of the catalyst (catalyst activity and the yield of C₁ products) will be illustrated on the example of nickel and cobalt clusters in Fischer-Tropsch reaction. Electrocatalysis. The study of the oxygen evolution reaction (OER) on size-selected palladium clusters supported on ultrananocrystalline diamond show pronounced size effects. While Pd₃ clusters show no reaction, Pd₄ and Pd₁₇ clusters are among the most active catalysts known (in terms of turnover rate per Pd atom). The system (soft-landed Pd₄, Pd₁₇, or Pd₁₇ clusters on an UNCD Si coated electrode) shows stable electrochemical potentials over several cycles, and the characterization of the electrodes show no evidence for evolution or dissolution of either the support. Theoretical calculations suggest that this striking difference may be a demonstration that bridging Pd-Pd sites, which are only present in three-dimensional clusters, are active for the oxygen evolution reaction in Pd₃Oₓ Li-air batteries. The studies show that sub-nm silver clusters have dramatic size-dependent effect on the lowering of the overpotential, charge capacity, morphology of the discharge products, as well as on the morphology of the nm size building blocks of the discharge products. The results suggest that by precise control of the active surface sites on the cathode, the performance of Li-air cells can be significantly improved.

4:18PM Q27.00006 Theoretical Study of Chemisorption on Small Palladium Clusters, AJIT HIRA, FRANK NARANJO, FELIPE MUNOZ, DANIELLE JARAMILLO, Northern New Mexico College — We continue our interest in the chemisorption of different atomic and molecular species on small clusters of metallic elements, by examining the interactions of H, H₂, Li and O adsorbates with Pdₙ clusters (n = 2 thru 20). Transition-metal clusters are specially suited for the study of quantum size effects and for formation of metallic states, and are ideal candidates for catalytic processes. Hybrid ab initio methods of quantum chemistry (particularly the DFT-B3LYP model) are used to derive optimal geometries for the clusters of interest. We compare calculated binding energies, bond-lengths, ionization potentials, electron affinities and HOMO-LUMO gaps for the clusters. Of particular interest are the comparisons of binding strengths at the three important types of sites: edge (E), hollow (H), on-top (T), threefold sites and fourfold sites. Effects of crystal symmetries corresponding to the bulk structures are investigated. The capacity of Pd clusters to adsorb H atoms will be compared to Ni clusters.

Research Supported by National Science Foundation

4:30PM Q27.00007 Role of electronic structure and surface structuring effects in the synergistic catalytic activity of Ni-Pd nanoparticles, LINN LEPPERT, Theoretical Physics IV, University of Bayreuth, 95440 Bayreuth, RHETT KEMPE, Inorganic Chemistry II, University of Bayreuth, 95440 Bayreuth, STEPHAN KUEMMEL, Theoretical Physics IV, University of Bayreuth, 95440 Bayreuth — Nickel-palladium nanoalloys show a drastically enhanced catalytic activity in a variety of hydrogenation reactions as compared to pure nickel or palladium nanoparticles. We explore the mixing behavior, electronic structure and magnetic properties of nickel-palladium clusters using density functional theory to gain insight into this synergistic effect. We show that the binding energy of hydrogen to the metal nanoparticle’s surface, which can be tuned via the nickel-palladium composition, is the decisive factor determining how efficiently the reaction can take place. The optimal magnitude of the binding energy for intermediate nickel-palladium ratios can be traced back to a purely electronic effect: a balanced hybridization of the hydrogen s with the metal particle d and s states. This explanation not only holds for small clusters, but also for nickel-palladium surfaces. Finally, we demonstrate that catalytic activity on nickel-palladium surfaces might not only benefit from alloying, but also from the formation of nanostructures on surfaces.

4:42PM Q27.00008 Ultrasmall Carbidic Nanospheres - Formation and Electronic Properties, PETRA REINKE, EHSAN MONAZAMI, University of Virginia, JOHN McCLIMON, University of Pennsylvania — Metallic nanoparticles are highly coveted but are subject to rapid Ostwald ripening even at moderate temperatures limiting study of their properties. Ultrasmall transition metal carbide “nanospheres” are synthesized by a solid-state reaction between fullerene as carbon scaffold, and a W surface. This produces nanospheres with a narrow size distribution below 2.5 nm diameter. The nanosphere shape is defined by the scaffold and densely packed arrays can be achieved. The metal-fullerene reaction is temperature driven and progresses through an intermediate semiconductor phase until the fully metallic nanospheres are created at about 350 C. The reaction sequence is observed with STM, and STS maps yield the local density of states. The reaction presumably progresses by stepwise introduction of W-atoms in the carbon scaffold. The results of high resolution STM/STS in combination with DFT calculations are used to unravel the reaction mechanism. We will discuss the transfer of this specific reaction mechanism to other transition metal carbides. The nanospheres are an excellent testbed for the physics and chemistry of highly curved surfaces.

Wednesday, March 4, 2015 2:30PM - 5:30PM — Session Q28 GMAG DMP: Focus Session: Honeycomb Antiferromagnets — 205 - James Analytis, University of California, Berkeley
but it changes to the antiferromagnetic Neel state with increase of the Hund's rule coupling. Interestingly enough, the valence bond solid (AKLT) state found for the noninteracting electrons survives the increase of the on-site (Hubbard) repulsion, making these states difficult to realize. Indeed, except for the one dimensional spin-

Institute of Science, Israel, DANIEL KHOMSKII, University of Cologne, ERAN SELA, Tel Aviv University — The models constructed by Affleck, Kennedy, Lieb, Modic, Ross McDonald, Arkady Shekter, Los Alamos Natl Lab, James Analytis, UC Berkeley, Brad Ramshaw, Los Alamos Natl Lab — We examine magnetic Hamiltonians for this family and show how a trio of nearest-neighbor exchanges, which arise from strong spin-orbit coupling, are sufficient for reproducing this spiral order on both lattices. We analyze the origin of this phenomenon by presenting a simple 1D model, transparently demonstrating how the counter-rotating spiral is stabilized by strong Kitaev exchange. We also discuss proximate quantum spin liquid phases which arise from spin-orbit coupling.

3:18PM Q28.00003 Unified theory of Kitaev-based spiral magnetism in the harmonic-honeycomb iridates $\alpha$, $\beta$, $\gamma$-Li$_2$IrO$_3$, ITAMAR KIMCHI, University of California, Berkeley, RADU COLDEA, University of Oxford, JAMES ANALYTIS, ASHVIN VISHWANATH, University of California, Berkeley — We review the recent theoretical developments triggered by the experimental discovery of remarkable 3D polymorphs of Li$_2$IrO$_3$, where $J=1/2$ moments form two new 3D lattices which generalize the 2D honeycomb lattice. Measurements on both compounds found that they magnetically order into remarkably similar spiral phases, exhibiting a pattern of non-coplanarity and counter-rotation. We examine magnetic Hamiltonians for this family and show how a trio of nearest-neighbor exchanges, which arise from strong spin-orbit coupling, are sufficient for reproducing this spiral order on both lattices. We analyze the origin of this phenomenon by presenting a simple 1D model, transparently demonstrating how the counter-rotating spiral is stabilized by strong Kitaev exchange. We also discuss proximate quantum spin liquid phases which arise from spin-orbit coupling.

3:30PM Q28.00004 Synthesis and doping of nonmagnetic honeycomb iridate single crystals, GILBERT LOPEZ, NICHOLAS BREZNAY, XUE FAN, JAMES ANALYTIS, Univ of California - Berkeley — The honeycomb iridare Na$_2$IrO$_3$ has been proposed to exhibit many unique properties, including possible spin liquid and topological insulator phases. Although the widely studied layered phase of Na$_2$IrO$_3$ is an antiferromagnetic Mott insulator, I will discuss single-crystal synthesis and electrical and thermodynamic properties of a weakly magnetic Na$_2$Ir$_{1-x}$O$_3$ relative. I will also discuss the effects of chemical doping on the electrical transport and magnetic properties of honeycomb iridate materials.

3:42PM Q28.00005 Thermodynamic Study of 3D “Harmonic” Honeycomb Li$_x$IrO$_3$, ALEJANDRO RUIZ, TONI HELM, NICHOLAS BREZNAY, GILBERT LOPEZ, JAMES ANALYTIS, Univ of California - Berkeley — Honeycomb iridates have been the focus of substantial interest due to the strong magnetic frustration that arises from their edge-shared bonding environment, which favors a strongly anisotropic Ising-like exchange between bonds. In materials with edge-shared IrO$_6$ octahedra, spin-anisotropy of the exchange between neighboring effective spin-1/2 states is enhanced by the interference of the two exchange paths across the planar Ir-O$_{5}$-Ir bond. In the honeycomb lattice, such an interaction couples different orthogonal spin components for the three nearest neighbors; no single exchange direction can be simultaneously satisfied, leading to strong frustration which can be described by the Kitaev-model. We have recently synthesized a new structure that retains the same bonding environment as the honeycomb lattice, and extends this physics to three-dimensions. Previous RMXD experiments on our orthorhombic $H^1$(-1)-Li$_2$IrO$_3$ samples revealed an incommensurate, non-coplanar magnetic structure with counter-rotating moments, suggesting that Kitaev exchange is the dominant spin interaction in this system. In this work, we study the thermal properties of our single crystals as a function of temperature and applied magnetic field.

1Berkeley Chancellor’s Fellowship & NSF-GRFP

3:54PM Q28.00006 Magnetic Anisotropy of a Three-Dimensional Honeycomb Iridate, KIMBERLY MODIC, ROSS MCDONALD, ARKADY SHEKTER, Los Alamos Nati Lab, JAMES ANALYTIS, UC Berkeley, BRAD RAMSHAW, Los Alamos Nati Lab — We present the magnetic anisotropy of a 3-dimensional honeycomb iridate, where the large spin-orbit coupling of iridium provides the possibility for exotic magnetic ground states. A complete angular dependence of magnetic torque provides evidence for highly spin-anisotropic exchange interactions at low temperature. An extension of these measurements to high magnetic fields shows that the magnetic anisotropy switches sign at 50 T and becomes five times larger than the anisotropy at low fields. The anisotropy continues to increase up to the largest applied fields suggesting the presence of new magnetically ordered states.

4:06PM Q28.00007 Valence bond solid (AKLT) state from $t_{2g}$ electrons, MACIEJ KOCH-JANUSZ, Weizmann Institute of Science, Israel, DANIEL KHOMSKII, University of Cologne, ERAN SELA, Tel Aviv University — The models constructed by Affleck, Kennedy, Lieb, and Tasaki (AKLT) describe gapped quantum spin liquids with fractionalized boundary spin excitations. The AKLT spin-spin interactions consist of projection operators onto the maximal possible spin formed between nearest neighbors, which involves a linear combination of powers of the Heisenberg coupling $(\vec{S}_i \cdot \vec{S}_j)^n$, making these states difficult to realize. Indeed, except for the one dimensional spin-1 case, simple antiferromagnetic Heisenberg interactions which are typically found in magnetic insulators, do not stabilize these spin liquid states, but rather generate conventional antiferromagnetically ordered states. We show that this type of interactions can be generated by orbital physics in multiorbital Mott insulators. Motivated by microscopic modeling of spin-orbit entangled Mott insulators such as the layered hexagonal lattices, we focus on $t_{2g}$ electrons on the honeycomb lattice and propose a physical realization of the spin-3/2 AKLT state. Interestingly enough, the valence bond solid (AKLT) state found for the noninteracting electrons survives the increase of the on-site (Hubbard) repulsion, but it changes to the antiferromagnetic Neel state with increase of the Hund’s rule coupling.


4:18PM Q28.00008 Competing quantum phases in the $K_1$-$K_2$ Kitaev model on the honeycomb lattice, JOHANNES REUTHER, Free University Berlin, RONNY THOMALE, University of Würzburg, STEPHAN RACHEL, Technical University Dresden — The Kitaev-spin model on the honeycomb lattice has attracted enormous interest in recent years as an exactly solvable 2D spin system. Research in this field has been fueled by the possibility to realize the Kitaev model in strongly spin-orbit coupled iridate compounds of the form $A_2$IrO$_3$. In these materials, the bond-dependent spin anisotropies of the Kitaev model are provided by spin-orbit entangled Kramers doublets. Experimental as well as theoretical investigations indicate that second neighbor honeycomb interactions are not necessarily small, which particularly applies to the second neighbor Kitaev exchange. We study the $K_1$-$K_2$ Kitaev model on the honeycomb lattice with nearest neighbor and second neighbor Kitaev couplings $K_1$ and $K_2$, respectively. Using a pseudo-fermion functional renormalization group approach for spin systems we map out the entire phase diagram of this model, allowing both couplings to be positive and negative. Aside from Kitaev-spin liquid phases at $K_2 = 0$ we find spin chain-like phases at $K_1 = 0$ where correlations only take place along effective 1D chains. Away from these special points we identify four different types of magnetic phases with collinear orders which retain a clear 1D character in large parts of the phase diagram.

4:30PM Q28.00009 Density matrix renormalization group study of triangular Kitaev-Heisenberg model, SHIGETOSHI SOTA, RIKEN, KAZUYA SJINJO, Yukawa Institute for Theoretical Physics, Kyoto University, TOMONORI SHIRAKAWA, RIKEN, TAKAMI TOHYAMA, Department of Applied Physics, Tokyo University of Science, SEIJI YUNOKI, RIKEN — Topological insulator has been one of the most active subjects in the current condensed matter physics. For most of topological insulators electron correlations are considered to be not essential. However, in the case where electron correlations are strong, novel phases such as a spin liquid phase can emerge in competition with a spin-orbit coupling. Here, using the density matrix renormalization group method, we investigate magnetic phase of a triangular Kitaev-Heisenberg (quantum compass) model that contains a spin-orbital interaction and spin frustration in the antiferromagnetic region. The triangular Kitaev-Heisenberg model is regarded as a dual model of the honeycomb Kitaev-Heisenberg model that is usually employed to discuss $A_2$CuO$_3$ ($A$=Na, K). Systematically calculating ground state energy, entanglement entropy, entanglement spectrum, and spin-spin correlation functions, we discuss the duality between the triangular and the honeycomb Kitaev-Heisenberg model as well as the ground state magnetic phases.

4:42PM Q28.00010 Dynamical properties of honeycomb-lattice magnets Na$_2$IrO$_3$, TAKAFUMI SUZUKI, University of Hyogo — We studied dynamical properties of magnetic effective models for Na$_2$IrO$_3$. The effective magnetic models have been much discussed to explain the zigzag magnetic ordering of this compound [1-6]. The most characteristic point of the proposed models is that the presence of the Kitaev type anisotropy is expected in addition to the Heisenberg coupling. Although there are several proposals for the coupling magnitude of the effective models, the qualitative and quantitative magnetic ordering have been still lacking from the viewpoint of dynamics. From the above background, we carried out numerical exact diagonalization and calculated the dynamical structure factors for the proposals in pioneering works [2,3,5,6]. The obtained results were compared with inelastic-neutron-scattering measurements [2]. We found that the parameter set proposed in ref. [6] well explains a characteristic boundary structure of the lowest excitation around Y point and an intensity distribution in the low energy region [2].

4:54PM Q28.00011 Theory of Magnetic Phases in Hyperhoneycomb and Harmonic-honeycomb Iridates, ERIC KIN HO LEE, YONG BAEK KIM, Univ of Toronto — Motivated by recent experiments, we consider a generic spin model in the $J_{ab} = 1/2$ basis for the hyperhoneycomb and harmonic-honeycomb (H-H) lattices via a combination of the Luttinger-Tisza approximation, single-Q variational ansatz, and classical Monte Carlo simulated annealing. The resulting phase diagrams on both systems show the existence of incommensurate, non-coplanar spiral magnetic orders as well as other commensurate magnetic orders. The spiral orders show counter-propagating spiral patterns, which may be favorably compared to recent experimental results on both iridates. The parameter regime of various magnetic orders and ordering wavevectors are quite similar in both systems. We discuss the implications of our work to recent experiments and also compare our results to those of the two dimensional honeycomb iridate systems.

5:06PM Q28.00012 CaMn$_2$Sb$_2$: Spin Waves Near a Tricritical Point of the Antiferromagnetic Honeycomb Lattice, DANIEL MCNALLY, Stony Brook University, JACK SIMONSON, SUNY Farmingdale, JED KISTNER-MORRIS, GREG SMITH, JULIAN HASSINGER, Stony Brook University, LISA DEBEER-SCHMIDT, ALEXANDER KOLESNIKOV, Spallation Neutron Source, Oak Ridge National Lab, MEIGAN ARONSON, Stony Brook University — The classical Heisenberg model for a honeycomb lattice of spins predicts at least three tricritical points, where three different long range ordered magnetic phases co-exist, depending on the relative strength of the nearest and next-nearest exchange interactions. J$_1-J_2$, where we performed inelastic neutron scattering at T = 5 K, $T_N = 85$ K on oriented single crystals of the antiferromagnetic insulator CaMn$_2$Sb$_2$, where the Mn spins $\mu = 2.8 \mu_B$/Mn form a corrugated honeycomb lattice. Spin wave excitations were observed up to E = 24 meV and these data were fit to the spin wave dispersion expected from the classical Heisenberg model to determine the individual exchange interactions $S_{J_1} = 8.22 \pm 0.23$ meV, $S_{J_2} = 1.29 \pm 0.09$ meV, $S_{J_3} = 0.56 \pm 0.04$ meV, where $J_i$ is the exchange interaction between honeycomb planes. The quantum fluctuations resulting from proximity to the tricritical point at $J_2/J_1 = 1/6$ are responsible for the relatively low ordering temperature of CaMn$_2$Sb$_2$, $T_N = 85$ K, much reduced from the mean field ordering temperature $T_{NFM} = 2\alpha J_1(S(S+1))^{1/3}$ $g = 560$ K.

1 Computations were performed on the GPC supercomputer at the SciNet HPC Consortium. This research was supported by the NSERC, CIFAR, and Centre for Quantum Materials at the University of Toronto.

5:06PM Q28.00012 CaMn$_2$Sb$_2$: Spin Waves Near a Tricritical Point of the Antiferromagnetic Honeycomb Lattice, DANIEL MCNALLY, Stony Brook University, JACK SIMONSON, SUNY Farmingdale, JED KISTNER-MORRIS, GREG SMITH, JULIAN HASSINGER, Stony Brook University, LISA DEBEER-SCHMIDT, ALEXANDER KOLESNIKOV, Spallation Neutron Source, Oak Ridge National Lab, MEIGAN ARONSON, Stony Brook University — The classical Heisenberg model for a honeycomb lattice of spins predicts at least three tricritical points, where three different long range ordered magnetic phases co-exist, depending on the relative strength of the nearest and next-nearest exchange interactions J$_1-J_2$, where we performed inelastic neutron scattering at T = 5 K, $T_N = 85$ K on oriented single crystals of the antiferromagnetic insulator CaMn$_2$Sb$_2$, where the Mn spins $\mu = 2.8 \mu_B$/Mn form a corrugated honeycomb lattice. Spin wave excitations were observed up to E = 24 meV and these data were fit to the spin wave dispersion expected from the classical Heisenberg model to determine the individual exchange interactions $S_{J_1} = 8.22 \pm 0.23$ meV, $S_{J_2} = 1.29 \pm 0.09$ meV, $S_{J_3} = 0.56 \pm 0.04$ meV, where $J_i$ is the exchange interaction between honeycomb planes. The quantum fluctuations resulting from proximity to the tricritical point at $J_2/J_1 = 1/6$ are responsible for the relatively low ordering temperature of CaMn$_2$Sb$_2$, $T_N = 85$ K, much reduced from the mean field ordering temperature $T_{NFM} = 2\alpha J_1(S(S+1))^{1/3} g = 560$ K.

1 We acknowledge the Office of the Assistant Secretary of Defense for Research and Engineering for providing the NSSEFF funds that supported this research.
offering a way to control the properties of domain wall propagation via electric gating. We show that the Walker breakdown threshold scales with the magnitude of a perpendicular electric field, the direction of the wall motion also is sensitive to an applied dc E field. Moreover, we determine the interaction between spin-transfer torque from an electric field. Waves exert magnetic torques in multiferroic materials can cause not only domain wall motion, but also magnetization dynamics for homogeneous magnetization.

3:18PM Q28.00013 Exotic magnetism on the FCC lattice of 5$d^n$ double perovskites. D.D. MAHARAJ, E. KERMARREC, C.A. MARJERISSLON, Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, L8S 4M1, Canada; C.M. THOMPSON, Department of Chemistry, McMaster University, Hamilton, Ontario, L8S 4M1, Canada; K. LEVIN, S. KROEKER, Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, L8S 4M1, Canada — In the search for exotic quantum states, the impact of strong spin-orbit interaction has been recently underlined with the discovery of the $J_{eff}=\frac{1}{2}$ spin-orbital Mott state in the 5$d^n$ layered perovskites iridates. The double perovskite structure can accommodate numerous 5$d$ ions and therefore offers a playground for systematic studies of the exotic ground states stabilized by strong spin-orbit coupling (SOC). Here, we report time-of-flight neutron scattering measurements on the antiferromagnetic (AF), frustrated system, Ba$_2$YOsO$_6$. This 5$d^3$ system undergoes a magnetic transition to a long range ordered AF state below $T_N=70K$. Our results reveal a large spin gap $\Delta=18(2)$meV, unexpected for an orbitally quenched $d^3$ system. We compare this result to the recent observation of a $\Delta=5$meV spin gap in the related 4$d^5$ system, Ba$_2$YRuO$_6$, and conclude to an effect of enhanced SOC.

Wednesday, March 4, 2015 2:30PM - 5:06PM

Session Q29 GMAG DMP FIAP: Focus Session: Spin-waves and Magnetization Dynamics

2:30PM Q29.00001 Excitation and detection of propagating spin waves at the single magnon level. ALEXY KARENOWSKA, ANDREW PATTERSON, MICHAEL PETERER, EINAR MAGNUSSON, PETER LEEK, University of Oxford — The fields of spin-wave dynamics and magnonics have made substantial contributions to our understanding of fundamental magnetism, and are increasingly widely acknowledged to be areas of solid-state physics with significant technological potential. To date however, experimental activity has focused on the study of possible applications of room-temperature systems operating within classical limits. Here, we report a series of experiments in which we demonstrate, for the first time, the excitation and detection of propagating spin waves at the single magnon level. Our results, which have been obtained at cryogenic temperatures using an yttrium iron garnet spin-wave waveguide, serve as evidence that the experimental tools now exist to permit us to create microwave (i.e. GHz frequency) quantum circuits incorporating dispersive magnon systems. This allows us to anticipate the possibility both of exploring quantum aspects of magnon physics with new experimental clarity, and of examining how this physics — in particular, the magnon’s highly tunable dispersion, its readily accessible nonlinearity, and its capacity to couple to optical excitations and electron-based spintronic systems — might have a role to play in new microwave quantum technologies.

2:42PM Q29.00002 Surface Acoustic Waves for Traveling Spin-Wave Resonance Spectroscopy. PRAVEEN GOWTHAM, Cornell University, TAKAHIRO MORIYAMA, Institute for Chemical Research, Kyoto University, DANIEL RALPH, ROBERT BUHRMAN, Cornell University, BUHRMAN/RALPH RESEARCH GROUP TEAM — Gigahertz frequency surface acoustic waves (SAWs) can, via the magnetoelastic interaction, generate effective RF pump fields that can resonantly excite spin waves in a thin-film ferromagnet. SAWs provide a powerful means to study spin waves because the pump field excites traveling spin waves with a definite nonzero wave-vector $\mathbf{q}$. This enables studies, at fixed $\mathbf{q}$, of the spin-wave self-interaction energies and damping. Here we report measurements of the angular dependence of SAW-induced magnetic resonance in Al(10)/AlO$_x$(2)/Ni(10)/Pt(15) structures (thicknesses in nm). We characterize the resonances by measurement of both the acoustical transmission loss in a SAW delay line and the inverse spin Hall voltage generated in the Pt layer by spin pumping. The measurements allow quantitative determinations of the effective RF field generated by the SAW, the magnetoelastic coupling, and damping. The angular dependence reveals that, within the range of $q$ studied, the spin-wave self-interactions are dominated by dipolar fields rather than exchange.

2:54PM Q29.00003 Control of Spin Wave Band Structure and Propagation in Two-Dimensional Magnonic Crystals. GLADE SIETSEMA, MICHAEL E. FLATTÉ, Department of Physics and Astronomy, University of Iowa — We have studied the properties of spin waves in two-dimensional magnonic crystals consisting of a magnetic material arranged in a lattice of cylinders and embedded in a second magnetic material. Dispersion curves, linewidths, and spin wave propagation patterns were obtained from the Landau-Lifshitz-Gilbert equation using the plane wave expansion method[1]. We have examined these results are affected by various parameters including the shape of the cylinders, the lattice structure, the material properties, and the spin-orbit interaction. Adjusting these values can open or close band gaps and drastically shift the frequency range of the band structure. The spin wave propagation patterns were found to exhibit high directionality dependent on the excitation frequency and can also be modified with the aforementioned parameters.[1]arXiv:1111.2506

3:06PM Q29.00004 Spin Wave Directional Coupler. KASUNI NAYAYAKKARA, ALEXANDER KOZHANOV, Center for Nano Optics, Department of Physics and Astronomy, Georgia State University, Atlanta, GA — Spin wave based logic devices are evolved as promising candidates for information processing due to potential in scaling and low power consumption. An element performing directional energy transfer between spin waveguides is required in order to implement existing proposed spin wave logic devices. Optical waveguide couplers are well studied and widely used in integrated and fiber optics applications. In this work we apply the concept of optical directional coupler to design and investigate the spin wave directional coupler comprised of the two ferromagnetic stripes separated by a nanometer scale air gap. Micromagnetic simulations and experimental spin wave energy transfer investigations using propagating spin wave spectroscopy were carried out. Spin waves are generated at one of the ends of the input waveguide while detected at remaining three ends of both spin waveguides. Spin wave coupling is investigated as the coupler geometry, bias magnetic field amplitude and orientation and the spin wave length are varied. Results are modeled as coupled backward volume magnetostatic spin wave modes.

3:18PM Q29.00005 Electric-Field Control over Spin-Wave and Current Induced Domain Wall Motion and Magnonic Torques in Multiferroics. IRYNA KULAGINA, JACOB LINDER, NTNU — We discover that the way spin waves and current exert magnetodynamic effects in multiferroic materials can cause not only domain wall motion, but also magnetization dynamics for homogeneous magnetization textures. Interestingly, the domain wall motion can be controlled via purely electrical means with the spin-waves being generated by an ac electric field E while the direction of the wall motion also is sensitive to an applied dc E field. Moreover, we determine the interaction between spin-transfer torque from an electric current and a magnetic domain wall in multiferroics and show that the Walker breakdown threshold scales with the magnitude of a perpendicular electric field, offering a way to control the properties of domain wall propagation via electric gating.
3:30PM Q29.00006 Generalized stochastic Landau-Lifshitz-Gilbert equation for yttrium-iron garnet films. ANDREAS RÜCKRIEGEL, PETER KÖPIETZ, Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt, Germany — We derive a generalization of the well-known stochastic Landau-Lifshitz-Gilbert equation starting from a microscopic Heisenberg model coupled to the lattice degrees of freedom. By integrating out the phonons we obtain a non-Markovian, stochastic equation of motion for the spin degrees of freedom satisfying a Fluctuation-Dissipation theorem. We apply our theory to study the parametric pumping and thermalization of spin excitations in thin yttrium-iron garnet films.

3:42PM Q29.00007 Angle-dependent 2D domain wall motion with Dzyaloshinskii-Moriya interaction1, JIN LAN, JIANG XIAO2, Department of Physics, Fudan University, Shanghai 200443, China, RUQIAN WU3, Department of Physics and Astronomy, University of California, Irvine, CA 92697-4575 — We explore the dependence of the 2D domain wall motion on the incident angle of magnons (spin waves), in the presence of the Dzyaloshinskii-Moriya interaction (DMI). It is found that the domain wall may either be dragged toward or be pushed away from the magnon source, depending on the incident angle of the magnons. This is mainly contributed by the linear momentum absorbed or released by the DMI when magnons pass through the domain wall. In addition, the total internal reflection of magnons beyond a critical incident angle from one side also contributes to the pushing effect. This adds a new mechanism for the magnetic domain wall motion.

3:54PM Q29.00008 ABSTRACT WITHDRAWN —

4:06PM Q29.00009 Field- and current- induced domain wall creep motions in Tb-based ferromagnetic alloys with varying compositions. MICHAEL QUINSAT, SHIHO NAKAMURA, TAKUYA SHIMADA, YASUAKI OOTERA, HIROFUMI MORISE, TSUYOSHI KONDO, Corporate R&D Center, Toshiba Corporation — Due to their tunable magnetization (Ms), Tb-based ferromagnetic alloys are expected as promising materials for spintronic devices utilizing current-induced domain wall motion (CIDWM) with low current-density. On this material system, we have investigated domain wall motions (DWM) induced by magnetic field $H$ or electric current $J$ in creep regime. We fabricated 2-µm-wide and 9-nm-thick wires made of Tb-based alloys of various composition ratios Tb/CoFe, resulting in Ms of 35-150 emu/cc. From the DW velocities $v$ - $H$ characteristics for the wires, we obtained creep exponents between 1 and 1/4 suggesting strong potential-disorder for DW in the samples[1]. In CIDWM experiments, we also identified creep with $J$ ranging from 5 to 20 MA/cm$^2$. It is found that the creep driven by $J$ is impeded more seriously by increasing the DW pinning strength observed in the creep by $H$, while the $J$-induced DW motion is in the electrons' flow. We infer that the observed DW motion by $J$ for the present samples is interfered with the potential disorders, unlike to the case of Co/Ni wires in a literature[e]. [1] A.B. Kolton et al., Phys. Rev. Lett. 94, 047002 (2005). [2] T. Koyama et al., Nature Materials 10, 194 (2011).

4:18PM Q29.00010 Comparison of Field and Drive Field Domain Wall Motion in Beaded Permalloy Nanowires1. ENNO LAGE, SUMIT DUTTA, CAROLINE A. ROSS, Massachusetts Institute of Technology — Domain wall based devices are promising candidates for non-volatile memory devices with no static power consumption. A common approach is the use of (field assisted) current driven domain wall motion in magnetic nanowires. In such systems local variations in linewidth act as obstacles for propagating domain walls. In this study we compare simulated field driven wall motion and current driven domain wall motion in permalloy nanowires with anti-notches. The simulations were obtained using the Object Oriented Micromagnetics Framework (OOMMF). The wires with a constant thickness of 8 nm exhibit linewidths ranging from 40 nm to 300 nm. Circular shaped anti-notches extend the linewidth locally by 10% to 30% and raise information about the domain wall propagation in such beaded nanowires. The results are interpreted in terms of the observed propagation behavior and summarized in maps indicating ranges of different ability to overcome the pinning caused by anti-notches of different sizes. Furthermore, regimes of favored domain wall type (transverse walls or vortex walls) and complex propagation effects like wall breakdown behavior or dynamic change between domain wall structures are identified

The authors thank the German Academic Exchange Service (DAAD) for funding.

3:42PM Q29.00012 Spin transport and dynamics in the F/N junction. HUA LI, KEVIN BEDELL, Boston College — We study the spin transport in the low temperature regime (often referred to as the precession-dominated regime) between a ferromagnetic Fermi liquid (FFL) and a normal metal metallic Fermi liquid (NFL), the F/N junction, which is considered one of the basic spintronic devices. In particular, we explore the propagation of spin waves and transport of magnetization through the interface of the F/N junction where non-equilibrium spin polarization is created on the normal metal side of the junction by spin injection. We calculate the probable spin wave modes in the precession-dominated regime on both sides of the junction especially on the NFL side where the system is out of equilibrium. Proper boundary conditions at the interface are introduced to establish the transport of the spin properties through the F/N junction. In the end, a possible transmission and dephasing electron spin resonance experiment is suggested on the F/N junction to see if the predicted spin wave modes could propagate through the junction.
In addition, the FePt has excellent structural properties with a high degree of L1\textsubscript{0} ordering. Granular FePt on TiN most often produces inter-connected, worm-like grains with low coercivity. We will show that by optimizing the deposition conditions, crystal structure and lattice constant as MgO, the higher surface energy of TiN causes more wetting of the FePt grains on the TiN surface. As a result, mechanically robust, TiN can be DC-sputtered, which produces fewer particles and has a faster deposition rate. Even though TiN has the same rocksalt sublayers beneath the MgO, there are possible concerns associated with using MgO in the media structure. MgO is highly sensitive to moisture, and perpendicular to the film plane and high perpendicular magnetic anisotropy. MgO is also an effective diffusion barrier between the FePt grains and the metallic underlayer material of choice for granular FePt thin film media for heat assisted magnetic recording, because MgO (001) seeds L1\textsubscript{0} ordering of element doping, optimization of preparation parameters, and temperature dependence of properties also will be discussed.

Wednesday, March 4, 2015 2:30PM - 5:30PM – Session Q30 MAG DMP: Focus Session: Magnetic Films and Magnetic Anisotropy 206B - David Sellmyer, University of Nebraska

2:30PM Q30.00001 Magnetic properties and structures of fibrous R\textsubscript{11}Ni\textsubscript{100} intermetallics (R = heavy rare earths), ALESSIA PROVINO, Dept of Chemistry, University of Genova, CLEMENS RITTER, ILL, Grenoble, KARL A. GSCHNEIDER, Ames Laboratory & DMSE, Iowa State University, PIETRO MANFRINETTI, Dept of Chemistry, University of Genova, SUDESH K. DHAR, CMP & MS Deptm, TIFR, Mumbai, India, VITALIJ K. PECHARSKY, Ames Laboratory & DMSE, Iowa State University — The existence and the unusual self-assembled nano/microfibrous morphology of the R\textsubscript{11}Ti\textsubscript{100} (R = rare earth, T = Ni, Pd, Pt) phases has been recently studied [1,2,3]. All the rare earths (but Sc, Eu, Yb) form this ternary compound (orthorhombic Ni\textsubscript{11}Pd\textsubscript{100} type, cC\textsubscript{4h}1, Cmmm). The bundles of fibers grow parallel to the temperature gradient and along the short c-axis. In this presentation we describe the results of a detailed investigation of the physical properties (electrical resistivity, heat capacity, magnetization measurements) of Tb\textsubscript{11}Ni\textsubscript{100}, Dy\textsubscript{11}Ni\textsubscript{100} and Ho\textsubscript{11}Ni\textsubscript{100} by orienting the fibers parallel and orthogonal, respectively, to the electric current and magnetic field. The unusual fibrous microstructure of these compounds leads to a strong anisotropy in their physical properties, with the c-axis of the orthorhombic cell being the easy magnetization and high electrical-conductivity direction. The magnetic structures of Tb\textsubscript{11}Ni\textsubscript{100} and Ho\textsubscript{11}Ni\textsubscript{100}, which have multiple magnetic orderings, have been investigated by neutron diffraction. The complex magnetic behavior found in these phases is a result of the competing ferrimagnetic (along the c-axis) and antiferromagnetic (on the a – b plane) orderings of the five R sublattices.

2:42PM Q30.00002 Structural, Magnetic and Electronic Transport Properties of Rapidly Quenched CoFeCrAl Nanostructures1, P. KHAREL, R. FUGLSBY, S. GILBERT, Y. HUH, Department of Physics, South Dakota State University, W. ZHANG, Nebraska Center for Materials and Nanoscience and Department of Physics and Astronomy, University of Nebraska, S. VALLOP-PILLY, Nebraska Center for Materials and Nanoscience, University of Nebraska, R. SKOMSKI, D.J. SELLMYER, Nebraska Center for Materials and Nanoscience and Department of Physics and Astronomy, University of Nebraska — Materials with moderate magnetization, high spin polarization at the Fermi level and high Curie temperature well above room temperature have huge potential for spin-based electronic devices. Several Heusler compounds including a quaternary compound CoFeCrAl are predicted to have these interesting materials properties. We have used a rapid quenching technique to prepare single-phase CoFeCrAl nanostructured ribbons in a cubic L2\textsubscript{1} crystal structure and have investigated the magnetic and electrical properties. As-quenched ribbons are ferrimagnetic at room temperature with a Curie temperature of about 500 K. The saturation magnetization is 1.9 \textmu\textsubscript{B}/f.u, which is very close to the value predicted by the Slater-Pauling Rule. The ribbons are conducting with a room temperature resistivity of about 80 m\Omega cm, but the resistivity is almost independent of temperature. The thermal coefficient of resistivity is very small and is negative. These ribbons show a small positive magnetoresistance (1.5% at 5 K) between 5 K and 300 K. We will also discuss the effect of vacuum annealing on the structural and magnetic properties of this material.

2:54PM Q30.00003 Control of anisotropy and magnetism of MnBi nanomaterials1, WENYONG ZHANG, DAVID SELLMYER, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE 68588 — High-anisotropy MnBi nanostructures have been fabricated by in-situ annealing of Bi/Mn/Bi multilayers and magnetic-field annealing of melt-spin Mn\textsubscript{100-x}Bi\textsubscript{x} ribbons. The ratio of Mn to Bi affects the concentration of NiAs-type MnBi, the degree of c-axis orientation, and phase distribution. For x = 50, the Mn\textsubscript{100-x}Bi\textsubscript{x} film exhibits the optimum nanostructure in which MnBi grains are uniformly separated by a thin layer of Bi. This has produced a record value of (BH)\textsubscript{max} = 16.3 MGOe for this compound. A good c-axis texture has been developed for Mn\textsubscript{90}Bi\textsubscript{10} ribbon with a remanence ratio of 0.94 after magnetic-field annealing and this result subsequently leads to (BH)\textsubscript{max} = 9.2 MGOe, the highest value for bulk MnBi materials. The reason for the much higher energy product for the Mn\textsubscript{90}Bi\textsubscript{10} film compared to the Mn\textsubscript{90}Bi\textsubscript{10} ribbon is that the ribbon has a comparatively lower coercivity induced by inhomogeneous distribution of intergranular Bi. The effect of element doping, optimization of preparation parameters, and temperature dependence of properties also will be discussed.

3:06PM Q30.00004 Well-isolated FePt grains with high coercivity on TiN underlayers for heat-assisted magnetic recording media, TIFFANY SANTOS, SHIKHA JAIN, AKEMI HIROTUNE, OLAV HELLWIG, HGST — MgO is the underlayer material of choice for granular FePt thin film media for heat assisted magnetic recording, because MgO (001) seeds L1\textsubscript{0} ordered FePt with c-axis perpendicular to the film plane and high perpendicular magnetic anisotropy. MgO is also an effective diffusion barrier between the FePt grains and the metallic underlayers beneath the MgO. However, there are possible concerns associated with using MgO in the media structure. MgO is highly sensitive to moisture, and hydration of MgO could potentially degrade film properties. In addition, many particulates are incorporated into the film during the RF-sputtering process, which can be sources of domain wall pinning points and magnetic loss. The low-flying recording heads, TiN is an attractive alternative to MgO because it is chemically and mechanically robust, and TiN can be DC-sputtered, which produces fewer particles and has a faster deposition rate. Even though TiN has the same rocksalt crystal structure and lattice constant as MgO, the higher surface energy of TiN causes more wetting of the FePt grains on the TiN surface. As a result, deposition of granular FePt on TiN most often produces inter-connected, worm-like grains with low coercivity. We will show that by optimizing the deposition of FePt and segregant material on the TiN underlayer, we are able to fabricate FePt media with well-isolated grains and high coercivity reaching nearly 4 Tesla. In addition, the FePt has excellent structural properties with a high degree of L1\textsubscript{0} atomic ordering and minimal c-axis in-plane oriented grains.
**3:18PM Q30.00005 Thickness Dependent Magnetoelastic Effects and Perpendicular Magnetic Anisotropy in the Ta/CoFeB/MgO system.** GREGORY STEIHL, PRAVEEN GOWTHAM, DANIEL RALPH, ROBERT BUHRMAN, Cornell University, Ithaca, New York, 14853 — We report the observation of strong thickness-dependent in-plane magnetoelastic coupling in Ta/CoFeB\(x=0.7-2\) nm/MgO multilayers. Measurements are made using a four-point bend test strain fixture, revealing the emergence of large effective surface and volume magnetoelastic couplings after post-deposition annealing. When such surface and volume magnetoelastic interactions are included in the standard Neel model of surface anisotropy, they provide a natural explanation for the nonmonotonic \(K_{\text{eff}}(x)\) vs. \(x\) curves measured for CoFeB films in the thickness range that yields perpendicular magnetic anisotropy (PMA). The magnitude of the magnetoelastic coupling terms suggest that enhanced control of thin film strains could be used to beneficially manipulate the PMA in CoFeB/MgO magnetic tunnel junctions and other thin film multilayer nanostructures.

**3:30PM Q30.00006 Tunable magnetic anisotropy in perpendicular exchange-coupled CoFeB/(Co/Pt) films.** LONG YOU, OUKJAE LEE, Department of Electrical Engineering and Computer Sciences, University of California at Berkeley, TERRÉLL GLENN, Department of Physics, Morehouse College, HARAM ABDEL-RAZIQ, SAYEEF SALAHUDDIN, Department of Electrical Engineering and Computer Sciences, University of California at Berkeley — Spintronic materials with strong perpendicular magnetic anisotropy (PMA), such as Co/Pd, Co/Pt and Co/Ni multilayers, have been introduced to improve the functional performance of STT devices (e.g. enhanced thermal stability, scalability and switching speeds of spin memory/logic). Furthermore, by coupling magnetic layers with PMA and longitudinal magnetic anisotropy (LMA), added benefits such as a variable magnetization tilt angle and tunable damping have been shown. In our study, we discuss how to precisely control the anisotropy tilt angle by coupling the PMA hard layer (Co/Pt) with an in-plane soft layer (IMA, CoFeB). Due to the competition between the PMA and IMA, the tilted angle can be tuned by varying thickness of IMA. The stack of Pt(5nm)/Co (1nm)/CoFeB(xnm)/MgO (2nm) \((x\) varied from 0 to 1nm) was deposited by magneto-sputtering system. The magnetic properties were measured by vibrating sample magnetometer and anomalous Hall effect. The electric transport of microscale devices comprised of that stack were also studied by our probe station with electromagnet. The experiments show the magnetic anisotropy can be tuned well by changing thickness of in plane layer and open a promising new avenue to next generation spintronic devices.

**3:42PM Q30.00007 ABSTRACT WITHDRAWN**

**3:54PM Q30.00008 Isothermal tuning of magnetic coercivity in NiFe/NiO/[Co/Pt] heterostructures with orthogonal easy axes.** ANDREW BARUTH, Department of Physics, Creighton University — Heterostructures of NiFe/NiO/[Co/Pt] with mutually orthogonal easy axes allow for isothermal tuning of the magnetic coercivity at room temperature with no associated shift in the hysteresis loop along the applied field axis. This is in contrast to what is typically seen in exchange biased heterostructures. The application of moderate dc magnetic fields of \(< 3 \text{kOe}\) enhances the NiFe coercivity from 14.5 to 105 Oe. The application of a similarly sized dc magnetic field perpendicular to the film completely resets this enhancement back to 14.5 Oe. We propose that the in-plane magnetization of both the NiFe and [Co/Pt] adjacent layers greatly influences the pinning of the antiferromagnetic NiO interlayer (with a blocking temperature expected to be well below 50 K at this thickness). In addition, these heterostructures show unique high and low-field training effects due to alignment of [Co/Pt] stripe domains during field cycling. The dynamic, yet predictable, behavior of isothermally tuning the magnetic coercivity without any permanent structural/chemical modifications has potential uses in advanced magnetic logic/storage, as well as tuning the interfacial coupling in spintronic applications.

**4:06PM Q30.00009 Controllable magnetic phase front in a vertically graded Ni,Cu\(_{1-x}\) alloy film.** BRIAN KIRBY, NIST - Natl Inst of Stds & Tech, H.F. BELLIVEAU, D.D. BELYEA, T. EGERS, University of South Florida, P.A. KIENZLE, A.J. GRUTTER, NIST - Natl Inst of Stds & Tech, P. RIEGO, A. BERGER, CIC nanoGUNE Consolidor, C.W. MILLER, Rochester Institute of Technology — We have used polarized neutron reflectometry to study the temperature and magnetic field dependent magnetization depth profile of a ferromagnetic 100 nm Ni,Cu\(_{1-x}\) alloy film with \(x\) that varies linearly from 0.61 - 0.70 along the growth axis. Modeling the data in terms of a mean-field exchange strength gradient theory, we find that with increasing temperature, the magnetized thickness of the film continuously decreases, indicating a continuous vertical distribution of effective ferromagnetic transition temperatures. For temperatures corresponding to a partially magnetized film, increasing the applied field from 5 mT to 500 mT is observed to significantly alter the shape of the profile, consistent with magnetization of an effectively paramagnetic region. Thus, we demonstrate that this system exhibits a vertical magnetic phase boundary that can be moved continuously along the growth axis with temperature. Such temperature and field control of the magnetized phase boundary could have important implications for our understanding of metamagnetic transitions, as well as for magnetoelastic and thermomagnetic device applications.

**4:18PM Q30.00010 Strain effect on magnetocrystalline anisotropy of 5d TM/Fe and TM/Fe/MgO(001) (TM=Ta, Ir, Pt, Au): A first principles study\(^1\).** PUREV TAIVANSAIKHAN, Department of Physics and Energy Harvest Storage Research Center, University of Ulsan, Ulsan 680-749, Republic of Korea, DORJ ODKHUU, Department of Physics, Incheon National University, Incheon 406-722, Republic of Korea, SUNG-HYON RHIM, SOON CHEOL HONG, Department of Physics and Energy Harvest Storage Research Center, University of Ulsan, Ulsan 680-749, Republic of Korea — Strain effect on magnetization and magnetocrystalline anisotropy (MCA) of TM/Fe(001) [TM=Ta, Ir, Pt and Au] with and without MgO(001) substrate has been investigated using first-principles calculations. It is found that perpendicular MCA of Pt/Fe(001) changes in-plane MCA in the presence of MgO substrate, where lattice is extended by 3.8% with respect to that without MgO. For Ta/Fe(001) and Au/Fe(001), PMCA is significantly enhanced by the MgO substrate, whereas MCA of Ir/Fe(001) remains in-plane. Furthermore, thickness dependence of MCA on both the TM and Fe layers will be also discussed.

\(^1\)Supported by Basic Research Program (2010-0008842) and Research Centers Program (2009-0093818) through National Research Foundation of Korea.

**4:30PM Q30.00011 Multilayer FeRh/MgO for an antiferromagnetic system.** GUOHUI ZHENG, ODKHUU DORJ, California State University Northridge, SANHUANG KE, Tongji University, Shanghai, China, RAMMOÖRTHY RAMESH, University of California Berkeley, MAOSHENG MIAO, NICKOLAS KIOUSSIS, California State University Northridge — Controlling the magnetocrystalline anisotropy (MCA) of ferromagnetic (FM) thin films by tunable strain and electric field has been pursued as an effective method of achieving low-power and highly scalable memory. Comparing with FM materials, AFM are much less sensitive to external magnetic field, a substantial advantage for memory devices. Inspired by recent work on AFM memory resistors based on FeRh, we carried out a systematic first-principles study of the MCA of multi-layer FeRh, either stand alone, or combined with MgO layers. FeRh is a unique material that undergoes a transition from AFM (type-II) to FM at elevated temperature of 370 K. Our calculations for thin films of FeRh from 5-15 atomic layers reveal that AFM is always the most stable configuration for Fe terminated films; while for Rh terminated films, there is a transition from FM to a configuration featured AFM at the center layers and FM at the surface layers (reconstructed). While applying the spin-orbit interactions (SOI) for the valence electrons, we found Fe-terminated films exhibit a relatively small MCA that varies and may change sign with film thickness, substrate and strain, providing a possibility of spin reorientation via the control of strain and electric field. The k-resolved MCA values reveals that the region around Gamma point adds the major contribution to the MCA.
Heat assisted magnetic recording (HAMR) is a promising approach for increasing the storage density of hard disk drives. To increase data density, information is recorded by using a laser to heat the magnetic medium to a temperature close to its Curie point, thereby reducing its coercivity, making it difficult to write the data with existing recording heads. This issue can be overcome by the technique of HAMR, where a laser is used to heat the recording medium to reduce its coercivity while retaining good thermal stability at room temperature due to the large anisotropy energy. One of the keys to the success of HAMR is the precise control of writing process. In this talk, I will propose a Monte Carlo simulation, based on an atomistic model, that would allow us to study the magnetic properties of L1₀ FePt and dynamics of spin reversal for the writing process in HAMR.

4:06PM Q30.00014 Atomistic modeling of L1₀ FePt: path to HAMR 5Tb/in² . TIANRAN CHEN, Department of Physics, West Chester University, West Chester, PA 19383, MOURAD BENAKLI, CHRIS REA, Seagate Technology, Bloomington, MN 55435 — Heat assisted magnetic recording (HAMR) is a promising approach for increasing the storage density of hard disk drives. To increase data density, information must be written in small grains, which requires materials with high anisotropy energy such as L1₀ FePt. On the other hand, high anisotropy implies high coercivity, making it difficult to write the data with existing recording heads. This issue can be overcome by the technique of HAMR, where a laser is used to heat the recording medium to reduce its coercivity while retaining good thermal stability at room temperature due to the large anisotropy energy. One of the keys to the success of HAMR is the precise control of writing process. In this talk, I will propose a Monte Carlo simulation, based on an atomistic model, that would allow us to study the magnetic properties of L1₀ FePt and dynamics of spin reversal for the writing process in HAMR.

5:18PM Q30.00015 Ferromagnetic thickness dependence of exchange bias: breaking of the inverse proportionality law1 . RAFAEL MORALES, Dept. Chemical-Physics & BCMaterials, UPV/EHU and IKERBASQUE Basque Foundation for Science, Bilbao, Spain, ALI C. BASARAN, Dept. of Physics and Center for Advanced Nanoscience, University of California San Diego, La Jolla, USA, J.E. VILLEegas, Uni 10 Mixte de Physique CNRS/Thales, Université Paris Sud, Orsay, France, D. NAVAS, IFIMUP-IN and Dept. Física e Astronomía, Universidade do Porto, Portugal, N. SORIANO, B. MORA, C. REDONDO, Dept. of Chemical-Physics, UPV/EHU, Leioa, Spain, X. BATLLE, Dept. de Física Fonamental and Instituto de Nanociencia i Nanotecnologia IN2UB, Universitat de Barcelona, Barcelona, Spain, IVAN K. SCHULLER, Dept. of Physics and Center for Advanced Nanoscience, University of California San Diego, La Jolla, USA — The exchange coupling between antiferromagnetic/ferromagnetic (AF/FM) materials shifts the hysteresis loop along the field axis by an amount known as exchange bias field. It is believed that the ferromagnetic thickness dependence of the exchange bias field follows an inverse proportionality law. This has experimentally and theoretically been confirmed for FM thicknesses below the FM domain wall width. In this work we demonstrate that this exchange bias dependence is broken for certain FM spin structures, even though in FM layers thinner than the FM domain wall width. We present experimental data of FeF₂/FeNi bilayers that deviate from the inverse proportionality law, as well as a theoretical calculation that accounts for the results.

5:38PM Q31.00002 5:38PM - 5:45PM — Session Q31 GMAG DMP FIAP: Focus Session: Spin-Dependent Phenomena in Semiconductors: Spin Injection 207A - Connie Li, Naval Research Laboratory

2:30PM Q31.00001 Spin-dependent transport across SrTiO₃-based heterostructures . ADRIAN SWARTZT, Stanford University — Identification of candidate spin-preserved materials is of crucial importance for the realization of functional spin logic devices. An oxide spin channel is particularly attractive because of the ease of epitaxial integration with other functional complex oxides, which could manipulate spins in transit. Electron-doped SrTiO₃ is one emerging material that has high mobility conductions has been realized at the interface between LaAlO₃ and SrTiO₃, as well as in more traditional semiconducting Nb-doped SrTiO₃ thin films. We have investigated spin injection in both systems using a three-terminal (3T) geometry with ferromagnetic electrodes and have observed magnetoresistance commonly attributed to dephasing of an ensemble spin population (Hanle effect), with associated spin lifetimes in the range of 40-130 ps, large enough for the realization of lateral spin transport devices. However, such a picture fails to explain all the experimentally observed behavior. Further experiments indicate contributions from magnetic-field modulation of spin-dependent transport through defect states in the barrier region, suggesting that the 3T approach does not uniquely probe spin accumulation in the SrTiO₃ channel.
3:06PM Q31.00002 Spin Transport Properties in Nondegenerate Si at Room Temperature
TAKAYUKI TAHARA, Kyoto University, HAYATO KOIKE, TDK Corporation and Osaka University, TOMOYUKI SASAKI, TDK Corporation, YUICHIRO ANDO, Kyoto University, MAKOTO KAMENO, YOSHISHIGE SUZUKI, Osaka University, MASASHI SHIRAISHI, Kyoto University, KYOTO UNIVERSITY TEAM, TDK CORPORATION COLLABORATION, OSAKA UNIVERSITY COLLABORATION — So-called beyond-CMOS technologies have been intensively investigated. Among them, Si spintronics is now a promising candidate, since Si has good spin coherence, enabling novel spin-based logic systems. We have been investigating spin transport properties in degenerate Si up to room temperature (RT) and recently, spin transport in a non-degenerate n-Si at RT was successfully achieved where the doping concentration of Si was $2 \times 10^{19} \text{ cm}^{-3}$. Spin drift in non-degenerate Si allows apparent modulation of Hanle spin signals under applications of bias- and gate-electric fields. The magnitude of the spin signals exceeds 1 mV under an bias electric current of 1 mA, which is ten times greater than previously reported values in degenerate-Si-based spin devices. The detail of the observation of large spin signals and other spin transport properties will be discussed in the presentation.

3:18PM Q31.00003 Investigation of spin drift velocity and the modulation of spin signals under spin drift in highly-doped n-type Si
MAKOTO KAMENO, Osaka University, YUICHIRO ANDO, TERUYA SHINJO, MASASHI SHIRAISHI, Kyoto University, HAYATO KOIKE, TOMOYUKI SASAKI, TOHRI OIKAWA, TDK Corporation, TOSHIO SUZUKI, AIT, OSAKA UNIVERSITY TEAM, KYOTO UNIVERSITY COLLABORATION, TDK CORPORATION COLLABORATION, AIT COLLABORATION — Spin drift enables to modulate a spin transport length scale in semiconductor. We have experimentally investigated a role of spin drift in spin transport in highly-doped n-Si, i.e., the modulation of a spin transport length scale by using an electrical spin transport method. The results directly show that spin drift becomes prominent in spin transport in semiconductor. In addition, spin drift velocity in the highly-doped Si channel was quantitatively estimated by introducing a new experimental technique. It was revealed that Hanle-type spin precession signals from the Si were modulated by spin drift and were theoretically reproduced.

3:30PM Q31.00004 Spin lifetime dependence on spin injection orientation in strained silicon films
JOYDEEP GHOSH, DMITRI OSIUTSEV, VIKTOR SVERDLOV, SIEGFRIED SELBERHERR, Institute for Microelectronics, TU Wien — Growing technological challenges and costs are guiding MOSFET scaling to an end. This accelerates the search of alternative devices principles, including concepts based on electron spin. As of the ongoing shift to thin silicon films and fins-based devices for the 14nm node and beyond, spin lifetime in such structures becomes a dominant issue. Large spin lifetime enhancement in (001) thin silicon films subjected to [110] uniaxial tensile stress was predicted for spin injected perpendicular to the film [1]. Here we find that the spin relaxation rate is further reduced and the spin lifetime is thus increased for spin injected in-plane. To explain the observed behavior we look at the spin relaxation hot spots. For an in-plane injection along OX the spin expectation value projections at the hot spots are: $\sigma_x = \sin^2(\arctan(p_x/p_y))$, $\sigma_y = -(p_y/p_x)\sigma_x$, $\sigma_z = 0$, while for spin injected perpendicular to the film the spin expectation value at the hot spots is zero, resulting in maximal spin randomization at any in-plane momentum $(p_x, p_y)$. Therefore the spin relaxation rate is the strongest for spin injected perpendicularly explaining the spin relaxation time increase for an in-plane spin injection. I.D. Osintsev et al., Solid-State Electron.90, 34 (2013).

This work is supported by the European Research Council through the grant #247056 MOSILSPIN.

3:42PM Q31.00005 Challenging the spin accumulation interpretation of local “3T” measurements
HOLLY TINKEY, IAN APPELBAUM, PENGKE LI, University of Maryland- College Park — The recent observation of magnetoresistance in local “three-terminal” (3T) measurements on ferromagnet/insulator/semiconductor junctions have spawned many claims of direct bulk spin injection or “accumulation”. We present a self-consistent model to rigorously calculate expected voltage changes due to electrochemical potential splitting from spin accumulation driven by pure elastic tunnel injection in such junctions, and find that the experimentally observed magnetoresistance vastly exceeds theoretical predictions in all doping, temperature, and bias voltage regimes. Our own experimental measurements using inelastic electron tunneling spectroscopy reveal that extrinsic impurities and defects within the junctions are responsible for the observed magnetoresistance signals, which cannot possibly be attributed to spin dephasing of polarized bulk electrons from elastic injection as claimed by proponents of the method.

3:54PM Q31.00006 Exchange Driven Spin Relaxation in Ferromagnet/Oxide/Semiconductor Heterostructures
YU-SHENG OU, YI-HSIN CHIU, The Ohio State University, DEPT OF PHYSICS, NICHOLAS HARMS, University of Iowa, DEPT OF PHYSICS, PATRICK O'DENTHAL, UNIV OF CALIFORNIA, RIVERSIDE, DEPT OF PHYSICS, ROLAND KAWAMAKI, THE OHIO STATE UNIVERSITY, DEPT OF PHYSICS, MICHAEL FLATTE, UNIVERSITY OF IOWA, DEPT OF PHYSICS, EZEKIEL JOHNSTON-HALPERIN, THE OHIO STATE UNIVERSITY, DEPT OF PHYSICS — Time-resolved Kerr rotation (TRKR) is employed to study the exchange coupling between spin ensembles in GaAs and a neighboring ferromagnet (FM) in an Fe/MgO/GaAs heterostructure. The time-resolved spin dynamics in GaAs provide local magnetometry, revealing the strength and sign of the exchange field as well as its impact on electron and nuclear spins. Consistent with previous studies, we see a hyperpolarization of the nuclei induced by the dynamic exchange at the Fe/MgO/GaAs interface that results in a large effective nuclear field on the electrons (Bn = 0.2 T). Unexpectedly, we observe that the spin relaxation time in GaAs, T2*, depends on the strength of the exchange-driven nuclear field rather than the applied field. In addition, the temperature dependence of T2* shows a crossovers of relaxation mechanism from hyperfine dominated to D'yakonov-Perel' (DP) dominated at temperatures above 40 K. These results not only resolve a long-lasting puzzle of the GaAs spin relaxation mechanism, but further demonstrate the ability to detect exchange-driven dissipation in FM/NM heterostructures. We discuss the potential for this work to define a novel detection scheme for exchange-driven spin injection in FM/semiconductor heterostructures, such as ferromagnetic resonance driven spin pumping.

1MRSEC (DMR-0820414 & DMR-1420451)
4:06PM Q31.00007 Non-local spin transport with two coupled channels: Manifestation of the inter-channel tunneling in the shapes of the Hanle curves1, MIKHAIL RAIKH, ROBERT ROUNY, MAGAN PRESTGARD, ASHUTOSH TIWARI, EUGENE MISHCHENKO, University of Utah — Dynamics of charge-density fluctuations in a system of two tunnel-coupled channels contains two diffusion modes with dispersion $\omega = Dq^2$ and $\omega = Dq^2 + \frac{\omega_L}{t}$, where $D$ is the diffusion coefficient and $\tau_s$ is the tunneling time between the channels. The dispersion of corresponding spin-density modes depends on magnetic field as a result of spin precession with Larmor frequency, $\omega_L$. The presence of two modes affects the shape of the Hanle curve, describing the non-local resistance between the injector and the detector. We calculate the shapes, $R_{11}(\omega_L)$ and $R_{12}(\omega_L)$, of the Hanle curves, for geometries in which detector is located, respectively, in the same and in the different channel than the detector. We demonstrate that the relative shapes of $R_{11}(\omega_L)$ and $R_{12}(\omega_L)$ depend on the ratio $\tau_s/\tau_L$, where $\tau_s$ is the spin-diffusion time. If the coupling between the channels is local, i.e. only at the point $x = 0$, then the shapes of the $R_{11}(\omega_L)$ and $R_{12}(\omega_L)$ curves reflects the difference in statistics of diffusive trajectories which “switch” or do not switch near $x = 0$.

1Supported by NSF through MRSEC DMR-1121252. E.M. is supported by the DOE Grant No. DE-FG02-06ER46313.

4:18PM Q31.00008 Detecting spin accumulation in FM/n-GaAs heterostructures using ferromagnetic resonance1, CHANGJIAN LIU, CHAD GEPPERT, KEVIN CHRISTIE, GORDON STECKLEIN, University of Minnesota, SAHIL PATEL, CHRIS PALMSTRØM, University of California, Santa Barbara, PAUL CROWELL, University of Minnesota — A distinguishing feature of spin accumulation in ferromagnet (FM)/semiconductor heterostructures is precession. This is the basis for detection techniques such as the Hanle effect, but these approaches become less effective as the spin lifetime in the semiconductor decreases. We report here on a technique in which the source magnetization is forced to precess at the ferromagnetic resonance frequency, allowing for the detection of spin accumulation even when the spin lifetime is short (less than 100 psec). The samples used in the experiments are MBE-grown FM/(001) n-GaAs heterostructures, in which the FM are the Heusler alloys Co2MnSi and Co2FeSi. These samples show non-local spin valve and Hanle signals in conventional electrical spin injection/detection measurements at low temperatures. Using the FMR technique, we detect the spin accumulation from 30 K to room temperature as a sharp resonance peak. The frequency dependence of the magnitude of the resonance peak allows for a measurement of the spin lifetime. Spin lifetimes as short as 40 psec are measured at room temperature in channels doped at 3x1016 cm$^{-3}$.

1This work was supported by the NSF under DMR-1104951, the NSF MRSEC program and C-SPIN, a SRC STARNET center sponsored by MARCO and DARPA.

4:30PM Q31.00009 Spin transport at high temperatures in epitaxial Heusler alloy/n-GaAs lateral spin valves1, TIMOTHY A. PETERSON, KEVIN D. CHRISTIE, University of Minnesota, SAHIL J. PATEL, University of California Santa Barbara, PAUL A. CROWELL, University of Minnesota, CHRIS J. PALMSTRØM, University of California Santa Barbara — We report on electrical injection and detection of spin accumulation in ferromagnet/n-GaAs lateral spin-valve devices, observed up to and above room temperature. The ferromagnet in these measurements is the Heusler alloy Co2FeSi, and the semiconductor channel is GaAs doped at 3x1016 cm$^{-3}$. The spin signal is enhanced by operating the detection contact under forward bias. The enhancement originates from drift effects at low-temperatures and an increase of the detection efficiency at all temperatures. The detector bias dependence of the observed spin-valve signal is interpreted by taking into account the quantum well (QW) which forms in the degenerately doped region immediately behind the Schottky tunnel barrier. In particular, we believe the QW is responsible for the minority spin accumulation (majority spin current) under large forward bias. The spin diffusion length and lifetime are determined by measuring the separation dependence of the non-local spin valve signal in a family of devices patterned by electron beam lithography. A spin diffusion length of 700 nm and lifetime of 46 picoseconds are found at a temperature of 295 K.

1This work was supported by the NSF under DMR-1104951, the NSF MRSEC program and C-SPIN, a SRC STARNET center sponsored by MARCO and DARPA.

4:42PM Q31.00010 g-factor modification by an in-plane electric field in a bulk In$_{0.03}$Ga$_{0.97}$As epilayer1, MARTA LUENGO-KOVAC, SIMON HUANG, RACHEL GOLDMAN, VANESSA SIH, Univ of Michigan - Ann Arbor — The response of an electron spin to a magnetic field, determined by the g-factor, is important for any spin-based device. The modification of the g-factor by a perpendicular electric field has been demonstrated in quantum wells and dots. This can be explained by the electric field shifting the electron wavefunction into the barrier. We found that the g-factor also changes when an in-plane electric field is applied across an In$_{0.03}$Ga$_{0.97}$As epilayer. We performed external magnetic field scans of the Kerr rotation of the InGaAs film in order to measure the g-factor independently of the spin-orbit fields. Measurements performed along the [110] and [1-10] crystal axes show the same electric-field dependence of the g-factor, indicating that this change in the g-factor is not related to the spin-orbit fields. Temperature and voltage dependent photoluminescence measurements were also performed, showing that change in the g-factor was not caused by channel heating by the electric field. As there is no quantum confinement along the direction of the electric field, this change in the g-factor is fundamentally different from that seen in quantum wells and dots.

1This work was supported by AFOSR, DTRA, NSF, and ONR.

4:54PM Q31.00011 Spin Lifetimes in annealed GaInNAs epilayers1, YUTSUNG TSAI, BIPLOB BARMAN, THOMAS SCRACE, ATHOS PETROU, SUNY at Buffalo, MIWA FUKUDA, IAN SELLERS, University of Oklahoma, MATTHIEU LEROUX, MOHAMED KHALFIOUI, CRHEA-CNRS, France, SUNY AT BUFFALO COLLABORATION, UNIVERSITY OF OKLAHOMA COLLABORATION, CRHEA-CNRS COLLABORATION — We have carried out Hanle measurements of the electron spin lifetime $T_{2\text{in}}$ optically pumped annealed GaInNAs epilayers (undoped and p-type doped). The samples were prepared in a 7T optical magnet cryostat with the magnetic field applied in the epilayer plane. The emitted light was collected along the normal to the epilayer. The PL was excited using the 1064 nm line from a Nd:YAG laser which gives a polarization P = 5% at B = 0. The transverse magnetic field results in a reduction of $P^*$, from which we determine $T_{2\text{s}}$. At $T = 50$ K, the electron spin lifetime $T_{2\text{in}}$ was measured to be 15 ps. As the sample temperature increases, $T_{2\text{in}}$ decreases ($T_{2\text{in}} = 7$ ps at $T = 150$ K). Our Hanle results are in agreement with the $T_{2\text{in}}$ values measured by Lombez et al. using time-resolved photoluminescence spectroscopy [2]. The observed sharp reduction in $T_{2\text{in}}$ annealed samples is interpreted as due to the D'yakonov-Perel' spin relaxation mechanism. In annealed samples the momentum relaxation time increases, resulting in a reduction of $T_{2\text{s}}$ [2]. L. Lombez et al, Appl Phys Lett 87, 252115(2005) [3] M.I. D’yakonov and V.I. Perel’, Soviet Physics JETP, 33, 1053(1971)

1The authors acknowledge support through the state of Oklahoma OARs program Grant No. 12.2-040.
Electric Field and Magnetoelectric Effects

We show that clockwise and counter-clockwise memristors can be tailored on the same sample yielding multiple resistance states. The memristive response is independent of the variation of the width or the height of the tunnel barrier. This yields a controlled sign change of the electroresistance upon polarization switching.

Heterostructure resulting from the controlled switching of polarization and/or oxygen vacancies may open new routes towards new computing architectures.

Ionized, can be manipulated by electric fields. We aim at using the strong electric fields building up in ultrathin tunnel barriers to generate and manipulate oxygen vacancies, by using the recently established model of Hanle effect taking into account the spin absorption by graphene with a large spin diffusion length, $\lambda$.

Thus $R$ in the range of 100 kOhm is generally not large enough to suppress the spin absorption, and taking into account the contacts is more important to characterize the real $r_\text{sf}$ in graphene with $\lambda$ in this range.

References:

Wednesday, March 4, 2015 2:30PM - 5:30PM –
Session Q32 GMAG DMP: Focus Session: Magnetic Oxide Thin Films and Heterostructures:
Electric Field and Magnetoelectric Effects

2:30PM Q32.00001 Oxygen vacancy control of a ferroelectric memristor, J. SANTAMARIA, GFMC Univ Complutense 28040 Madrid, YAOHUA LIU, S. G. E. TE VELTHUIS, Argonne National Laboratory, Illinois 60439, USA., D. HERNANDEZ-MARTIN, A. PEREZ MUNOZ, M. CABERO, G. SANCHEZ-SANTOLINO, J. TORNOS, M. VARELA, C. LEON, Z. SEFRIOUI, GFMC Univ Complutense 28040 Madrid, S. J. PENNYCOOK, University of Tennessee, Tennessee 37996-2200 — The rich phenomenology exhibited by correlated oxide interfaces can be expanded by considering the control and manipulation of point defects. In particular, oxygen vacancies can be induced by electro forming processes at redox active electrodes and, when ionized, can be manipulated by electric fields. We aim at using the strong electric fields building up in ultrathin tunnel barriers to generate and manipulate oxygen vacancies in Ag/BaTiO$_3$/La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO) micron-size structures defined by optical and electronic lithography techniques. Controlling accumulation of oxygen vacancies in the BTO or LSMO interfaces allows modification of the magnetic state of the LSMO at the interface, enabling independent variation of the width or the height of the tunnel barrier. This yields a controlled sign change of the electroresistance upon polarization switching.

We show that clockwise and counter-clockwise memristors can be tailored on the same sample yielding multiple resistance states. The memristive response is independent of the variation of the width or the height of the tunnel barrier. This yields a controlled sign change of the electroresistance upon polarization switching.

2:42PM Q32.00002 Memristive Switching and Interfacial Magnetoelectricity in LCMO/PBCO Heterostructure, XIAO SHEN, Vanderbilt University, TIMOTHY J. PENNYCOOK, Oxford University, DAVID HERNANDEZ MARTIN, ANA PÉREZ, MARIA VARELA, Universidad Complutense de Madrid, YEVGENIY S. PUZYREV, Vanderbilt University, CARLOS LEON, ZOUHAIR SEFRIOUI, JACOBO SANTAMARIA, Universidad Complutense de Madrid, SOKRATES T. PANTELIDES, Vanderbilt University — New phenomena emerge at the interfaces of transition metal oxides. Here we report memristive switching in a La$_{0.7}$Sr$_{0.3}$MnO$_3$/PrBa$_2$Cu$_3$O$_7$ bilayer structure with an On/Off ratio greater than 10$^3$ that originates from a new type of interfacial magnetoelectricity. Using DFT calculations, we show that at the LCMO/PBCO interface, a “magnetic dead layer” (MDL) can be switched on and off by a small displacement of the interfacial Mn atoms generated by an external voltage. Initially, the LCMO is ferromagnetic with no MDL. This is the Low Resistance State (LRS) as majority-spin carriers tunnel through the PBCO. A negative voltage creates an electric field that displaces the interfacial Mn atoms towards the bulk LCMO by a few hundredths of an Angstrom. In such a position, the interfacial Mn layer is coupled anti-ferromagnetically to the bulk LCMO, whereby a MDL is present, adding a barrier for the majority-spin carriers to tunnel and thus the bilayer is at High Resistance State (HRS). A positive bias drives the Mn atoms back to their original positions that favor ferromagnetic coupling, thus destroying the MDL and switching the bilayer back to LRS.

Enhanced magneto-ionic switching of interface anisotropy in Pt/Co/GdOx films, AIK JUN TAN, UWE BAUER, GEOFFREY BEACH, Massachusetts Inst of Tech-MIT, BEACH GROUP TEAM — Voltage control of magnetic anisotropy is of great interest for reducing the switching energy barrier in spintronic devices. It has recently been shown that electric field-driven oxygen ion migration near the interface of ferromagnet/oxide bilayers can lead to very large changes in magnetic anisotropy [1], but these changes required elevated temperature and a voltage dwell time on the order of minutes. Here, we examine magneto-ionic switching in ultrathin Co/GdOx films with perpendicular anisotropy, in which the GdOx gate dielectric acts as an oxygen ion conductor. We examine the switching efficiency as a function of GdOx layer thickness and electrode geometry, and show that the voltage, operating temperature, and switching timescale can be significantly reduced by optimizing the GdOx thickness and defect structure. We demonstrate reversible toggling of magnetic properties for >50 cycles, and correlate the magnetic switching behavior with changes in the electrical properties of the GdOx. 1. U. Bauer et al., arXiv:1409.1843v1(2014)
3:06PM Q32.00004 Dual field effects in spinel ferrite field effect devices: electrostatic carrier doping and redox reactions , HIDEKAZU TANAKA, Institute of Scientific and Industrial Research, Osaka University — Spinel ferrite is a good candidate as a tunable magnetic semiconductor with high $T_C$. Here, we report the gate-induced conductance modulation of $(\text{Fe}_3\text{Zn}_5\text{O}_4)\text{O}_2$ solid solution to demonstrate the dual contributions of volatile and non-volatile field effects arising from electronic carrier doping and redox reactions using field effect device structure with a ferroelectric Pb(Zr,Ti)O$_3$ and an ionic liquid DEME-TFSI. In the Pb(Zr,Ti)O$_3$/(Fe$_2$,$\text{Zn}$,$\text{O}_4$)$_2$ FET, the gate voltage dependence of channel conductance on the $(\text{Fe}_{2.2}\text{Zn}_{0.8})\text{O}_4$ layer shows the typical hysteresis behavior reflecting the ferroelectric polarization, indicating the static carrier modulation [1]. In contrast, in the DEME-TFSI/(Fe$_2$,$\text{Zn}$,$\text{O}_4$)$_2$ FET, a large hysteresis observed in the drain current vs gate voltage characteristics is not accounted for solely by electrostatic doping, strongly suggesting the presence of chemical reactions[2]. In more details, the characteristic hysteresis virtually disappears for the heavily Zn substituted system $(\text{Fe}_{2.2}\text{Zn}_{0.8})\text{O}_4$ with less carrier concentration [3]. These observations revealed the coexistence of two types of field effects in the Fe$_{3-x}$Zn$_x$O$_4$ devices, and the tuning of field-effect characteristics via composition engineering should be extremely useful for fabricating high-performance oxide field-effect devices. References; [1] Appl Phys Lett. 98 (2011) 102506, [2] Adv. Mater. Interfaces 1 (2014) 1300108, [3] Sci. Rep. 4 (2014) 5818.

3:42PM Q32.00005 Tuning magnetic and electronic properties of (La$_{1-x}$Pr$_x$)$_6$Ca$_{0.33}$MnO$_3$ thin films by composition spread deposition and electrolyte gating , XIAOHANG ZHANG, Y.G. LIANG, S. FACKLER, J.M. SHIN, ICHIRO TAKEUCHI, Department of Materials Science and Engineering, University of Maryland, A.T. N’DIAYE, E. ARENHOLZ, Lawrence Berkeley National Laboratory — The magnetic and electronic properties of mixed-valence mangetites are known to be sensitive not only to chemical doping but also to oxygenation. However, it is difficult to consistently attain exactly the same set of deposition conditions and treatment history for samples that are fabricated individually. In order to perform systematic studies on each of the two effects, we fabricated epitaxial (La$_{1-x}$Pr$_x$)$_6$Ca$_{0.33}$MnO$_3$ (LPCMO) composition spread thin films with the Pr concentration changing continuously across 1 cm to ensure that all the sample segments of interest experience the same processing history. X-ray magnetic circular dichroism (XMCD) and electronic transport measurements indicated that the Curie temperatures and the metal-insulator transition temperatures change continuously from ~ 260 K to ~ 120 K as the Pr concentration is varied from 0 to 0.33. Systematic comparison between experimental data obtained on as-grown and post-annealed samples reveals the role of oxygen in the observed magnetic and electronic transitions. Moreover, changes in the magnetic and electronic properties of LPCMO films under electrolyte-gating have also been observed. A proposed mechanism to explain the effect will be discussed.

3:54PM Q32.00006 Aspects of bulk and surface magnetism of magnetoelectric Fe$_2$TeO$_6$ , SAI MU, KIRILL BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska-Lincoln — Magnetoelastic anti-ferromagnets can be used to implement voltage-controlled magnetism, but materials design for above room-temperature operation is a challenge. Here we focus on the trirutile Fe$_2$TeO$_6$ magnetoelectric and use first-principles calculations to develop several strategies for increasing its Neel temperature $T_N$ above the bulk 210 K value. We find that substitution of larger ions like Zr or Hf for Te increases $T_N$ by increasing the superexchange angles. The compensating O vacancies tend to form bound complexes with such dopants, preserving the electronic band gap. Substitution of N for O is favorable due to the decreased charge-transfer gap.

4:06PM Q32.00007 Designing asymmetric multiferroics with strong magnetoelectric coupling , XUEZENG LU, Northwestern University, HONGJUN XIANG, Fudan University, JAMES RONDINELLI, Northwestern University, MATERIALS THEORY AND DESIGN GROUP TEAM — Multiferroics offer exciting opportunities for electric-field control of magnetism. Single-phase multiferroics suitable for such applications are often exclusive or weakly coupled in bulk. In this talk, we will discuss how superlattices of perovskites can be designed from first principles to achieve high-electric field magnetism and use first-principles calculations to develop several strategies for increasing its Neel temperature $T_N$ above the bulk 210 K value. We find that substitution of larger ions like Zr or Hf for Te increases $T_N$ by increasing the superexchange angles. The compensating O vacancies tend to form bound complexes with such dopants, preserving the electronic band gap. Substitution of N for O is favorable due to the decreased charge-transfer gap.

4:18PM Q32.00008 Magnetoelectric multiferroic superlattices and interfaces: Designing spintronic materials from first principles , ZEILIA ZANOLLI, Forschungszentrum Jülich — The research challenges of the near and far future in electronics focus on the quest for new materials and novel device concepts to achieve low energy consumption, increased reliability and high device density. These can be obtained by designing active elements and interconnects whose operating principle is not (only) based on the electron charge but on the spin degree of freedom of the electron. The nanoscale size of the materials calls for atomicistic and parameter free (ab initio) simulations, which have proven to be crucial in achieving the necessary accuracy and predictive power. Materials which present a coupling between ferroelectricity and magnetism, i.e. magnetoelectric (ME) multiferroics, have been proposed as fundamental building blocks for spintronic devices [1]. However ferroelectricity and magnetism are often exclusive or weakly coupled in bulk. In this talk, we will discuss how superlattices of perovskites can be designed from first principles to achieve strong coupled MO and, hence, control the weak magnetization via an electric field [2]. Most important, advanced epitaxial techniques allow one to actually grow such magnetoelectric superlattices [3]. Another route to optimize spintronic devices is to exploit the unique electronic and transport properties of Carbon-based nanomaterials [4]. The latter present spin diffusion lengths up to 100 μm and high electron velocity. However, a large spin diffusion length comes at the price of small Spin Orbit coupling, which limits the possibility of manipulating electrons via an external applied field. Further, to achieve graphene-based devices one also needs to open its vanishing electronic gap. We use first principle techniques to show that placing graphene on a ME substrate can overcome these limitations by inducing magnetism and opening an electronic band-gap in the hybrid organic-magnetoelectric material.

3:06PM, 3:42PM, 3:54PM, 4:06PM, 4:18PM


Z.Z. acknowledges EC support under the Marie-Curie IEF (PIEF-Ga-2011-300036), computational resources from the PRACE-3IP project (FP7 RI-312763) and the JARA-HPC project (jara0088) of RWTH Aachen University.
4:54PM Q32.00009 Electric Field Control of the Ferromagnetic CaRuO$_3$/CaMnO$_3$ Interface
ALEXANDER GRUTTER, BRIAN KIRBY, NIST Center for Neutron Research, NIST, MATTHEW GRAY, CHARLES FLINT, Department of Materials Science and Engineering, Stanford University, YURI SUZUKI, Department of Applied Physics, Stanford University, JULIE BORCHERS, NIST Center for Neutron Research, NIST — Electric field control of magnetism has been recognized as one of the most important goals in nanoscale magnetics research. The most popular routes towards achieving magnetoelectric (ME) coupling have focused on heterostructures incorporating multiferroics or ferroelectrics. Such studies often rely on voltage induced distortion to induce strain in the magnetic film and alter the magnetic properties. However, successful attempts to induce ME coupling through interface effects or interfacial interactions remain relatively rare. The ferromagnetic interface between the antiferromagnetic insulator CaMnO$_3$ and the paramagnetic metal CaRuO$_3$ is a promising candidate for direct magnetization control. This interfacial ferroagnetism is stabilized through the competition between interfacial double exchange and antiferromagnetic superexchange between adjacent Mn$^{4+}$ so that the system is expected to be very sensitive to small changes in interfacial carrier density. Using polarized neutron reflectometry, we have probed the electric field dependence of the interfacial magnetization of CaRuO$_3$/CaMnO$_3$ bilayers deposited on SrTiO$_3$. We find that electric fields of $\pm 8$ kV/m are sufficient to switch the interfaces from largely ferromagnetic to completely antiferromagnetic.

5:06PM Q32.00010 Simultaneous Kerr and Faraday investigations of boundary magnetization and order parameter switching in voltage-controllable exchange bias films
JUNLEI WANG, WILL ECHTENKAMP, MIKE STREET, CHRISTIAN BINEK, University of Nebraska-Lincoln — Magnetoelastic oxides are of great interest for ultra-low power spintronics. A key property for the realization of electrically switchable state variables is the voltage-controlled boundary magnetization in magnetoelastic antiferromagnets. It allows electric switching of an adjacent exchange coupled ferromagnetic layer in the absence of dissipative currents. Previous surface sensitive measurements of boundary magnetization in thin films of the archetypical magnetoelastic antiferromagnet chromia lacked explicit demonstration of the predicted rigid coupling between the bulk antiferromagnetic order parameter and the boundary magnetization. We designed a magneto-optical setup allowing simultaneous measurement of Kerr and Faraday rotation. Our experiments correlate electric field induced bulk magneto-optical effects (non-reciprocal rotation), including the response on switching of the antiferromagnetic order parameter, with the boundary magnetization. Our results suggest that switching of a ferromagnetic film strongly exchange coupled to a magnetoelastic antiferromagnetic ultra-thin film allows switching of the antiferromagnetic order parameter. We investigate the possibility that this switching phenomenon might induce a voltage pulse via a generalized variation of the inverse linear magnetoelectric effect.

5:18PM Q32.00011 Voltage Controlled Exchange Bias in a Cr$_2$O$_3$ based heterostructure
WILL ECHTENKAMP, MIKE STREET, CHRISTIAN BINEK, University of Nebraska — Controlling magnetism by electrical means is a key challenge in the field of spintronics, and electric control of exchange bias is one of the most promising routes to address this challenge. Isoelectric control of exchange bias has been achieved near room temperature using bulk, single crystal, magnetoelastic Cr$_2$O$_3$, which has a voltage controlled net magnetization at the (0001) surface. Voltage control of magnetism in a Cr$_2$O$_3$ thin film system has presented significant challenges. In this study we explore the electric control of exchange bias in an all-thin-film system of decreasing chromia film thickness with significant implications for scalability of ultra-low power memory and logical devices. Cross-sectional HRTEM indicates that grain boundaries in the metallic bottom electrode propagate into the Cr$_2$O$_3$ thin film with detrimental effects on leakage currents. We address this issue via a three-step growth method for the deposition of epitaxial Pd on sapphire. The resulting microstructure of the films is analyzed by reflection high-energy electron diffraction, tunneling electron microscopy and x-ray diffraction.

Wednesday, March 4, 2015 2:30PM - 4:18PM Session Q33 FEd: Physics Education Research 208 - Monica Plisch, American Physical Society

2:30PM Q33.00001 Potential Utility of Non-Cognitive Constructs in Graduate Admissions
CASEY MILLER, Rochester Inst of Tech — It is becoming clear that the methods employed by many graduate admissions committees need updating. Regarding outcomes, we cannot select students that will actually graduate much better than would a coin toss. Further, the GRE is often misused. For example, the most recent GRE general test data (2006-2007) shows that for US citizens in the physical sciences, a cut-off score of ~64th percentile (700/1550 on old/new test) would eliminate from eligibility: 63% of women vs 42% of men; 76% of all under-represented minorities vs 38% of Asian and 47% of White applicants. Fortunately, Organizational Psychologists have identified and validated several “non-cognitive constructs” for admissions: aspects of personality (conscientiousness); and self-management factors. Some intriguing facts about these parameters: they are measurable with the help of social scientists; they do not show race/ethnicity/gender performance differences; they are orthogonal to cognitive metrics measured by GPA and tests scores. These are proven to enhance both validity and diversity in admissions. My goals for this talk are to overview the non-cognitive constructs with the most potential for being used in physics graduate admissions, and to suggest example admissions protocols.

2:42PM Q33.00002 Beyond detection: nuclear physics with a webcam in an educational setting
ARTHUR PALLONE, Norwich University — Nuclear physics affects our daily lives in such diverse fields from medicine to art. I believe three obstacles — limited time, lack of subject familiarity and thus comfort on the part of educators, and equipment expense — must be overcome to produce a nuclear-educated populace. Educators regularly use webcams to actively engage students in scientific discovery as evidenced by a literature search for the term webcam paired with topics such as astronomy, biology, and physics. Inspired by YouTube videos that demonstrate alpha particle detection by modified webcams, I searched for examples that go beyond simple detection with only one education-oriented result — the determination of the in-air range of alphas using a modified CCD camera. Custom-built, radiation-hardened CMOS detectors exist in high energy physics and for soft x-ray detection. Commercial CMOS cameras are used for direct imaging in electron microscopy. I demonstrate charged-particle spectrometry with a slightly modified CMOS-based webcam. When used with inexpensive sources of radiation and free software, the webcam charged-particle spectrometer presents educators with a simple, low-cost technique to include nuclear physics in science education.

2:54PM Q33.00003 Unveiling Angular Momentum
STEPHEN ROBINSON, Belmont University — Angular momentum is a notoriously difficult concept to grasp. Visualization often requires three-dimensional pictures of vectors pointing in seemingly arbitrary directions. A simple student-run laboratory experiment coupled with intuitive explanations by an instructor can clear up some of the inherent ambiguity of rotational motion. Specifically, the precessional period of a suspended spinning bicycle wheel can be related to the spinning frequency through a simple algebraic expression. An explanation of this precession apart from the concept of angular momentum will be given.

This project was supported by SRC through CNFD, an SRC-NRI Center, by C-SPIN, part of STARnet, and by the NSF through MRSEC DMR-0820521.

This project was supported by SRC through CNFD, an SRC-NRI Center, by C-SPIN, part of STARnet, and by the NSF through MRSEC DMR-0820521.

Supported by the National Science Foundation.
3:06PM Q33.00004 Tracking student progress in a game-like physics learning environment with a Monte Carlo Bayesian knowledge tracing model. GEY-HONG GWEON, HEE-SUN LEE, Univ of California-Santa Cruz, CHAD DORSEY, ROBERT TINKER, WILLIAM FINZER, DANIEL DAMELIN, The Concord Consortium — In tracking student learning in on-line learning systems, the Bayesian knowledge tracing (BKT) model is a popular model. However, the model has well-known problems such as the identifiability problem or the empirical degeneracy problem. Understanding of these problems remain unclear and solutions to them remain subjective. Here, we analyze the log data from an online physics learning program with our new model, a Monte Carlo BKT model. With our new approach, we are able to perform a completely unbiased analysis, which can then be used for classifying student learning patterns and performances. Furthermore, a theoretical analysis of the BKT model and our computational work shed new light on the nature of the aforementioned problems.

1 This material is based upon work supported by the National Science Foundation under grant REC-1147621 and REC-1435470.

3:18PM Q33.00005 Quality of Undergraduate Physics Students’ Written Scientific Arguments: How to Promote Students’ Appropriation of Scientific Discourse in Physics Laboratory Reports? MEHMET AYDENIZ, KUBRA YETER-AYDENIZ, The University of Tennessee, Knoxville — In this study we challenged 18 undergraduate physics students to develop four written scientific arguments across four physics labs: 1) gravity-driven acceleration, 2) conservation of mechanical energy, 3) conservation of linear momentum and 4) Boyle’s law, in a mechanics and thermodynamics laboratory course. We evaluated quality of the written scientific arguments developed by the participants using the Claim, Evidence, Reasoning and Rebuttal (CERR) rubric. The results indicate that while students developed adequate scientific explanations that summarized the findings of their experiments, they experienced unique difficulties in using a persuasive and critical discourse in their written arguments. Students experienced the most difficulty in considering alternative explanations in formulating their written scientific arguments. We elaborate on the implications of these findings for teaching physics laboratories and assessing students’ learning in physics laboratories. We especially focus on the importance of framing in helping students to appropriate the epistemic norms of science in writing scientific arguments.

3:30PM Q33.00006 Comparison of Students’ Ability to Measure Distance using Wavelength in 1D and 2D Settings. GARY WHITE, The George Washington University — When physics students are asked to measure the distance between two fixed locations using a concrete object like a pencil, virtually all respond successfully; however, in some settings, when asked to perform a similar measurement using wavelength as a ruler, there is less success, especially if the students are first asked to note that the “ruler” to be used is not fixed in length (see “Is a Simple Measurement Task a Roadblock to Student Understanding of Wave Phenomena?”, by M. Kryjevskaia, M. Stetzer, and P. Heron, The Physics Teacher 51, 560, (2013) and references therein). I will show some data from introductory classes (algebra- and calculus-based) that replicate this latter result, and also show some interesting features when comparing particular 1D and 2D contexts.

3:42PM Q33.00007 Can you build intuition about quantum mechanics through a game? CHARLES TAHAN, None — We made an app called Meqanic for iOS. To the world, it is a pattern matching game whose rules are very unusual. In reality, it is a functional quantum simulator designed to visualize quantum states and to challenge the user to reconstruct them. The app was released on the Apple App Store in 2014. Here’s what we learned.

3:54PM Q33.00008 Facts and Methods need to be taught GEORGE ZIMMERMAN, Boston University, Emeritus — Current trends in the K-12 educational establishment tend to concentrate on “understanding”, both the “understanding” of how the student thinks and the student’s “understanding” of a concept. In many cases the teaching of facts upon which the student might base his/her “understanding” is neglected. The lack of facts is amplified in our digital age where the exposure to reality is replaced by a virtual experience. This is one of the reasons for the limitations our college students exhibit. Examples in physics and math will be discussed, as well as possible remedies.

4:06PM Q33.00009 Assessing student reasoning in upper-division electricity and magnetism at Oregon State University. JUSTYNA ZWOLAK, Florida International University, CORINNE MANOGUE, Oregon State University — Standardized assessment tests that allow researchers to compare the performance of students under various curricula are highly desirable. There are several research-based conceptual tests that serve as instruments to assess and identify students difficulties in lower-division courses. At the upper-division level, however, assessing students difficulties is a more challenging task. Although several research groups are currently working on such tests, their reliability and validity are still under investigation. We analyze the results of the Colorado Upper-Division Electrostatics diagnostic from Oregon State University and compare it with data from University of Colorado. In particular, we show potential shortcomings in the Oregon State University curriculum regarding separation of variables and boundary conditions. Our work complements and extends the previous findings from the University of Colorado by highlighting important differences in student learning that may be related to the curriculum, illuminating difficulties with the rubric for certain problems and verifying decay in post-test results over time.

Wednesday, April 3, 2015 2:30PM - 5:06PM

Session Q34 DFD: Fluid Dynamics - General 210A - Thomas Solomo, Bucknell University

2:30PM Q34.00001 Time Transient Effects in Heterogeneous Permselective Systems. YOAV GREEN, SINOY BARK, Technion-Israel Institute of Technology — The passage of an electric current through a permselective medium (membranes/nanochannels) under an applied electric field is characterized by the formation of ionic concentration gradients which result in regions of depleted and enriched ionic concentration at opposite ends of the medium, i.e. concentration polarization (CP). In this work, we study the time-transient behavior of the concentration and electric potential distributions in a realistic two dimensional and three layered system (i.e. microchannel-permselective medium-microchannel device). We provide an analytical solution for the concentration under the simplifying assumptions of local-electroneutrality, ideal permselectivity and negligible convection while the electric potential is solved numerically. It is shown that time transient effects occur over the diffusive time scale until steady-state is achieved. The numerical steady state solution is compared with previous analytical results and good quantitative behavior is observed.

2:42PM Q34.00002 Bistability in Inhomogeneity – Effects of Flow Coherent Structures on the Fate of a Bi-stable Reaction ADITYA DHUMUNTARAO, WENBO TANG, Arizona State University — A numerical study on the mixing process of a chemical reaction model between two stable states adjacent to each other in water is presented. The two stable states are equilibriums and are homogenized by fluid stirring and diffusion, and settle into a single stable state. With all other parameters fixed, we find the dependence of the final state on the reacting speed. Interestingly, with the existence of coherent structures, at a range of intermediate speeds, the final state also depends on the flow topology. The exact dependence on flow topology is explored in detail. For this bistable reaction, the elliptic flow structures help maintain scalar concentration and preserve the small impurity. These results attribute to the fundamental connection between the underlying flow topology and the domain transitions of dynamic biogeochemical processes.

1 The authors would like to thank the NSF Grant DMS-1212144.
2:54PM Q34.00003 Convective velocity profiles as a function of applied fields in a magnetic fluid. JUN HUANG, Department of Physics, University of Central Florida, Orlando, TIANSHU LIU, Department of Mechanical and Aerospace Engineering, Western Michigan University, WEILI LUO, Department of Physics, University of Central Florida, Orlando — Natural convection occurs when there is a horizontal temperature gradient across a sample. We have found previously [1] that the convective flow in magnetic fluid responds to applied magnetic fields differently, depending on the relative direction of the gradient of temperature to that of the field. In this work we report the velocity profiles from these flows obtained from optical flow method based on images from temperature-sensitive paint technique. Results from perturbation fields show the direction change of velocity vectors and crossover from two-dimensional to three-dimensional flow for higher fields. The streamline plots indicate formation of local flow structures that could explain the slowing down of the heat transfer when the temperature gradient is anti-parallel to the field gradient. We will discuss the different responses to the applied magnetic fields for two different sample configurations in terms of relative orientation of the temperature and field gradients. [1] Jun Huang and Weili Luo “Heat Transfer Through Convection in a Quasi-One-Dimensional Magnetic Fluid.” Journal of Thermal Analysis and Calorimetry, 113, p449 (2013).

3:06PM Q34.00004 Manifolds and front propagation barriers in advection-reaction-diffusion systems. TOM SOLOMON, Bucknell University — We present experiments on the propagation of reaction fronts in laminar, vortex-dominated flows. The fronts are produced by the excitable Belousov-Zhabotinsky chemical reaction. The flows studied are driven by magnetohydrodynamic forcing techniques and are composed of a single vortex, chains or arrays of vortices, or spatially-disordered flows. In all of these cases, one-way barriers appear that either inhibit front propagation or, in some cases, pin the reactions fronts. We analyze this behavior with a recent theory of burning invariant manifolds (BIMs) that are a generalization of the theory of invariant manifolds developed in the past to characterize chaotic mixing and transport of passive impurities. We demonstrate that the BIMs are responsible for the reaction barriers observed experimentally, and we discuss the applicability of this BIM formalism to a range of flows: time-independent, time-periodic and time-aperiodic.

3:18PM Q34.00005 Tweaks to Turing Patterns, Wavelength Transitions in CDIMA. DELORA GASKINS, EMILY PRUC, MILOS DOLNIK, IRVING EPSTEIN, Brandeis University — Alan Turing predicted that stationary patterns could arise from a uniform state in a system through the processes of reaction and diffusion. Beyond the Turing instability, there exist spatially periodic states with different wavelengths. Pattern transitions, including those transitions to patterns of differing wavelengths are of interest in reaction-diffusion systems including ecological systems with patterned biomass prone to desertification. We study pattern transitions in the chlorine dioxide-iodine-malic acid (CDIMA) system which is the prototypical system for the study of Turing patterns in chemical systems. Additions of selected halides (bromides and chlorides) to the system in its patterned state have led to the observation of up to a five fold increase in wavelength. With the concentration of these halides as bifurcation parameter we observe that these large wavelength patterns are bistable with the uniform steady state. We explore the pattern wavelength selection of this system. Wavelength halving and super lattice structure formation result from transitions between patterns of different wavelengths.

3:30PM Q34.00006 Simplistic Approach to Characterize Sloshing Phenomena using CFD Simulation. MD MAHMUD, Lamar University, RAFIGUL KHAN, Cameron Corporation, QIANG XU, Lamar University — Liquid sloshing in vessels caused by forced acceleration has been the subject of intense investigations for last several decades both by experiments and numerical simulations. Many studies are done to minimize the sloshing induced forces on the vessel internals and some studies focused on different ways to describe the sloshing patterns. Most of the sloshing characterization methods are done using complex mathematical manipulation and more simplified method may be useful for better practical understanding. In this study, simple/easily understandable methods are explored to describe sloshing phenomenon through Computation Fluid Dynamics (CFD) simulation. Several parameters were varied including liquid level/tank length ratio, wave induced vessel motions, motion frequency, amplitudes in various sea state conditions. Parameters such as hydrodynamic force, pressure, moments, turbulent kinetic energy, height of the free surface, vorticity are used to quantify the sloshing intensity. In addition, visual inspections of sloshing motion are done through gas-liquid/oil-water interface fluctuation, streamlines, vector profiles. An equation connecting independent variables to resultant quantities will be established that will be established that will make it easier to describe the sloshing.

3:42PM Q34.00007 Onset of motion of a particle attached to a wall in a linearly sheared fluid flow. ARSHAD KUDROLLI, DAVID SCHEFF, BENJAMIN ALLEN, Department of Physics, Clark University — We examine the onset of motion of particle on a bumpy surface which is exposed to a linear shear fluid flow by means of moving a top surface parallel to the bottom surface on which the particle rests with a prescribed shear rate. This system can be considered as a particularly simple limit of a granular bed exposed to a fluid flow, where forces and torques acting on the particles can be clearly determined. The control parameters available to us include the relative size of the particle to the bumps, the relative size of the particle to the gap thickness, and the flow Reynolds number controlled by the density of the particle and the viscosity of the fluid. Further, the degree of exposure of the particle to the fluid flow is measured by means of adding tracer particles to the fluid and measuring the flow field around the particle. By measuring the critical shear rate at onset of motion as a function of control parameters, we estimate the relative magnitude of forces and torques acting due to drag, lift, and gravitational forces on the particle. We contrast the torque balance and force balance conditions obtained using analytical expressions and numerical simulations with those observed in our experiments.

3:54PM Q34.00008 Kelvin wake pattern and wave resistance at large Froude numbers. MICHAEL BENZAQUEN, ALEXANDRE DARMON, ELIE RAPHAËL, UMR CNRS 7083 Gulliver, ESPCI ParisTech — Recently, M. Rabaud and F. Moisy provided an analysis of airborne observations of ship wakes [1]. Their conclusion that the angle of the wake was no longer constant when varying the hull Froude number Fr drew the attention of the scientific community, as it was in contradiction with Kelvin’s century old theory of ship waves. We perform a mathematical study to understand these surprising observations [2]. Modelling the moving object by a pressure field symmetrical about a point, we analytically show that the angle delimiting the wake region outside which the surface is essentially flat actually remains constant and equal to the Kelvin angle, whereas the angle corresponding to the maximum amplitude of the waves indeed decreases to the Froude number, scaling as 1/Fr for large Froude numbers. To correctly reflect the elongated geometry of boats, we extend our calculations to anisotropic objects and show that the angle corresponding to the maximum amplitude of the waves also depends on the aspect ratio W of the object and scales as $\sqrt{W/Fr}$ for large Froude numbers [3].

Increased swimming efficiency using thickness-varying flexible fins. PETER YEH, YUANDA LI, ALEXANDER ALEKSEEV, Georgia Institute of Technology — We use three dimensional computer simulations to probe the hydrodynamics and deformation of oscillating flexible fins with varying thickness. We model the fin as an elastic rectangular plate undergoing a plunging motion at its leading edge. Since we assume that the thickest part of the fin is very small compared to its other length scales, the plate is modeled as infinitely thin. We simulate the thickness gradient by introducing an appropriate mass gradient and stiffness gradient in the plate. We characterize the steady state swimming velocity, input power, and swimming efficiency as a function of driving frequency and thickness ratio (between the thickest and thinnest part). Our simulations show that the swimming economy, the ratio between the velocity and input power, is increased when the trailing edge is thinner. These findings help to identify the physical mechanisms that allow fish to have high swimming efficiency.

Nozzle Spray Delivery Studies for High-Viscosity Shear-Thinning Fluids. SMITA AGRAWAL, MIKE CLOETER, YUXI ZHANG, JANA RAJAN, JAIME CURTIS-FISK, PUSPENDU DEO, BILLY SMITH, The Dow Chemical Company — Experiments were performed to explore the spray of shear-thinning polymer solutions through various nozzles. High speed images near the nozzle exit, drop size distributions, and spatial mass flow distributions were analyzed with the shear-thinning fluids and deionized water for comparison for seven different nozzles with pressure drops up to 40 psi. The nozzles tested include full cone, hollow cone, and flat fan nozzles. The aim was to identify suitable nozzles that would give droplet sizes in the range of 100-2000 µm for the shear-thinning fluids. It was found in general that the shear-thinning fluids led to formation of ligament like structures whereas sheet perforation was more predominant with deionized water. The spray break up was delayed with the shear-thinning fluids. The spray of the shear-thinning fluids also led to an increase in the median drop size with the extent of increase being dependent on the nozzle type. The spray angle was found to be reduced by around 20° at a distance of 12" when compared to that of distilled water. This study lends fundamental insights into spray characteristics for a wide range of spray nozzles with high viscosity shear-thinning solution as compared to spraying deionized water with the same nozzles.

Designing a Micromixer for Rolling Circle Amplification in Cancer Biomarker Detection. HAYRIYE ALTURAL, Department of Electrical and Computer Engineering, Boston University — Rolling circle amplification (RCA) is an alternative method to the Polymerase Chain Reaction based amplification for point-of-care (POC) diagnosis. In future personalized cancer diagnostic for POC applications, smaller, faster and cheaper methods are needed instead of costly and time-consuming laboratory tests. Microfluidic chips can perform the detection of cancer biomarkers within less analysis time, and provide for improvement in the sensitivity and specificity required for biochemical analysis as well. Rapid mixing is essential in the chips used in cancer diagnostic. The goal of this study is to design a micromixer for rapid RCA-based analysis and develop the assay time in cancer biomarker detection. By combining assays with micromixers, multi-step bioapplications in microfluidic chips may be achieved with minimal external control. Here, simulation results related to the micro mixer are obtained by COMSOL software.

This work was supported by the NSF grant No. DMR-1147430. E.J.T.H. acknowledges partial support by CONACYT, Mexico.

Wednesday, March 4, 2015 2:30PM - 5:30PM – Session Q35 DAMOP: Many-body Localization and Disordered Optical Lattices

Quantum computation using many-body localization. SOONWON CHOI, SARANG GOPALAKRISHNAN, Harvard Univ, NORMAN YAO, University of California Berkeley, MIKHAIL LUKIN, Harvard Univ — Conventional wisdom holds that a stable quantum bit — the building block for a quantum computer — requires an isolated degree of freedom. Here, we explore a new approach to quantum information processing based on many-body localization (MBL). In condensed-matter physics, MBL occurs when many-body interactions confine quantum dynamics to a localized phase. Unlike in other phases of matter, no emergent symmetry is realized in MBL — the quasiparticles are indistinguishable, and density matrices are highly entangled. The presence of MBL is characterized by quantum phase transitions, which can be monitored using a number of unique features of an MBL phase: a lack of thermalization, a locally gapped spectrum, and slow dephasing. We illustrate our main idea using a spin-1 model, and develop the assay time in cancer biomarker detection. By combining assays with micromixers, multi-step bioapplications in microfluidic chips may be achieved with minimal external control. Numerical simulations based on the boundary integral method showed a good agreement with the experimental findings.

Rapid mixing is essential in the chips used in cancer diagnostic. The goal of this study is to design a micromixer for rapid RCA-based analysis and develop the assay time in cancer biomarker detection. By combining assays with micromixers, multi-step bioapplications in microfluidic chips may be achieved with minimal external control. Here, simulation results related to the micro mixer are obtained by COMSOL software.

Traveling Wave Electrophoresis Due To Selective Currents At Electrodes. WILLIAM BOOTH, BOYD EDWARDS, Utah State University — Abstract Using COMSOL finite element modeling software we simulate a 2D traveling-wave electrophoresis (TWE) device for microfluidic chromatography and electrophoretic concentration. A periodic array of four electrodes each produce AC potentials shifted by a quarter-period from one another. This yields an electric wave which travels down the channel. Ions of varying mobilities in solution are carried along with the electric wave or left behind at different rates. We employ a simplified model for asymmetric reactions at the electrodes in order to solve the issue of electric double layer shielding at the electrodes. The selective reactions allow for the formation of diffusion layers of ions which attempt to follow the traveling electric wave. We examine the formation of these diffusion layers and how various system parameters affect motion of various ions through the system. With easy control over the traveling electric wave’s frequency and direction one may employ this method for concentrating or separating bands of electrolytes.

Travelling Wave Electrophoresis Due To Selective Currents At Electrodes. WILLIAM BOOTH, BOYD EDWARDS, Utah State University — Abstract Using COMSOL finite element modeling software we simulate a 2D traveling-wave electrophoresis (TWE) device for microfluidic chromatography and electrophoretic concentration. A periodic array of four electrodes each produce AC potentials shifted by a quarter-period from one another. This yields an electric wave which travels down the channel. Ions of varying mobilities in solution are carried along with the electric wave or left behind at different rates. We employ a simplified model for asymmetric reactions at the electrodes in order to solve the issue of electric double layer shielding at the electrodes. The selective reactions allow for the formation of diffusion layers of ions which attempt to follow the traveling electric wave. We examine the formation of these diffusion layers and how various system parameters affect motion of various ions through the system. With easy control over the traveling electric wave’s frequency and direction one may employ this method for concentrating or separating bands of electrolytes.

Floating Wave Electrophoresis Due To Selective Currents At Electrodes. WILLIAM BOOTH, BOYD EDWARDS, Utah State University — Abstract Using COMSOL finite element modeling software we simulate a 2D traveling-wave electrophoresis (TWE) device for microfluidic chromatography and electrophoretic concentration. A periodic array of four electrodes each produce AC potentials shifted by a quarter-period from one another. This yields an electric wave which travels down the channel. Ions of varying mobilities in solution are carried along with the electric wave or left behind at different rates. We employ a simplified model for asymmetric reactions at the electrodes in order to solve the issue of electric double layer shielding at the electrodes. The selective reactions allow for the formation of diffusion layers of ions which attempt to follow the traveling electric wave. We examine the formation of these diffusion layers and how various system parameters affect motion of various ions through the system. With easy control over the traveling electric wave’s frequency and direction one may employ this method for concentrating or separating bands of electrolytes.

Dynamics of interacting quantum systems near the transition to a many-body localization phase. E. JONATHAN TORRES-HERRERA, Department of Physics, Yeshiva University, New York, NY 10016 and Instituto de Fisica, Benemerita Universidad Autonoma de Puebla, Puebla 72570, Mexico, LEA F. SANTOS, Department of Physics, Yeshiva University, New York, NY 10016, USA — Many-body localization (MBL) has become a very active field of research. The interest in the subject is motivated by indications of the existence of a MBL phase transition and by advances in experiments with optical lattices, which may serve as testbeds for corroborating theoretical predictions. A paradigmatic system that exhibits a MBL phase transition is the one-dimensional Heisenberg model with on-site disorder. Here, we study the dynamics of these systems. In particular, we report the observation of a power-law decay of the fidelity (survival probability) near the MBL transition. We provide numerical evidence suggesting that the exponent of this decay is related to the multifractal structure of the eigenstates through the so-called correlation dimension.

This work was supported by the NSF grant No. DMR-1147430. E.J.T.H. acknowledges partial support by CONACYT, Mexico.
to the inclusion of interatomic interaction effects are also discussed. Hamiltonian, as well as in terms of an effective model consisting of an open quantum system with a small number of degrees of freedom. Preliminary approaches strength; and the distance over which the harmonic trap is displaced. We analyse these results in terms of the population of eigenstates of the post-quench experiment, the pre-quench potential consists of an optical lattice, a harmonic trap, and uncorrelated site disorder (produced, for example, by exposing the

We present results for the post-quench evolution of the density profile as the following parameters are varied: the pre-quench chemical potential; the disorder dependence for sample-to-sample density fluctuations. We, furthermore, examine the equilibration of the system to generalized thermodynamic statistical properties of the single-particle disordered wave functions and analyze their behavior as a function of disorder. In particular, we find a non-monotonic from a thermal environment. We relate several physical observables of the system (including their temporal as well as sample-to sample fluctuations) to the localization-delocalization transition? In particular, does the system thermalize at the transition? In this talk, I will show that certain general considerations involving the behavior of entanglement entropy close to the transition imply that at a continuous many-body localization transition, the system is fully thermalized in the sense that critical eigenstates show ergodic behavior.

Numerical data, obtained by exact diagonalization and time-evolving block decimation methods, suggests a direct transition between the two phases. Our results in terms of an extensive number of emergent local integrals of motion (LIOM), which naturally explains the spectral and dynamical properties of this phase.

PONTE, ZLATKO PAPIC, Perimeter Institute for Theoretical Physics, FRANCOIS HUVENEERS, University of Paris — We consider disordered many-body systems with periodic time-dependent Hamiltonians in one spatial dimension. By studying the properties of the Floquet eigenstates, we identify two distinct phases: (i) a many-body localized (MBL) phase, in which almost all eigenstates have area-law entanglement entropy, and the eigenstate thermalization hypothesis (ETH) is violated, and (ii) a delocalized phase, in which eigenstates have volume-law entanglement and obey the ETH. MBL phase exhibits logarithmic in time growth of entanglement entropy for initial product states, which distinguishes it from the delocalized phase. We propose an effective model of the MBL phase in terms of an extensive number of emergent local integrals of motion (LIOM), which naturally explains the spectral and dynamical properties of this phase. Numerical data, obtained by exact diagonalization and time-evolving block decimation methods, suggests a direct transition between the two phases. Our results show that many-body localization persists for sufficiently weak periodic driving, and that MBL-delocalization transition can be induced by sufficiently strong driving. [1] P. Ponte, Z. Papic, F. Huveneers, D. A. Abanin, arXiv:1410.8518 [2] P. Ponte et al., arXiv:1403.6480

PONTE, Z. Papic, Perimeter Institute for Theoretical Physics, UC Santa Barbara — It has been recently found that sufficiently disordered, isolated quantum systems may fail to thermalize leading to a ‘many-body localized’ phase. In this phase the basic tenet of equilibrium statistical mechanics, namely, the equal likelihood for all microstates with the same energy, breaks down. A fundamental question is what happens as the disorder becomes weaker so that one approaches the localization-delocalization transition? In particular, does the system thermalize at the transition? In this talk, I will show that certain general considerations involving the behavior of entanglement entropy close to the transition imply that at a continuous many-body localization transition, the system is fully thermalized in the sense that critical eigenstates show ergodic behavior.

We theoretically study a quantum quench in a fermionic lattice model that exhibits Anderson localization, in which a disorder potential is suddenly turned on in isolation from a thermal environment. We relate several physical observables of the system (including their temporal as well as sample-to-sample fluctuations) to the statistical properties of the single-particle disordered wave functions and analyze their behavior as a function of disorder. In particular, we find a non-monotonic disorder dependence for sample-to-sample density fluctuations. We, furthermore, examine the equilibration of the system to generalized thermodynamic ensembles. We relate several of the observed features to the crossover from extended to localized behavior.

In our proposed experiment, the pre-quench potential consists of an optical lattice, a harmonic trap, and uncorrelated site disorder (produced, for example, by exposing the atoms to laser speckle). The post-quench potential is the same, but with the centre of the harmonic trap shifted to one side. In the non-interacting case, we present results for the post-quench evolution of the density profile as the following parameters are varied: the pre-quench chemical potential; the disorder strength; and the distance over which the harmonic trap is displaced. We analyze these results in terms of the population of eigenstates of the post-quench Hamiltonian, as well as in terms of an effective model consisting of an open quantum system with a small number of degrees of freedom. Preliminary approaches to the inclusion of interatomic interaction effects are also discussed.
4:18PM Q35.00010 Exact mobility edge in one dimensional quasiperiodic lattices

SRIRAM GANESHAN, University of Maryland, College Park — We present localization properties of a family of nearest neighbor tight binding models with quasiperiodic onsite modulation. We prove that this family is self-dual under a generalized transformation. The self-dual condition for this general model turns out to be a closed form function of model parameters and energy. We numerically verify that this self-dual line is a mobility edge separating the localized and extended states. Our model is a first of its kind example of a nearest neighbor tight binding model with duality symmetry manifesting mobility edge. Our model provides analytical insight into the mobility edge physics of Anderson localization, a feature occurring in three or more dimensions. Quasiperiodic 1D lattices have been realized in ultracold atoms by a standing wave arrangement of two laser beams with mutually incommensurate wave vector. The quasiperiodic potentials we considered in this work can be systematically engineered by a controlled application of series of standing wave laser beams. We present a concrete schematic to realize our results in optical lattices and photonic waveguides.

3Supported by JQI-NSF-PFC.

4:30PM Q35.00011 Phase diagram of bosons trapped in a two-dimensional quasi-periodic lattice

CHAO ZHANG, Homer L. Dodge Department of Physics and Astronomy, The University of Oklahoma, Norman, Oklahoma, 73019, USA, ARGHAVAN SAFAVI-NAINI, JILA and Department of Physics, University of Colorado, 440 UCB, Boulder, CO 80309, USA, BARBARA CAPOGROSSO-SANSONE, Homer L. Dodge Department of Physics and Astronomy, The University of Oklahoma, Norman, Oklahoma, 73019, USA — We report on results of Quantum Monte Carlo simulations for bosons in a two dimensional quasi-periodic optical lattice. We study the ground state phase diagram at unity filling and confirm the existence of three phases: superfluid, Mott insulator, and Bose glass. At lower interaction strength, we find that sizable disorder strength is needed in order to destroy superfluidity in favor of the Bose glass. On the other hand, at large enough interaction, superfluidity is completely destroyed in favor of the Mott insulator (at lower disorder strength) or the Bose glass (at larger disorder strength). At intermediate interactions, the system undergoes an insulator to superfluid transition upon increasing the disorder, while a further increase of disorder strength drives the superfluid to Bose glass phase transition.

4:42PM Q35.00012 Superfluid - Insulator transition for bosons in disordered and quasi-periodic potentials


4:54PM Q35.00013 Characterizing the Bose Glass Phase in Disordered Optical Lattices

ERIC WELCH, ADAM CHALUPA, BYOUNGHAK LEE, Texas State Univ-San Marcos — We present a theoretical study of disordered optical lattices using a mean-field approach to the Bose-Hubbard model. Through analyses on simple disorder configurations, such as binary and ternary random disorder potentials, we find that the phase transition at each lattice site is directly between Mott insulator and superfluid, contrary to the spatially averaged phase, where the transition between Mott insulator and superfluid is through the Bose glass phase. We also discuss the instability of the Bose glass phase in uniformly disordered systems in the terms of spatially averaged pure systems with chemical potential offsets.

5:06PM Q35.00014 Searching for the Bose glass in disordered optical lattices with center-of-mass dynamics

MI YAN, VITO SCAROLA, Virginia Tech — Ultracold atomic gases placed in optical lattices realize distinct many-body phases, including superfluids and Mott insulators. The addition of controlled disorder induces an additional phase, a Bose-Glass phase, that is difficult to unambiguously identify experimentally. We apply the time-dependent Gutzwiller mean-field method to model the transport properties of interacting bosons confined in disordered optical lattices after a sudden displacement of the underlying harmonic trapping potential. The edge superfluid is used to distinguish Bose glass and Mott insulator phases in the center of the trap by different center-of-mass dynamical signatures. We find that the edge superfluid oscillates after collision with the central Mott state. But the edge superfluid only drifts through a central Bose glass with a characteristic linear signature in long-time dynamics. Our work provides a method for experimental identification of the Bose glass in cold atom systems.

5:18PM Q35.00015 Impurity-doped Bose-Einstein Condensates in Multi-mode Cavities

SHAHRIAR SHADKHOO, ROBJIN BRUINSMA, Univ of California - Los Angeles — We study impurities in a Bose-Einstein Condensate (BEC), trapped in a multi-mode cavity which is transversely laser-pumped. The pure system has been proposed to exhibit emergent crystallinity for sufficiently strong pumping, and is therefore described by the quantum version of the fluctuation-induced first order phase transitions. We address the ground state of a quantum impurity coupled to the BEC, away from and near the phase transition. We show that this model system supports various perturbative and non-perturbative excitations around the particle. Light impurities form large and small polarons, whereas solitonic solutions may appear around heavier impurities. The effects of quantum and thermal fluctuations are also investigated.

Wednesday, March 4, 2015 2:30PM - 5:18PM – Session Q36 DPOLY: Focus Session: Self-assembled Block Copolymers and Soft Nanoparticles in Solution II
2:30PM Q36.00001 Topologically Active Soft Materials for Cellular Delivery, CECILIA LEAL, University of Illinois, Urbana-Champaign — Lyotropic lipid liquid crystalline materials having nanostructures that deviate from the conventional flat bilayer arrangement such 2D hexagonally packed lipid tubes and bicontinuous channels have been increasingly recognized as relevant materials for the applications of gene and drug delivery as well as linked to the functionality of cellular organelles comprising lipid-membranes. The simple argument that non-bilayer phases such as bicontinuous cubic having 3D nanostructured interwoven channels have a higher surface-to-volume ratio enabling more point contacts with cell surfaces while having a larger encapsulation power to host drug/gene molecules might be insufficient to completely describe the experimental findings. In this work we will show our recent efforts in stabilizing topologically rich lipid-based materials incorporating drugs or nucleic acids in diverse morphologies such as: i) bulk, ii) dispersed in an aqueous solution, iii) as well as thin film coatings. We utilize a combinatorial technical approach including Small/Wide Transmission/Grazing Incidence X-ray Scattering structural characterization and Cell Culture methods to demonstrate that a judicious choice of lipid materials allows an incredibly rich phase behavior in bulk, solution, and thin film platforms. Furthermore, the systems can be tailored to be adaptive in response to a number of environmental cues. The general finding is that lipid-based materials comprising negative Gaussian curvature membranes are able to most efficiently deliver their cargo across cell membranes by lowering the energy cost of forming a membrane pore. These new materials have great potential in the particular field of responsive and self-healing materials for surface-based and systemic drug/gene delivery devices as well as bioadhesive drug delivery.

3:06PM Q36.00002 Control of Nanostructure of Block Copolymer Particles through Size and Aspect Ratio-controlled Nanoparticle Surfactants, KANG HEE KII, JAE MAN SHIN, HYUNSEUNG YANG, BUMJOON J. KIM, KAIST — Due to the high surface area of nanometer-sized colloidal particles relative to their volume, the interfacial interaction between block copolymer (BCP) chains and surfactant surrounding the emulsion droplet greatly affects the final internal morphology of BCP particles. Convex lens-like functional BCP particle with defect-free porous cylindrical channels was created via precise design of interfacial interactions between Nanoparticle (NP) surfactants and BCPs. The effect of size and aspect ratio of nanorod (NR) surfactants on the shape and internal morphology of BCP particles was systemically investigated using polystyrene-b-poly(4-vinylpyridine), Au NPs, and CuPt NPs. Both size and shape-induced segregation of NPs generated the balanced interfacial interaction between BCPs and water, and this neutralized interface combined with the directionality of solvent generated defect-free, vertically ordered porous channels within the particles. Furthermore, these particles could possess unique optical, chemical and catalytic property by loading various metal nanoparticles into the porous channels.

3:18PM Q36.00003 Multiple Phases of Binary Micellar Crystals Derived from Aqueous Solutions of Charged Block Copolymers, KOOKHEON CHAR, SEYOUNG KIM, Seoul National University, SOO-HYUNG CHOI, Hongik University, SHENG LI, DuPont Central Research and Development — Amphiphilic block copolymer containing weak polyelectrolyte blocks can induce surface-charged block copolymer micelles (BCM) in aqueous media and, at the same time, their charge densities can be finely tuned by pH of the media. Poly(styrene-block-poly(acrylic acid) and poly(styrene-block-poly(4-vinylpyridine) BCMs, whose signs of surface charges are opposite in a relevant pH window, can self-assemble together via electrostatic interactions. By mixing of these charge-tuned BCMs, we obtained binary micellar complexes showing strong crystalline habits and assigned their crystal structures with small-angle neutron scattering and other techniques. We demonstrate multiple phases of binary micellar crystals derived from a set of BCM mixtures of which size and charge ratios are varied. The dependence of the size ratio of individual phases is proven to be different from that of rigid nanoparticles such as inorganic nanocrystals. We believe that this deviation from the hard-matter superlattices is due to the deformability of BCMs based on soft building units. That is to say that BCMs can be readily deformed by good solvent and can modify their structure from spheres to other anisotropic shapes while they assemble together.

3:30PM Q36.00004 Structure and Self-Assembly of Thermoreversible Triblock Copolymer Micelles and Gels, VIVEK PRABHU, NIST, 100 Bureau Drive, Gaithersburg, Maryland, SHRINIVAS VENKATARAMAN, YI YANG, Institute of Bioengineering and Nanotechnology, 31 Biopolis Way, The Nanos Singapore, JIM HEDRICK, IBM Almaden Research Center, San Jose, California — The polymer physics of hierarchical, self-assembled block copolymer solutions remains an active area of research for both advanced materials and biomaterial applications. Of current interest is the development of aliphatic polycarbonates for biomedical applications [1]. For instance, cholesterol-functionalized aliphatic polycarbonate diblock copolymers of polyethylene glycol formed disk and stacked disk-like self-assembled morphologies that are nano-carriers for hydrophobic molecules [2]. The hydrophobic nature of the cholesterol block provides a versatile platform to form complex morphologies in solution. The presentation will describe the phase diagram, structure and dynamics of the micelles and gels formed by well-defined triblock copolymers prepared with cholesterol and fluorene hydrophobic end-groups. The hierarchical structure of these thermoreversible gels as a function of hydrophobic end-group molecular weight was studied by small-angle neutron scattering and static and dynamic light scattering covering nm-to-micron length scales and microsecond-to-second time scales. [1] F. Suriano, O. Coulembier, J.L. Hedrick, P. Dubois, Polym. Chem. 2, 528 (2011). [2] S. Venkataraman, A.L. Lee, H.T. Maune, J.L. Hedrick, V.M. Prabhu, and Y.Y. Yang, Macromolecules 46, 4839 (2013).

3:42PM Q36.00005 BREAK —

3:54PM Q36.00006 Assembly of Block Copolymer-Nanoparticles Conjugates Towards Sub-10-nm Hybrid Ordered Nanostructures, ZHIWEI LIN, PENGTAO LU, CHIH-HAO HSU, STEPHEN CHENG, Univ of Akron — Precisely controlled locations of nanoparticles (NPs) in block copolymers (BCP) and design of BCP/NPs hybrid nanostructures have attracted numerous research interests over the past several decades. In this work, two series of BC-NP conjugates, composed of a hydrophilic fullerene (AC60) NP tethered with a polystyrene-block-poly(ethylene oxide) (PS-b-PEO) at the PS chain end (AC60-b-PS-b-PEO) or the junction point (PS-AC60-b-PEO), were utilized to investigate assemblies of these two series conjugates in the bulk. It was revealed that the incorporation of AC60 NPs induces the nano-phase separation of intrinsically disordered PS-b-PEO with low molecular masses. A variety of ordered nanostructures were found including lamellae, double gyroids and cylinders with domain sizes smaller than 10 nm. The different architectures of these conjugates provided evidence of how the NPs are located and distributed within the nano-phase separated PS-b-PEO, and in turn, demonstrated significant effects of these NPs on the stabilization of these originally unstable structures.

4:06PM Q36.00007 Giant Molecules based on Precisely Functionalized POSS Nano-atoms: Tuning from Crystals to Frank-Kasper and Quasicrystal Phases, STEPHEN Z. CHENG, MINGJUN HUANG, KAN YUE, CHIH-HAO HSU, ZHIWEI LIN, University of Akron — In order to create new functional materials for advanced technologies, precisely control over functionalities and their hierarchical structures as well as orders is vital for obtaining the desired properties. Among all the giant molecules, giant surfactants and giant polyhedra draw us the special focus. Giant surfactants are constructed via tethering polymers tails to the precisely functionalized polyhedral oligomeric silsesquioxane (POSS) or fullerene (C60) molecular nano-particles (MNPs) (so called “nano-atoms”) heads. The heads and tails thus have drastic chemical differences to impart amphiphilicity. Giant polyhedra were created by integrating polyhedron framework with differently functionalized POSS nano-atoms, which further introduce the designed symmetry breaking of positional interactions. A series of novel giant surfactants with multiple polymer tails and giant tetrahedra are utilized as building blocks to construct into hierarchically ordered suprastructure systems ranging from crystals, to Frank-Kasper and quasicrystal phases in the condensed bulk state and thin films. This reveals evidently the interconnections between soft matters and hard matters in sharing their common structures and fundamental knowledge.
4:18PM Q36.00008 Kelvin Problem and Sphericity Metric in the Packing Structures of Soft Particles, SANGWOO LEE, Rensselaer Polytechnic Institute, CHRIS LEIGHTON, FRANK BATES, University of Minnesota — Attractive hard spheres are known to prefer to form close-packing structures. In contrast, soft particles develop non-close-packing structures, e.g., body-centered cubic (BCC), which Kelvin proposed a century ago as the array of densely packed monodisperse soft particles with lowest surface area per unit volume. Remarkably, nearly all packing structures by self-assembled soft particle domains in surfactants, dendrimers, and block polymers are also non-close-packed and appear a set of common symmetries. We found this commonality can be reasoned based on careful observations on the equilibration process occurring in the formation of a Frank-Kasper σ-phase in a poly(1,4-isoprene-b-DL-lactide) diblock polymer specimen. The formation of a low symmetry σ-phase occurred by statistically selective mass-exchanges between particle domains, which resulted in volume multiplicity and this process eventually lowered the surface area per unit volume, i.e., better sphericity of particle domains. This example demonstrates that the isovolume condition in the Kelvin problem, which also was assumed in the Wearn-Phelan (A15) structure is not necessary for the natural systems.

4:30PM Q36.00009 Tunable Encapsulation Structure of Block Copolymer Coated SWNTs in Aqueous Solution, YOUNGYU HAN, SUK-KYUN AHN, ZHE ZHANG, GREGORY S. SMITH, CHANGWOOD DO, Oak Ridge National Laboratory — Nano-sized and shape-tunable molecular building blocks can provide great opportunities for the fabrication of precisely controlled nanostructures. In this work, we have fabricated a molecular building block of single-walled carbon nanotubes (SWNTs) coated by block copolymers whose encapsulation structure can be controlled via temperature or addition of small molecules. The structure and optical property of SWNT-block copolymer have been investigated by small angle neutron scattering (SANS), ultraviolet-visible (UV-vis) spectroscopy, atomic force microscopy (AFM), and molecular dynamics (MD) simulation. The structure of hydrated block copolymer layer surrounding SWNT can be controlled reversibly by varying temperature as well as irreversibly by adding 5-methylsalicylic acid (5MS). Increasing hydrophobicity of the polymers with temperature and strong tendency of 5MS to interact with both block copolymers and π orbitals of SWNTs are likely to be responsible for the significant structural change of the block copolymer encapsulation layer. Our results show an efficient and simple way to fabricate and manipulate carbon-based nano building blocks in aqueous systems with tunable structure.

4:42PM Q36.00010 Pickering emulsion stabilized by highly luminescent carbon nanodots, MINXIANG ZENG, ZHENGDONG CHENG, Texas A&M Univ — Graphene quantum dots as a novel form of nanocarbons have been attracting increasing interest in the past decade owing to their low cytotoxicity, chemical inertness, cost effectiveness, and biocompatibility. However, few work has been done regarding applying carbon-based quantum dots in surfactant synthesis. The diversity and facility of surface chemistry on graphene quantum dots make them strong candidate as novel amphiphilic materials. The tunable assembly of graphene surfactant dots were synthesized and stabilized emulsions of water/oil were investigated. Also, the amphiphilicity of graphene quantum dots is tunable upon various organic functional groups. The ease synthesis of chemically modified graphene quantum dots would enable new opportunities in applying carbon-based materials on solution processing, such as enhanced oil recovery.

4:54PM Q36.00011 Preparation of uniform-sized block copolymer particles by membrane emulsification, JAE-MIN SHIN, KAIST, MINSOO KIM, GI-RA YI, Sungkyunkwan University, BUMJOON KIM, KAIST, SUNGKYUNKWAN UNIVERSITY COLLABORATION — Block copolymer (BCP) particles have been intensively studied due to their unique internal and surface structures, but their applications have been limited mainly due to inherent polydispersity in the particle size arising from the fabrication technique. Here, monodisperse polystyrene-block-polybutadiene (PS-b-PB) BCP particles with unique internal morphology were successfully prepared using Shirasu Porous Glass membrane emulsification. Systematic study on the process parameters in the membrane emulsification, such as membrane pore size, operation pressure, and surfactant concentration was performed to obtain the uniform-sized BCP particles, which generally showed coefficient of variation (CV) value under 10%. Moreover, we successfully extended our method of membrane emulsification to other polystyrene-block-poly(4-vinylpyridine) (PS-b-P4VP) particles, in which P4VP domains were selectively metallized, producing uniform-sized BCP hybrid particles.

5:06PM Q36.00012 Highly luminescent polymer particles driven by thermally reduced graphene quantum dot surfactants, HYUNSEUNG YANG, DONG JIN KANG, KANG HEE KU, HAN-HEE CHO, CHAN HO PARK, JUNHYUK LEE, DOH C. LEE, Korea Advanced Institute of Science and Technology(KAIST), PULICKEL M. AJAYAN, Rice University, BUMJOON J. KIM, Korea Advanced Institute of Science and Technology(KAIST), RICE UNIVERSITY COLLABORATION — We report the use of highly luminescent graphene quantum dot surfactants to drive Pickering emulsions and novel polymer particles. To generate the QGD surfactants, the surface properties of 10 nm sized, non-reduced QGDs (nQGDs), which have strong hydrophilicity, were synthesized and modified in a systematic manner by the thermal reduction of oxygen-containing groups at different treatment times. In stark contrast to the behavior of the nQGDs, thermally reduced QGDs (rQGDs) can produce highly stable Pickering emulsions of oil-in-water systems. To demonstrate the versatility of the rQGD surfactants, they were applied in a mini-emulsion polymerization system that requires nanoparticle surfactants to synthesize submicron-sized polystyrene particles. In addition, the use of rQGD surfactants can be extended to generating block copolymer particles with controlled nanostructures. Particularly, the polymer particles were highly luminescent, a characteristic produced by the highly fluorescent QGD surfactants, which has great potential for various applications, including bioimaging, drug delivery, and optoelectronic devices. To the best of our knowledge, this is the first report in which nanosized QGDs were used as surfactants.

Wednesday, March 4, 2015 2:30PM - 5:30PM
Session Q37 GQI: Focus Session: Semiconductor Qubits - Hybrid Systems and Electrons Floating on Liquid Helium 212A - Steve Lyon, Princeton University

2:30PM Q37.00001 Semiconductor double quantum dot micromaser, YINYU LIU, Department of Physics, Princeton University, Princeton, New Jersey 08544 — The coherent generation of light, from masers to lasers, relies upon the specific structure of the individual emitters that lead to gain. Circuit quantum electrodynamics (cQED) allows strong coupling between microwave photons and a solid-state quantum device. Photon emission has recently been observed from a cavity coupled double quantum dot. Here we demonstrate a two atom maser that is created by coupling two double quantum dots (DQDs) to a microwave cavity. Charge transport through the DQDs results in a gain as large as 1000 in the cavity transmission. With no cavity drive, the free emission spectrum has a linewidth of 34 kHz, which corresponds to a coherence length of 3 km. We verify maser action by comparing the statistics of the emitted microwave field above and below the maser threshold.

1Research was performed in collaboration with Jiri Stehlik, Christopher Eichler, Michael Guillans, Jake Taylor and Jason Petta. We acknowledge support from the Sloan and Packard Foundations, ARO, DARPA, and the NSF.

Magnetic Fields, NODAR SAMKHARADZE, PASQUALE SCARLINO, ALESSANDRO BRUNO, LEONARDO DI CARLO, LIEVEN VANDERSYPEN.

...is the typically poor performance of these resonators in high magnetic fields. We present a novel design of microwave resonators based on NbTiN nanowires, which retain intrinsic quality factors above $10^5$.

...The crossover from the strong coupling regime to the weak coupling regime is observed at 200 mK allowing for the generation of entanglement between spatially separated spin qubits [1].

...Our findings can be used to scale up spin quantum bit architectures.

...We observe a hysteretic evolution of the phase of the microwave signal as a function of the external magnetic field, stemming from the spin valve behavior of the double quantum dot (DQD) maser. In characterizing the gain of this device we find that, in addition to the direct stimulated emission of photons, there is a large contribution from transitions that involve the simultaneous emission of a photon and a phonon. This phonon assisted process controls the lasing transition because it dominates the gain in the region of large population inversion. These theoretical results are compared to experiment. The broadband nature of this phonon assisted process implies that the maser operation is robust against charge noise and fabrication imperfections. In addition, due to the sharp threshold behavior of the lasing transition, this work indicates that the maser can serve as an extremely sensitive probe of the mesoscopic environment of the DQD.

...The main goal in the recent development of hybrid circuit quantum electrodynamics with quantum dots is to find efficient means to couple single spins to cavity photons. So far though, only the coupling of photons to the charge degree of freedom could be demonstrated. Here, we demonstrate a large and coherent spin photon coupling in a cQED architecture at the single spin level. Our scheme relies on the use of a non collinear spin valve which realizes an artificial spin orbit interaction. Thanks to that interaction we are able to couple electronic states which are sensitive to the external magnetic field to cavity photons. We observe a hysteretic evolution of the phase of the microwave signal as a function of the external magnetic field, stemming from the spin valve behavior of the device. This demonstrates an efficient spin/photon coupling and illustrates a new method for manipulating the quantum mechanical spin degree of freedom. Our findings can be used to scale up spin quantum bit architectures.

...the circuit quantum electrodynamics architecture may allow for the generation of entanglement between spatially separated spin qubits [1]. This approach has introduced the challenge of fabricating high quality factor superconducting resonators on multilayered semiconductor substrates. Here we present electric field simulations which show that 30% of the resonator electric field resides in the 675 µm thick Si substrate on which the Si/SiGe heterostructure is grown, 55% resides in the 3.5 µm thick SiGe relaxed buffer and 300 nm of Si$_2$Ge$_{0.7}$ grown above the relaxed buffer, and 15% resides in the remaining Si/SiGe heterostructure. We evaluate the performance of Nb coplanar waveguide resonators fabricated on top of a strained Si/SiGe quantum well at 4.2 K and 10 mK. The tested resonators exhibit a high quality factor despite the presence of an accumulated two-dimensional electron gas beneath the resonator center pin.

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4:18PM Q37.00008 Electron Spin Resonance Spectroscopy of Bismuth donors in Silicon using a Parametric Amplifier. YUIMARU KUBO, AUDREY BIENFAIT, MICHAEL STERN, DENIS VION, DANIEL ESTEVE, PATRICE BERTET, Quantumics Group, SPEC, CEA-Saclay, JARRYD PLA, CHEUK CHI LO, JOHN MORTON, London Centre for Nanotechnology, University College London, CHRISTOPH WEIS, THOMAS SCHENKEL, Accelerator and Fusion Research Division, Lawrence Berkeley National Laboratory, MICHAEL THEWALT, Department of Physics, Simon Fraser University — Bismuth donor spins in Silicon are well suited to implement a quantum memory for superconducting qubits [1], owing to their long coherence times and large hyperfine interaction leading to a zero-field splitting of 7.35GHz [2]. We report low-field electron-spin resonance spectroscopies of ensembles of Bismuth spins with a concentration of 5 \(10^{16}\) cm\(^{-3}\) in an isotopically purified 26Si sample at 10 mK, at which the electronic spin is expected to be fully polarized. The spectrometer consists of a superconducting resonator patterned on top of the substrate, with a quality factor of 10\(^7\). The signal coming from the spins is amplified using a Josephson Parametric Amplifier [3].


4:30PM Q37.00009 Entanglement of Two, Three, and Four Quantum Dots in Hybrid Quantum Dot/Plasmonic Systems. MATTHEW OTTEN, Department of Physics, Cornell University, Ithaca, NY and Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL, RAMAN SHAH, NORBERT SCHERER, Department of Chemistry and The James Franck Institute, The University of Chicago, IL, MISUN MIN, Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL, MATTHEW PELTON, Department of Physics, University of Maryland, Baltimore County, Baltimore, MD, STEPHÉN GRAY, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL — We use cavity quantum electrodynamics to study systems composed of two, three, and four two-state quantum dots in proximity to a plasmonic system such as a metal nanoparticle or an array of metal nanoparticles. We find that significant essential (all dot) entanglement, as measured by concurrence, in the two and four quantum dot cases is possible. At present the three quantum dot case lacks an easily applied measure of entanglement, but multiple bipartite entanglements are demonstrated. Moreover, we show that one can induce entanglement in two and three quantum dot systems starting from the ground state by use of pulsed excitations. These results represent a promising advance for the eventual use of quantum dots, coupled to one another through a dissipative structure such as a plasmonic system, in quantum computation.

4:42PM Q37.00010 Ripplonic Lamb shift for electrons on liquid helium. DENIS KONSTANTINOv, Okinawa Institute of Science and Technology, Japan, KONO KIMITOSHI, RIKEN, Japan, MICHAEL LEA, Royal Holloway, University of London, UK, MARK DUKYMAN, Michigan State University, USA — We resolve a long-standing controversy regarding the electrons on the surface of helium and their coupling to capillary waves, ripplons. The direct two-ripplon coupling to short-wavelength ripplons is strong. It leads to a strong power-law ultraviolet divergence of the shifts of the electron energy levels and to a high energy relaxation rate of the excited states. We use the Bethe-type approach to show that one-ripplon processes, taken to the higher order of the perturbation theory, compensate the divergence of the level shifts. The resulting shifts, which are ripplonic analogs of the Lamb shift, are small. The transition frequencies display characteristic temperature dependence. The calculation of this dependence with no adjustable parameters for transitions between the two lowest subbands of motion along the surface is in good agreement with our experimental data. We also show that one-ripplon processes renormalize the energy relaxation rate, which for highly excited electron states is determined by two-ripplon emission. As a result, energy relaxation is much slower than the lowest-order theory predicts. This is important for applications of electrons on helium in quantum information.

4:54PM Q37.00011 Isolating Electrons on the Surface of Superfluid Helium. MAIKA TAKITA, C. SPENCER NICHOLS, STEPHÉN LYON, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544 — Electrons on helium have been suggested as promising mobile spin qubits. Electrons floating on the surface of superfluid helium can be transferred extremely efficiently in narrow channels with underlying gates. The channels are filled with superfluid helium by capillary action and electrons on the surface can be clocked over a billion pixels in a 3-phase charge coupled device (CCD) without any detectable transfer errors. To use electrons as qubits, we need to reliably obtain a single electron per pixel. We demonstrate an electron turnstile operating across 78 parallel channels for isolating electrons. First, electrons are accumulated over wide 2.3um channels and clocked using the CCD gates into the narrow 0.8um wide turnstile regions. When large packets of electrons are clocked from the wide channels through the narrow regions, the number of electrons per pixel decreases. Using the narrow underlying gates in the turnstile region, the electron packets are repeatedly split. We find a plateau in the electron signal as a function of the applied gate voltages indicating a quantized number of electrons per pixel in each of the 78 parallel channels.

5:06PM Q37.00012 Modeling Strongly Interacting Electrons on Helium Coupled to a Microwave Resonator. GE YANG, University of Chicago, DAVID G. REES, National Chiao Tung University Institute of Physics, LEONIDAS OCOLA, DAVID CZAPLEWSKI, Argonne National Laboratory Center for Nanoscale Materials, GERWIN KOOLSTRA, DAVID MCKAY, DAVID I. SCHUSTER, University of Chicago — Electrons on helium is a unique two-dimensional electron gas system formed at the interface of a quantum liquid (superfluid helium) and vacuum. If single electrons on helium can be isolated, the motional and spin states could form the building blocks for hybrid quantum computing [1,2]. However, to trap single electrons we must start from a 2-dimensional gas of many electrons, which is a strongly interacting classical gas. In our experiment, we trap mesoscopic samples of electrons in a micron-sized trap, at the end of a centimeter-long quarter wavelength microwave cavity, and interrogate the system via the change in the microwave resonance frequency. Here, we will present a simple numeric model that we developed to understand the coupled cavity-electron on helium system in a micron-sized trap, and insights towards building a single electron quantum dot. [1] S. Lyon, Phys. Rev. A. 74, 9 (2006) [2] D.I. Schuster, et al. Phys. Rev. Lett. 105, 040503 (2010)

5:18PM Q37.00013 Entanglement dynamics of capacitively coupled spin qubits in the presence of stray inductance. MICHAEL WOLFE, SHAWN CHISHOLM, JASON KESTNER, University of Maryland, Baltimore County — A pair of spin qubits formed by electrons confined in a pair of double quantum dots can be entangled at distances on the order of microns via a floating metallic top gate that mediates capacitive coupling [1]. The double-well biasing, and hence the coupling through the top gate, can be controlled through voltage leads connected to an arbitrary waveform generator. We theoretically examine how the entanglement dynamics of the system are affected by inductance of the coupling element when the biases are driven at high frequencies. We numerically simulate the von Neumann entropy of the reduced density matrix as a function of time in various parameter regimes. In particular, we examine the behavior when the qubits are driven near the resonance frequency of the coupling element.

were calculated from a quadratic Hamiltonian that had the given ground state, and the probability that the D-Wave Two found the ground state was measured. RST problem was solved up to 100 times and the number of times the ground state energy was found was recorded. This procedure was repeated for square over all spanning trees of G. In the first study, 100 RSTs with random clusters of 8 qubits. Problem input consists of values for the fields H, for n > Hc, there is formed a local condensate of spins with nonzero z-component around the defect. It grows with further decreasing H. We then consider a point defect that corresponds to the change δJ in the coupling constant between n and n+1 spins. For δJ > Hc, there emerges a pair of localized excitations for large H. As H decreases, for some δJ-dependent H > Hc, there is formed a local cloud of spins with nonzero z-component around the defect. It grows with further decreasing H. Remote defects interact very weakly. For small but nonzero temperatures, different defects should be able to align in the opposite directions, leading to nucleation of kinks between them. We study the evolution of the system as H decreases, the possibility of forming kinks, kink tunneling, and the ultimate approach of the system to the ground state. We also study the case of antiferromagnetic defects.

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4:30PM Q38.00009 Reexamining classical and quantum models for the D-Wave One processor , TAMEEM ALBASH, University of Southern California, TROELS RONNOW, MATTHIAS TROYER, ETH Zurich, DANIEL LIDAR, University of Southern California — We revisit the evidence for quantum annealing in the D-Wave One device (DW1) based on the study of random Ising instances. We consider measures that account for ground state degeneracy and the distributions of excited states, and present evidence [1] that for these new measures neither SQA nor the classical rotor model correlate perfectly with the DW1 experiments, despite both models correlating very well with the DW1 ground state success probabilities [2,3]. We thus provide evidence that SQA and the classical rotor model, both of which are classically efficient algorithms, do not satisfactorily explain all the DW1 data.


4:42PM Q38.00010 Optimal annealing in p-spin model , KOSTYANTYN KECHEDZHI, QuAIL NASA Ames Research Center Mail Stop 269-3, Moffett Field, CA 94035 and USRA RIACS, 615 National Ave, 94043 Mountain View CA, VADIM SMELYANSKIY, QuAIL NASA Ames Research Center Mail Stop 269-3, Moffett Field, CA 94035 — In this work we are looking to understand the physical mechanisms of quantum speedup in quantum annealing devices. We consider a simplified Hamiltonian that can be addressed analytically using a semiclassical approximation. The Hamiltonian models a typical potential barrier that can trap the system in a metastable state and thus prevent it from reaching the ground state. This situation is common in complex optimization problems such as a spin glass. The model we consider consists of Ising spins forming a fully connected graph with interaction energy proportional to a product of p individual spin operators (p = 2 would correspond to the pair interaction in, for example, a ferromagnet). At p > 2 this model demonstrates 1st order phase transition associated with exponential scaling of the quantum annealing computation time with the system size. We analyze the characteristics of the potential barrier that determine the efficiency of quantum annealing. We also identify the optimal regime for quantum annealing.

4:54PM Q38.00011 Isothermal quantum annealing of the 1D transverse Ising chain , DAVIDE VENTURELLI, VADIM SMELYANSKIY, ALEJANDRO PERDOMO-ORTIZ, NASA Ames Research Center, SERGEI ISAKOV, Google, SERGEY KNYSYH, NASA Ames Research Center, MARK DMYKMAN, Michigan State University — We present a quantum annealing strategy to solve optimization problems that relies on the effect of the external environment on the quantum system (isothermal protocol). We define the isothermal complexity as the scaling of the longest instantaneous relaxation time with the number of qubits in the region after the critical point where the first excitation gap equals to the temperature. We calculate this complexity for the case of 1D transverse field Ising chain coupled to the bosonic environment. We show that the quantum annealing complexity bottleneck is determined by the quantum diffusion limited recombination of the fermions that represent system excitations. We present the analytical results as well as numerical study of the system dynamics and annealing complexity.

5:06PM Q38.00012 Role of Collective Tunneling in a Quantum Annealer , HARTMUT NEVEN, Google, VADIM SMELYANSKIY, NASA, SERGIO BOIXO, ALIREZA SHABANI, SERGEI ISAKOV, Google, MARK DMYKMAN, Michigan State University, VASIL DENCHEV, Google, MOHAMMAD AMIN, ANATOLY SMIRNOV, D-Wave, MASOUD MOHSENI, Google — We show that quantum resources in the D-Wave Two processor enhance the probability to reach the global minimum of an optimization problem. We implemented a series of structural primitives on the device governed by non-convex optimization landscapes consisting of just one global and one false local minima. The quantum adiabatic evolution path over product states connects the initial global minimum with the final false minimum. The final global minimum can only be reached by traversing an energy barrier. Experimentally we found that the D-Wave Two quantum annealer returns the solution that minimizes the energy with consistently higher probability than physically plausible models of the hardware that only employ product states and thermal activation over the barrier and do not allow for multiqubit tunneling transitions. On the contrary open system quantum mechanical models are in very close correspondence with the hardware data without using any fitting parameters. We additionally performed a series of experiments in which we varied the temperature of the chip. We find that the observed correlation between the temperature and success probability is consistent only with quantum models. We also demonstrate that the success probabilities of path integral Monte Carlo are consistently low.

5:18PM Q38.00013 Collective dissipative tunneling during quantum annealing on D-Wave II device1 , VADIM SMELYANSKIY, NASA Ames Research Center, SERGIO BOIXO, ALIREZA SHABANI, SERGEI ISAKOV, Google, MARK DMYKMAN, Michigan State University, VASIL DENCHEV, Google, MOHAMMAD AMIN, ANATOLY SMIRNOV, D-Wave Systems, MASOUD MOHSENI, HARTMUT NEVEN, Google — We develop theory based on NIBA Quantum Master Equation to describe the multiqubit tunneling in the evolution of a programmable quantum annealer. We describe D-Wave II’s performance in the non-convex problems realized by frustrated networks of qubit clusters with strong intra-cluster coupling. We show that the collective effect of the environment is suppressed near the avoided crossing leading to coherent tunneling in that region. In a later stage of the annealing z-magnetizations of qubit clusters increase steeply as a manifestation of the spontaneous symmetry breaking giving rise to a substantial polaronic effect. Transition to the final solution state proceeds via tunneling of one of the qubit clusters as a whole, accompanied by the reorganization of the environmental degrees of freedom and absorption of the residual energy from the qubit system. Transition rate decreases exponentially fast with time after avoided crossing leading to the freezing of the qubit population in the local minimum. We used noise parameters from the single qubit MRT experiments taken on the same device. Model predictions for multiqubit quantum annealing on the above problems are in a very close correspondence with the data collected on D-Wave II device without using any fitting parameters.

1The work of V.N.S. was supported in part by the ODNI and IARPA via IAA 144583; by the AFRL ID under grant F4HBKC4162G001.

5:30PM Q38.00014 Optimising simulated quantum annealing, simulated annealing and a mean-field algorithm to find ground states of Ising spin glasses , DAMIAN S. STEIGER, ETH - Zurich, TROELS F. RØNNOW, ETH - Zurich and Nokia Technologies, Cambridge (UK), MATTHIAS TROYER, ETH - Zurich — We report on benchmarks of finding the ground states of Ising spin glasses on chimera graphs using simulated annealing, simulated quantum annealing and a mean-field quantum annealing algorithm. We analyze the performance of these algorithms by calculating the empirical time-to-solution distribution function and extrapolating their tails, which describe the hard instances. All algorithms show an increasing fat-tail with larger system size, and therefore the average time-to-solution is dominated by the run-times of the hard instances. These tails can be significantly reduced by optimizing the annealing time and temperature. Especially the hard instances of simulated quantum annealing are solved much faster by using a shorter annealing time or higher temperature.

Wednesday, March 4, 2015 2:30PM - 5:18PM
Session Q39 DPOLY: Focus Session: Polymer Nanocomposites - Active Particles and Dynamics
213AB - Jacinta Conrad, University of Houston

1Support from US National Science Foundation (CMMI-0800237, CMMI-106910)

Metal nanoparticles under continuous-wave (cw) optical excitation resonant with their localized surface plasmon exhibit a photothermal effect, efficiently converting the incident light into heat [1] originating from the particle. Gold nanorods (GNRs) dispersed within a transparent material are utilized as such remotely-controlled, nano-sized heaters [2], with heating properties which can be manipulated and monitored by using control of the polarization direction [3, 4] of the excitation and probe light fields. Steady-state average temperatures within a polymer matrix embedded with GNRs undergoing cw photothermal heating are determined in the immediate vicinity of the GNR by observing the rate of driven physical rotation of the nanorods, and simultaneously across the entire sample by using an independent fluorescence method. Comparing these two observations as the concentration of dispersed GNRs is varied reveals the interplay between local and global heating in these polymer nanocomposite materials.

Support from US National Science Foundation (CMMI-0800237, CMMI-106910)

Metal nanoparticles embedded within polymeric systems can be made to act as localized heat sources thereby aiding in-situ polymer processing. This is made possible by the surface plasmon resonance (SPR) mediated photothermal effect of metal (in this case gold) nanoparticles, wherein incident light absorbed by the nanoparticle generates a non-equilibrium electron distribution which subsequently transfers this energy into the surrounding medium, resulting in a temperature increase in the immediate region around the particle. Here we demonstrate this effect in polymer nanocomposite systems, specifically electrosyn polystyrene oxide nanofiber mats, which have been annealed at temperatures above the glass transition. A non-contact temperature measurement technique utilizing embedded fluorophores (perylene) has been used to monitor the average temperature within samples. The effect of annealing methods (conventional and photothermal) and annealing conditions (temperature and time) on the fiber morphology, overall crystallinity, and mechanical properties is discussed. This methodology is further utilized in core-sheath nanofibers to crosslink the core material, which is a pre-cured epoxy thermoset.

1NSF Grant CMMI-1069108

Using computer simulations, we model an array of flexible fibers that are embedded in a lower critical solution temperature (LCST) thermo-responsive gel, which swells at lower temperatures and collapses at higher temperatures. The system is immersed in a solution containing dispersed nanoparticles and this fluid is driven to flow by an imposed shear. When the gel is heated, it collapses to expose the fibers, and thereby, triggers the “catch” process. Namely, the fibers can act like “arms” that wrap around the nanoparticle and bring it from the outer solvent into the gel layer. Moreover, we show that depending on the flexibility and hydrophobicity of the fibers, as well as the imposed shear, we can position the nanoparticles at the desired height within the gel layer. Our approach can be utilized for the detection and separation of components in fluids and for the controlled insertion of nanoparticles within a hydrogel at a particular distance from the gel interface.

Support from US National Science Foundation (CMMI-0829379, CMMI-106910)

Using dissipative particle dynamics (DPD), we model a monolayer formed at the water-oil interface, which comprises stimuli-responsive nanoparticles. The solid core of the nanoparticle encompasses beads arranged in an fcc lattice structure and its surface is uniformly grafted with stimuli-responsive polymer chains. The surface-active nanoparticles adsorb to the interface by characterizing the detailed adsorption kinetics. We explore the microstructure of the monolayer at different surface coverage, including the particle crowding and ordering, and elucidate the response of monolayer to external stimuli. The collective behavior of the particles within the monolayer is demonstrated quantitatively by vector-vector autocorrelation functions. This study provides a fundamental understanding of the interfacial behavior of stimuli-responsive nanoparticles.

3:30PM Q39.00006 Using Gold Nanorods to Probe the Local Environment within Polymer Nanocomposites 1, LAURA CLARKE, SOMSUBHRA MAITY, WEI-CHEN WU, JOSEPH TRACY, JASON BOCHINSKI, North Carolina State University — Active metal nanoparticles embedded within polymeric materials can generate internal photothermal heating [1,2] to enable processing, such as shape memory actuation [3] or thermal annealing [4], with outcomes unrealizable by conventional means. When gold nanorods are utilized [5, 6], their anisotropic-shape provides additional capabilities: using the nanoparticle as an optical probe allows quantitative measurement of the local polymer environment, particularly in the melt phase. Specifically, one surface plasmon excitation can heat while the other monitors particle orientation (altered by rotational diffusion) to make a temperature measurement in the region near the nanorod [6]. We describe results from this approach with examples of the differing local environments within the polymer due to changes in processing.

1Support from US National Science Foundation (CMMI-0829379, CMMI-106910)
3:42PM Q39.00007 Contrasting nanoparticles diffusion in synthetic and biopolymer solutions
SHARMINE ALAM, INDERMEET KOHLI, ASHIS MUKHOPADHYAY, Wayne State Univ — We investigated the dynamics of gold nanospheres (AuNS) and nanorods (AuNR) in synthetic polymer (polyethylene glycol) and biopolymer (bovine serum albumin and mucin) solutions. The variables are particle size and shape, polymer volume fraction, etc. The fluctuation correlation spectroscopy (FCS) was used to measure the translational ($D_T$) and rotational diffusion ($D_R$) of gold nanoparticles. Comparison will be made for the nano-viscosities at different length scales. The nanoparticle dynamics within the mucus gel will be presented.

3:54PM Q39.00008 Embedded Gold Nanorods as Microscale Thermochromic Temperature Sensors
W. JOSHUA KENNEDY, KEITH SLINKER, Universal Technology Corporation, Air Force Research Laboratory (WPAFB), HILMAR KOERNER, GREGORY EHLERT, JEFFERY BAUR, Air Force Research Laboratory (WPAFB) — Gold nanorods (AuNRs) are known to undergo a shape transformation via surface melting at temperatures far below the bulk melting temperature of gold. Because the optical scattering by the AuNRs depends on both particle morphology and the surrounding local dielectric constant, the opto-thermal properties of polymer-AuNR nanocomposites depend strongly on the chemical and mechanical characteristics of the polymer host. We have measured the optical absorption of polymer nanocomposites consisting of AuNRs in a variety of polymer systems as a function of temperature, time, molecular weight, and crosslink density. Our results show that the shape transformation of the AuNRs is not well described by a simple kinetic model, and that multiple contributors to the surface energy play significant roles in the process. We show that the dynamics of the shape transformation may be controlled in a nanocomposite such that the optical absorption spectrum of the material may be used as a local sensor of both temperature history and degree of cure. We demonstrate the usefulness of this technique by measuring (ex situ) the temperature of an internally heated epoxy resin with a lateral spatial resolution of <10 μm.

1Principal Investigator

4:06PM Q39.00009 Supramolecular Nanocomposites Under Confinement: Chiral Optically Active Nanoparticle Assemblies and Beyond
PETER BAI, SUI YANG, WEI BAO, MIQUEL SALMERON, XIANG ZHANG, TING XU, Univ of California - Berkeley — Block copolymer-based supramolecules provide a versatile platform to direct the self-assembly of nanoparticles (NPs) into precisely controlled nanostructures in bulk and thin film geometries. A supramolecule, PS-b-P4VP(PDP), composed of the small molecule 3-pentadecylphenol (PDP) hydrogen bonded to a diblock copolymer, polystyrene-block-poly(4-vinylpyridine) (PS-b-P4VP), was subjected to 2-D volume confinement in cylindrical anodic aluminum oxide (AAO) membrane pores. TEM and 3-D TEM tomography reveal that the morphologies accessible by the supramolecule and supramolecule/NP composites, such as NP clusters, arrays, stacked rings, and single and double helical ribbons, are significantly different from those in the bulk or thin film. Furthermore, single molecule dark field scattering measurements demonstrate strong chiral optical response of single helical Au NP ribbon nanostructures in the near infrared wavelength regime. These studies demonstrate 2-D confinement to be an effective means to tailor self-assembled NP structure within supramolecule nanocomposites and pave the way for this assembly approach to be applied towards next generation chiral metamaterials and optoelectronic devices.

4:18PM Q39.00010 Harnessing Biomimetic Catch Bonds to Create Mechanically Robust Nanoparticle Networks
ANNA BALAZS, University of Pittsburgh — Using computer simulations, we investigate the mechanical properties of a network of polymer-grafted nanoparticles (PGNs) that are interlinked by labile “catch” bonds. In contrast to conventional “slip” bonds, the life time of catch bonds can potentially increase with the application of force (i.e., the rate of rupture can decrease). In effect, the bond becomes stronger under an applied force (if the strain rate is sufficiently high). Subjecting the PGN networks to a tensile deformation, we find that the networks encompassing catch bonds exhibit greater ductility and toughness than the networks interconnected by slip bonds. Moreover, when the applied tensile force is released, the catch bond networks exhibit lower hysteresis and faster relaxation of residual strain than the slip bond networks. The effects of the catch bonds on the mechanical behavior are attributed to transitions between two conformational states, which differ in their sensitivity to force. The findings provide guidelines for creating nanocomposite networks that are highly resistant to mechanical deformation and show rapid strain recovery.

4:54PM Q39.00011 Microwave Induced Welding of Carbon Nanotube-Thermoplastic Interfaces for Enhanced Mechanical Strength of 3D Printed Parts
CHARLES SWEENEY, MICAH GREEN, Texas A&M University, MOHAMMAD SAED, Texas Tech University — Three-dimensional (3D) printed parts produced by fused-filament fabrication of a thermoplastic polymer have become increasingly popular at both the commercial and consumer level. The mechanical integrity of these rapid-prototyped parts however, is severely limited by the interfiller bond strength between adjacent extruded layers. In this report we propose for the first time a method for welding thermoplastic interfaces of 3D printed parts using the extreme heating response of carbon nanotubes (CNTs) to microwave energy. To achieve this, we developed a coaxial printer filament with a pure polylactide (PLA) core and a CNT composite sheath. This produces parts with a thin electrically percolating network of CNTs at the interfaces between adjacent extruded layers. These interfaces are then welded together upon microwave irradiation at 2.45GHz. We investigated the dielectric properties of the PLA/CNT composites at microwave frequencies and performed in-situ microwave thermometry using a forward-looking infrared (FLIR) camera to characterize the heating response of the PLA/CNT composites upon microwave irradiation. Finally, computational models were developed to verify the microwave heating response of the percolating CNT composites according to their measured dielectric properties.

5:06PM Q39.00012 Smart Hybrids made of Polymer Brushes and Gold Nanospheres
STEPHANIE CHRISTAU, FELIX BROSE, TIM MOELLER, RALF KOEHLER, ZULEYHA YENICE, Technical University Berlin, JAN GENZER, North Carolina State University, REGINE VON KLITZING, Technical University Berlin — The modification of surfaces by coating with polymer brushes has attracted much interest in the past few years due to numerous potential applications in material and life science for the development of smart surfaces. They can be used as 3D matrices for the immobilization of nanoparticles, resulting in nanocomposite materials with interesting mechanical, optical, or catalytic properties with tailored functions [1]. Studying the mutual influence of the brush matrix and the attached AuNPs on the structure of the resulting brush/AuNP hybrid will allow fine-tuning of the particle loading and distribution ... this study, responsive poly-(N,N-dimethylamino)ethyl methacrylate (PDMAEMA) and poly-(N-isopropylacrylamide) (PNIPAM) brushes are used as a matrix for the attachment of spherical gold nanoparticles (AuNPs). We find that the uptake and distribution of nanoparticles in polymer brush matrices depends greatly on the brush thickness [2], brush grafting density [3], polymer chemistry, particle surface functionalization and particle size. References: [1] S. Christau et al. Z. Phys. Chem., 2014 [2] S. Christau et al. Polymers, 2014, 6, 1877. [3] S. Christau et al. Langmuir, 2014, 30, 13033

Wednesday, March 4, 2015 2:30PM - 5:30PM – Session Q41 DPOLY DMP: Focus Session: Organic Electronics and Photonics - Structure-Property Relationships
2:30PM Q41.00001 Quantifying Order in Semiconducting Polymers, CHAD SNYDER, NIST - Natl Inst of Stds & Tech — Semiconducting polymers form the basis for the burgeoning flexible electronics industry. However, quantifying their order can be challenging due to the nanophase separation induced by the side chains which are used to impart solubility, their propensity to form mesophases, and their often high levels of paracrystalline disorder. Recent successes in our laboratory in understanding these materials and quantifying their order will be presented.

2:42PM Q41.00002 Multi-scale Modeling Study of poly(3-hexylthiophene) and [6,6]-phenyl-C_61-butyric acid methyl ester Towards Organic Photovoltaic Cell Application, HANJONG YOO, KI CHUL KIM, SEUNG SOON JANG, Georgia Inst of Tech — To date, organic photovoltaic cells have gained attention due to their promising potential in the industry. Its efficiency needs to be improved through constructing better morphologies. There are three morphological quantities that affect the efficiency. The domain size of the electron donor phase has to be small and the interface-to-volume ratio of the blend must be large. The percolation ratio has to be high. To investigate the morphological properties of the active layer systems, the state-of-the-art multi-scale modeling is employed. In this study, P3HT and PCBM blends have been used as our active layer candidates. We have developed our own force field parameters to accurately describe potential energy surfaces in the layer systems. Subsequently, coarse-grained force field for P3HT and PCBM have been developed based on the improved atomistic force field parameters in order to simulate larger systems. The results from coarse-grained models are validated through the comparison with those from the full atomistic models. Using the molecular dynamics simulations, the newly developed coarse-grained models will be further used to study how the crystallinity of P3HT affects the morphological properties in the active layers.

2:54PM Q41.00003 Structure and segmental dynamics in amorphous conjugated polymers, PENGFEI ZHAN, JANNA MARANAS, ENRIQUE GOMEZ, The Pennsylvania State University — Although it is well established that the microstructure strongly affects charge transport in organic semiconductors, the role of fluctuations of the structure on charge mobilities is still not well understood. We have examined the dynamics and structure in amorphous conjugated polymers poly(3-alkylthiophene) (P3ATs) with neutron and x-ray scattering. We measured the segmental dynamics in amorphous P3ATs with quasi-elastic neutron scattering (QENS). The structure of amorphous P3ATs is measured with small-angle neutron scattering (SANS) and grazing incidence X-ray diffraction (GIXRD). Using SANS, we observe phase separation between the backbone and side-chains in all polymer samples for regiorandom P3ATs. Additionally, the analysis of the QENS data shows that longer side-chains relax faster compared with shorter side-chains and our further analysis of the elastic incoherent structure factor (EISF) suggests that the amplitude of proton motion on the thiophene rings increases by a factor of 3 as the side-chain length increases from 6 to 12, demonstrating that longer side-chains lead to enhanced motion of conjugated rings.

3:06PM Q41.00004 Pushing structural limits to reveal fundamental mechanisms of organic solar cell operation, BARRY RAND, Princeton University — Organic-based solar cells are beginning to emerge with the potential to compete with other thin film photovoltaic technologies, with efficiencies of 12% recently demonstrated. Unique to the function of organic photovoltaics are the creation of tightly bound excitons that can only be efficiently separated at a donor/acceptor (D/A) interface capable of providing the necessary energetic driving force for dissociation. The consequences of this are the need for long exciton diffusion lengths and the presence of charge transfer (CT) states, ground state complexes that exist at the D/A interface. We have that charge transfer states are more easily separated into free charge if they are delocalized; an aspect that becomes most feasible for highly ordered systems. I will discuss our recent efforts to template and control film morphology and molecular orientation. These studies allow us to understand the importance of molecular orientation, crystallite size, and crystal phase. We will show templated devices utilizing neat films as well as bulk heterojunctions, with crystallite dimensions spanning from the more standard nano-sized grains to those with highly ordered micron-sized crystalline domains revealing unprecedented thin film exciton diffusion lengths of 100s of nm. In these highly ordered films, owing to significant delocalization, we are able to directly measure photocurrent from multiple CT states, an aspect which has important consequences for the design of more efficient photocurrent generation.

3:42PM Q41.00005 Predicting X-ray absorption spectra of semiconducting polymers for electronic structure and morphology characterization, GREGORY SU, SHRAYESH PATEL, Univ of California - Santa Barbara, C. DAS PEMMARAJU, Lawrence Berkeley National Laboratory, EDWARD KRAMER, Univ of California - Santa Barbara, DAVID PRENDERGAST, Lawrence Berkeley National Laboratory, MICHAEL CHABINCY, Univ of California - Santa Barbara — Core-level X-ray absorption spectroscopy (XAS) reveals important information on the electronic structure of materials and plays a key role in morphology characterization. Semiconducting polymers are the active component in many organic electronics. Their electronic properties are critically linked to device performance, and a proper understanding of semiconducting polymer XAS is crucial. Techniques such as resonant X-ray scattering rely on core-level transitions to gain materials contrast and probe orientational order. However, it is difficult to identify these transitions based on experiments alone, and complementary simulations are required. We show that first-principles calculations can capture the essential features of experimental XAS of semiconducting polymers, and provide insight into which molecular model, such as oligomers or periodic boundary conditions, are best suited for XAS calculations. Simulated XAS can reveal contributions from individual atoms and be used to visualize molecular orbitals. This allows for improved characterization of molecular orientation and scattering analysis. These predictions lay the groundwork for understanding how chemical makeup is linked to electronic structure, and to properly utilize experiments to characterize semiconducting polymers.

3:54PM Q41.00006 Phase Separation and Development of a Scanning Time of Flight Microscope to Study Charge Transport in Structured Organic Semiconductors, SANJOY PAUL, Dept. of Physics, Kent State University, ŠUVAGATA TRIPATHI, Dept. of Chemistry, Kent State University, GAUTAM SINGH, Dept. of Physics, Kent State University, ROBERT TWIEG, Dept. of Chemistry, Kent State University, SATYENDRA KUMAR, BRETT ELLMAN, Dept. of Physics, Kent State University — A scanning time-of-flight microscope (STOFm) has been developed to study charge transport in liquid crystalline organic semiconductors (LCOSCs). The STOFm combines the well-known pulsed laser time-of-flight technique with simultaneous polarized light transmission measurements, both on length scales of ~ 10 µm. In parallel, we have fabricated devices via photopolymerization and phase separation of a monomer/LCOSC mixture. The resulting structure has the LCOSC confined to small regions separated by an insulating polymer. We will discuss fabrication of these systems, as well as their characterization using the STOFm. Finally, we will show results on position-dependent charge transport in various pure LCOSC samples.

4:06PM Q41.00007 ABSTRACT WITHDRAWN
4:18PM Q41.00008 Nanoscale Orientation Effects on Carrier Transport in a Low-Band-Gap Polymer, BAN DONG, BINGYUAN HUANG, AARON TAN, PETER GREEN, University of Michigan — We show that the out-of-plane hole mobility of the low-band-gap polymer poly[4,8-bis-(2-ethylhexyloxy)-benzo[b][1,2-b:4,5-b']dithiophene-2,6-diyl-alt-4-(2-ethylhexyloxy-l-one)thieno-[3,4-b][thiophene-2,6-diyl] (PBDDTTT-C) is film thickness dependence; and this behavior is associated with the morphology. Due to a geometric confinement and to polymer/substrate interactions, the average orientation of the chains in the thinnest films was predominantly parallel to the substrate. In this thickness range, the out-of-plane hole mobilities \( \mu \) were necessarily low and \( \beta \), a measure of the strength of the field dependence of the mobility, was largest. Within the framework of the Gaussian Disorder model, the relative value of \( \beta \) suggests that the largest effect of positional disorder on the carrier transport was most significant in the thinnest films. The hole mobility \( \mu \) increased and depended less on the electric field (\( \beta \) decreases in magnitude) with increasing thickness, due evidently to the increased degree of orientation of the domains with respect to the direction of the field (normal to the interfaces). These findings demonstrated the profound impact of the substrate on the morphology and of the morphology on the charge carrier mobility.

4:30PM Q41.00009 Directed alignment of conjugated polymers for enhanced long-range photocurrent collection, ANTON LI, DAVID BILBY, BAN DONG, JINSANG KIM, PETER GREEN, Univ of Michigan - Ann Arbor — To realize the full potential of conjugated polymers, possessing anisotropic structure and properties, it is often desirable to extend their organization to larger length scales. An epitaxy-directing solvent additive 1,3,5-trichlorobenzene was combined with an off-center spin-casting technique to produce poly(3-hexylthiophene) (P3HT) fibers with uniaxial in-plane alignment on the centimeter scale, which were incorporated into planar heterojunction solar cells with PCBM acceptor. Topography and photocurrent were mapped by photoconductive AFM; in devices with aligned P3HT, local photocurrent measured on fibers was over 4 times higher than in control devices with unaligned polymer. Even at large distances (> 200 \( \mu \)m) between laser spot (carrier excitation) and conductive probe (charge extraction), significant long-range photocurrent was measured in the aligned devices, especially when the separation was oriented parallel to the fiber alignment. Complementary TFE measurements of neat P3HT fibers revealed that the anisotropy of in-plane carrier mobilities was greater than a factor of 3. Together, these findings highlight the importance of conjugated polymer alignment for improving carrier transport and ultimately the performance of solar cells and other devices.

4:42PM Q41.00010 Modifying Photoluminescence Emission from Thin Polymer Films through Local Deformation Zones\(^1\), PO-JUI CHEN, XUAN LONG HO, JONATHON DAVID WHITE, Yuan Ze University, Taiwan — Controlling light extraction is important for applications ranging from LEDs to the weakly emissive thin films used for trace chemical detection. The commercial importance of GaN photodiodes, has resulted in the majority of work being concentrated on increasing light extraction efficiency \( (\eta) \) as GaN’s high refractive index results in up to 96% of light being trapped and reabsorbed. Various methods, such as embedding photonic crystals and surface texturing, have been proposed and employed to improve \( \eta \). Our focus is not on optimizing this quantity but rather on understanding the effect of surface modification on the angular, spatial and spectral characteristics of the emitted radiation. We do this by simulating the effect of a one-dimensional perturbation of thickness on the outputted radiation of a weakly absorbing fluorescent polymer film. While such a perturbation increases the \( \eta \) by a factor of two over a wide range of parameters, the film’s other emission properties are quite sensitive to the surface structure. For instance, adjusting the spatial period, allows the spectral peak of the emission to be tuned over a 10nm range and the output to be localized in specific regions of the film. Adjusting the edge angle, allows one to fine tune the direction of radiation escaping the film. Finally, we will discuss tradeoff between structural parameters involved in optimizing light emission for specific detector geometries.

\(^1\)Supported by the Ministry of Science and Technology of Republic of China

5:44PM Q41.00011 Photocatalytically Active Oligomeric Graphitic Carbon Nitride: Conformational Flexibility, Electronic Levels, Carrier Localization, VOLKER BLUM, Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC, USA, VINCENT LAU, Max Planck Institute for Solid State Research, Stuttgart, Germany, TAIJO BOTARI, WILLIAM HUHN, Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC, USA, BETTINA V. LOTSCH, Max Planck Institute for Solid State Research, Stuttgart, Germany, and University of Munich (LMU), Munich, Germany — Polymers consisting of bridged heptazine units (often called “graphitic carbon nitride” or “g-C\(_3\)N\(_4\)”) show considerable promise as photocatalysts for solar hydrogen evolution. Recent experimental evidence suggests that oligomeric rather than fully polymerized “g-C\(_3\)N\(_4\)” exhibits intrinsic photocatalytic activity. Using density-functional theory (DFT; van der Waals corrected PBE functional for conformers, hybrid DFT and GW for electronic levels), we show that considerable conformational flexibility exists for the heptazine trimers and tetramers. Analysis of HOMO and LUMO locations as well as trends in photocatalytic activity among heptazine oligomers and polymers reveals the NH\(_2\) groups of the oligomers as potential charge-transfer sites. We show that conformational variations of the oligomers can lead to significant, electrostatically motivated carrier localization effects. We suggest that NH\(_2\) side groups and the intrinsic conformational variations of the oligomeric species lead to the observed enhanced catalytic activity.

5:06PM Q41.00012 ABSTRACT WITHDRAWN –

5:18PM Q41.00013 Development and Studies of Nematic Liquid Crystalline Organic Semiconductors, SALMA BEGUM, SANJOY PAUL, SUVAGATA TRIPATHI, ROBERT TWIEG, BRETT ELLMAN, Kent State Univ - Kent — A huge body of knowledge exists on the creation and alignment of films of nematic liquid crystals (LCs), raising the promise of electronic devices (OFETs, LEDs, etc.) where the structure of the semiconductor is simply controlled with major implications for device parameters. Nematic LCs, however, typically possess low mobilities due to disorder, and are also susceptible to effects due to ionic conduction and screening. We will present material classes of more practical nematic organic semiconductors as well as novel characterization techniques to measure the effects of ionic motion in the nematic phase.

Wednesday, March 4, 2015 2:30PM - 5:30PM –
Session Q42 DPOLY DCOMP: Focus Session: Theory and Simulation of Macromolecules I
214B - Lisa Hall, Ohio State University

2:30PM Q42.00001 Computation of the Gibbs free energy difference between polymorphs\(^3\), DANIEL W. SINKOVITS, SANAT K. KUMAR, Columbia University — Semi-crystalline polymers commonly crystallize into several different polymorphs; for example, the alpha and beta phases of isotactic polypropylene. While it is possible to favor particular polymorphs by kinetic means, such as with varying degrees of supercooling or through the use of different solvents in solution casting, we focus on the question of thermodynamic stability; that is, which polymorph possesses the lowest Gibbs free energy for a given temperature and pressure. We implement a version of the Bennett Acceptance Ratio method and find phase diagrams for several polymers. We also demonstrate agreement with phonon analysis in the quasi-harmonic approximation. The advantages and drawbacks of these methods will be discussed.

\(^3\)Multidisciplinary University Research Initiative (MURI)
The development of a molecular theory for dense polymer systems ranks among the most challenging problems in the statistical mechanics of complex matter. These difficulties become compounded when considering the influence of molecular details on thermodynamic properties of thin polymer films, properties deviating from those of the bulk phases. A new theory of dense polymer films is developed as a significant generalization of methods used to devise lattice cluster theory, an extension of Flory-Huggins theory that includes details of monomer structure and short range correlations (neglected in FH theory) and that has successfully been applied to a wide range of polymer systems. The new theory incorporates the essential “transport” constraints of Helfand and focuses on the strict imposition of excluded volume constraints, appropriate to dense polymer systems, rather than the maintenance of chain connectivity as appropriate for lower densities and implemented in self-consistent theories of polymer adsorption at interfaces. The theory is illustrated by presenting examples of the computed density and chain end profiles for free standing films as a function of bulk density, chain length, temperature, and chain semi-flexibility.

2:42PM Q42.00002 New Molecular Theory for Dense, Thin Polymer Films, KARL FREED, James Franck Institute, University of Chicago — The development of a molecular theory for dense polymer systems ranks among the most challenging problems in the statistical mechanics of complex matter. These difficulties become compounded when considering the influence of molecular details on thermodynamic properties of thin polymer films, properties deviating from those of the bulk phases. A new theory of dense polymer films is developed as a significant generalization of methods used to devise lattice cluster theory, an extension of Flory-Huggins theory that includes details of monomer structure and short range correlations (neglected in FH theory) and that has successfully been applied to a wide range of polymer systems. The new theory incorporates the essential “transport” constraints of Helfand and focuses on the strict imposition of excluded volume constraints, appropriate to dense polymer systems, rather than the maintenance of chain connectivity as appropriate for lower densities and implemented in self-consistent theories of polymer adsorption at interfaces. The theory is illustrated by presenting examples of the computed density and chain end profiles for free standing films as a function of bulk density, chain length, temperature, and chain semi-flexibility.

3:06PM Q42.00004 Molecular Dynamics Simulations of Homogeneous Crystallization in Polymer Melt, BIN KONG, Chinese Academy of Sci (CAS) — Molecular mechanisms of homogeneous nucleation and crystal growth from the melt of polyethylene-like polymer were investigated by molecular dynamics simulations. The crystallinity was determined by using the site order parameter method (SOP), which describes order due to the chain folding. Snapshots of the simulations showed evolution of the nucleation and the crystal growth through SOP images clearly. The isothermal crystallization kinetics was determined at different temperatures. The rate of crystallization, $K_c$, and the Avrami exponents, $n$, were determined as a function of temperature. The formation of nuclei was traced to reveal that the nuclei were formed with more ordered cores and less ordered shells. A detailed statistical analysis of the MD snapshots and trajectories suggested conformations of the polymer chains changed smoothly from random coil to chain folded lamella in the crystallization processes.

3:18PM Q42.00005 Molecular dynamics simulation of electromechanical breakdown of polyolefins under a high electric field, MAYANK MISRA, DANIEL SINKOVITS, SANAT KUMAR, Columbia University — Polymers are finding increasing use as dielectric materials. Due to their flexibility, polymer dielectrics in the presence of an electric field may undergo large deformations that result in mechanical instability, which leads to detrimental failures. We study this mechanical instability in polyolefins using all-atom molecular dynamics. We vary the simulated external electric field from 0 to 1200 V/µm to study the effect of high electric fields on polyolefins. At critical conditions, we observe a thinning effect leading to electromechanical breakdown. We also determine the critical voltage using theoretical models and relate it to the thinning effect detected in the molecular dynamics simulations.

3:30PM Q42.00006 Recovery of polymer folding landscapes from univariate time series and its dimensionality reduction using machine learning, JIANG WANG, Department of Physics, University of Illinois at Urbana-Champaign, ANDREW FERGUSON, Materials Science and Engineering, University of Illinois at Urbana-Champaign — The stable conformations and motions of polymers and macromolecules are governed by their underlying free energy surface. By integrating ideas from dynamical systems theory with nonlinear manifold learning, we have developed an approach to recover single-molecule free energy surfaces from univariate time series of a single system observable. Using the method of delays, we expand the time series into a high dimensional phase space in which, by Takens' Theorem, the dynamics are equivalent to those of the molecule in real space. We then apply nonlinear manifold learning algorithm (diffusion maps and nonlinear PCA) to extract a low-dimensional representation of the free energy surface that is diffeomorphic (i.e., a smooth transformation) to that which would have been recovered from a complete knowledge of all system degrees of freedom. We have validated our approach in molecular dynamics simulations of a C$_2$H$_4n$-alkane chain, demonstrating that the free energy surface extracted from the atomistic simulation trajectory is geometrically and topologically equivalent to that recovered from a knowledge of only the head-to-tail distance of the chain. Our approach lays the foundations to extract empirical single-molecule free energy surfaces directly from experimental data.

3:42PM Q42.00007 Flow-Induced Crystallization and Nucleation in Isotactic Polypropylenes, SCOTT MILNER, Pennsylvania State University — Flow-induced crystallization (FIC) occurs when a brief interval of strong flow precedes a temperature quench; many more nuclei form, resulting in a much more fine-grained solid morphology and better material properties. Commercial industrial polymer processing (injection molding) depends on FIC, which has been the subject of many experimental studies, most commonly on isotactic polypropylene (iPP). The prevailing hypothesis is that FIC results from flow aligning chains in the melt, increasing the melt free energy with respect to the crystal, hence acting like undercooling. Here, I combine experimental results for FIC and homogeneous nucleation with theoretical estimates for critical nuclei; to assess the prevailing hypothesis. Current best information supports the view that chain stretching (not just alignment) is necessary and sufficient to explain the observed increase in nucleation rate. Important puzzles remain: 1) shear applied at temperatures well above the equilibrium melting temperature Tm = 187 °C is effective for FIC, and 2) a shear sample may be held for hours above Tm, and still crystallize faster when quenched.

4:18PM Q42.00008 Emergent tilt order in zigzagging polymer liquids, BENJAMIN LOEWE, ANTON SOUSLOV, PAUL M. GOLDBART, Georgia Institute of Technology — We study a liquid of zigzagging two-dimensional polymers that have bending rigidity. These are directed polymers whose conformations lie along the paths followed by pieces on a checkerboard. We observe that in the continuum limit the statistical physics of one such polymer can be described in terms of the Dirac equation for a particle having an imaginary mass. We exploit this observation to study the effect of high electric fields on polyolefins. At critical conditions, we observe a thinning effect leading to electromechanical breakdown. We also determine the critical voltage using theoretical models and relate it to the thinning effect detected in the molecular dynamics simulations.

1Multidisciplinary University Research Initiative (MURI)

2This work was supported in part by NSF grant DMR 12 07026.
Simulations are used to study the behavior of two polymers under confinement in a cylindrical tube. We measure the free energy and the end-to-end distance of the tails. The tails do not follow the worm-like chain model and exhibit a stretched conformation. This picture for the adsorbed layer is akin to the de Gennes blob scaling model. For finite tubes, a tail and an adsorbed segment dominate the chain conformation of the adsorbed layer. Also, the mean-square end-to-end distance normal to the substrate is proportional to the normal component of the mean-square end-to-end distance to the substrate. Both quantities agree with Silberberg’s derivation for an ideal chain in the presence of a reflecting wall. We characterized the conformation near the substrate. This is demonstrated in the chain center-of-mass distribution normal to the substrate and the probability of a polymer chain ends to be the closest to the substrate. The finite element approach allows use of arbitrarily shaped systems and is ideal for studying confinement effects. We explore how this framework works on a few examples for polymers confined to a sphere.

Parallel framework for wormlike chains using self consistent field theory. The Gaussian chain model commonly used in Self Consistent Field Theory (SCFT) does not account for confinement effects. The wormlike chain model makes no assumption about the form of confinement and systems such as liquid crystals where alignment effects are critical. The orientations accounted for in a wormlike chain model can correctly capture the physics of these systems. The primary problem with a wormlike chain model is the computational cost of implementation, which far exceeds that of the Gaussian chain model. We address this problem through a parallel SCFT framework for wormlike chains incorporating orientation interactions. The framework can scale to 10s of thousands of processors using an efficient finite element (FE) approach. Orientations are treated with an FE in FE method which overlays a surface orientation mesh on top of the spatial geometry mesh. The finite element approach allows use of arbitrarily shaped systems and is ideal for studying confinement effects. We characterize the adsorbed chains and counted the number of loops and tails. For stiff chains, a tail and an adsorbed segment dominate the chain conformation of the adsorbed layer. Also, the mean-square end-to-end distance normal to the substrate is proportional to the normal component of the mean-square end-to-end distance of the tails. The tails do not follow the worm-like chain model and exhibit a stretched conformation. This picture for the adsorbed layer is akin to the polysaccharide model envisioned by Guiselin. We probe the dynamics of the segments by calculating the layer- resolved intermediate coherent collective dynamics structure factor, \( S(q,t,z) \), for values equivalent to the bond length. The segment dynamics is slower for stiffer chains. In the adsorbed layer, dynamics is slowed down and can be described by two relaxation times.
2:54PM Q43.00003 A hybrid Brownian Dynamics model for yielding, aging, and rejuvenation in deforming polymeric glasses1, WEIZHONG ZOU, RONALD LARSON, Department of Chemical Engineering, University of Michigan, Ann Arbor — We describe the rheology of polymeric glasses by combining a simple constitutive equation for the fast segmental modes, borrowed from Fielding, et al.[1], with Brownian dynamics (BD) simulations of the slow polymer modes. The BD simulations determine the polymeric stress from ensembles of finitely extensible bead-spring chains, where the bead drag coefficient is governed by solutions to the equation for segmental relaxation. Thus the model treats the short glassy segmental mode as “solvent” for the polymer modes. With rubbery modulus for the slow-relaxing polymer modes as one of our model parameters, stress-dependent relaxation, physical aging, flow rejuvenation as well as strain-hardening and recovery can be successfully accounted for in uniaxial extension and steady shear, without the use of an artificial “crinkle factor” used to account for recoil dynamics in previous work [1]. Our simulation results remarkably agree with the experimental data from Lee et al.[2] A comparison between our model and the barrier-hopping theory [3] is also made.


The authors acknowledge discussions with M. E. Cates and S. M. Fielding.

3:06PM Q43.00004 Structural Recovery of Glass-Forming Materials, SINDEE SIMON, Texas Tech University — The glass transition and structural recovery of glass-forming materials, including polymeric, small-molecule, and inorganic network glasses, have been studied in our laboratory using dilatometry and calorimetry. Of particular interest have been the relative timescales to reach equilibrium for different properties, whether the extrapolated liquid line is reached at equilibrium, the ability of phenomenological models to describe the structural recovery process, and behavior at the nanoscale. Recent work using a commercial rapid-scanning calorimeter has extended the time and temperature range to times as short as 0.01 s and temperatures up to 15 K above the nominal Tg. Our results will be discussed in the context of unanswered questions in the field.

3:42PM Q43.00005 Quantitative relaxation dynamics of supercooled liquids from first principles, LIESBETH JANSSEN, Columbia University, PETER MAYER, ThinkEco, Inc., DAVID REICHMAN, Columbia University — Understanding the liquid-to-glass transition remains one of the deepest unsolved problems in condensed matter science. Here we present a novel first-principles framework, referred to as generalized mode-coupling theory (GMCT), which can predict the microscopic dynamics of glass-forming systems with near-quantitative accuracy using only simple static information as input. The theory is based on the well-established standard mode-coupling theory (MCT) of the glass transition, but rigorously incorporates higher-order dynamic density correlations neglected in standard MCT. We demonstrate that GMCT can accurately describe the dynamics of quasi-hard spheres over an unprecedentedly large time and density domain, supporting the view that activated glassy behavior is inherently dynamic in origin. Finally, our schematic results show that GMCT is capable of predicting novel types of glass transitions, including type-A, type-B, and avoided transitions, as well as different types of relaxation-time scaling behaviors. This suggests that GMCT may constitute the first microscopic, first-principles theory that can account for different fragilities in glass-forming materials.

3:54PM Q43.00006 Using s-ensemble to probe glasses formed by cooling and aging, DAVID CHANDLER, University of California, Berkeley, JUAN P. GARRAHAN, University of Nottingham, AARON S. KEYS, University of California, Berkeley — Space-time phase transitions can be studied within the context of large-deviation formalism. Numerical implementations of this formalism to lattice models and atomistic models have demonstrated the existence of such transitions between liquid-like (i.e., dynamically active) and glassy (i.e., dynamically inactive) phases. Here, in terms of an emergent nonequilibrium correlation length and formulas derived from dynamical facilitation theory [1,2], we describe how glassy states obtained from the large-deviation formalism (i.e., the s-ensemble) are equivalent to the glassy states obtained from nonequilibrium cooling protocols. We test the formulas with lattice models, and we demonstrate that the formulas are consistent with nonequilibrium calorimetry experiments [3].


4:06PM Q43.00007 Nontrivial correlation length distinguishes melt from glass in a large-scale atomistic non-equilibrium simulation of a glass transition1, KRANTHI MANDADAPU, Lawrence Berkeley National Laboratory, ALEXANDER HUDSON, DAVID CHANDLER, University of California Berkeley — Dynamical facilitation theory [1,2] predicts the emergence of a non-trivial correlation length from the cooling process that transforms the reversible melt to the irreversible glass [3]. A decrease in cooling rate produces an increase in correlation length, and an increase in correlation length coincides with an increase in stability and aging rate of the glass. Here, we present results from a large-scale non-equilibrium numerical simulation that provide the first demonstration of the emergent nonequilibrium correlation length for an atomistic model. The study also tests the ability of the theory to predict the value of the nonequilibrium length and its corresponding glass transition temperature in terms of material properties and cooling protocols.


4:18PM Q43.00008 Thwarting Crystallization through Hydrogen Bonding in Triazine Molecular Glasses, AUDREY LAVENTURE, University of Montreal, ARMAND SOLDERA, University of Sherbrooke, OLIVIER LEBEL, Royal Military College of Canada, CHRISTIAN PELLERIN, University of Montreal — Using irregular shaped molecules interacting weakly with each other is the most intuitive choice of material properties and cooling protocols. In this presentation, we will show that variable-temperature infrared spectroscopy is a tool of choice to probe the vitreous state of these compounds. We take advantage of the selectivity of this technique to correlate their molecular features to their thermal properties. Quantitative monitoring of hydrogen bonds during vitrification will be addressed.
4:30PM Q43.00009 Theory of the Role of Attractive Forces in the Dynamics of Supercooled Liquids under Isochoric and Isobaric Conditions, ZACHARY E. DELL, KENNETH S. SCHWEIZER, University of Illinois at Urbana-Champaign — Microscopic, force-level, dynamical theories of supercooled liquids (e.g., mode-coupling, elastically cooperative nonlinear Langevin equation (ECNLE)) employ a projection approximation that replaces the real forces by a single effective force determined by the equilibrium pair structure. Recent isochoric simulations by Berthier and Tarjus suggest that under isochoric conditions such theories fail to capture the effect of attractions which might not change structure but can strongly slow relaxation. We propose a hybrid dynamical theory where the ECNLE approach with effective forces is employed for repulsions, and for attractions a new projection-less description is developed where the attractive forces directly enter. The theory is applied to the Lennard-Jones and repulsive WCA fluids in the supercooled regime. Under isochoric conditions, we find qualitative agreement with the recent simulations, where attractive forces are important depending on the specific density. Under isobaric conditions, attractive forces are found to be unimportant due to the combined effect of thermal contraction and increasing effective particle size upon cooling. The new theory exhibits density scaling, and realistically predicts the relaxation time of molecular liquids over 14 decades in time.

4:42PM Q43.00010 Relation of dynamics and local structure to glass-formability in a crystallizable bead-spring polymer model, HONG NGUYEN, TYLER SMITH, ROBERT HOY, Univ of South Florida, NIKOS KARAYIANNIS, Universidad Politecnica de Madrid, Madrid, Spain — We relate the dynamics and local structure of equilibrium and supercooled polymer melts using a model wherein a single parameter (bending stiffness) controls the morphology of the equilibrium, low-temperature crystal. The dynamical slowing down in strongly glassforming systems correlates directly to the increasing presence of microstructural features that are incompatible both with each other and with crystalline order. Systems which more readily crystallize also exhibit rich behavior since their solid-state morphology can be varied from nearly amorphous to highly crystalline by varying their thermal preparation protocol. We tie the “critical” cooling rates, across which this behavior varies, to the lifetimes of structural features such as small crystalline nuclei and stable liquid-like clusters. The role such structures play is analogous to that recently demonstrated for colloidal systems [S. R. Williams, arXiv:0705.0203, 2007], but is considerably enriched both by the dynamical constraints imposed by covalent connectivity and by the presence of a second characteristic length scale (the polymer Kuhn length) controlled by chain bending stiffness.

5:06PM Q43.00012 Dynamic Odd-Even Effects in a Network-Forming Ionic Glass Homologue, KE YANG, Univ of Illinois - Urbana, MADHUSSUDAN TYAGI, NIST Center for Neutron Research, NIST, JEFFREY MOORE, YANG ZHANG, Univ of Illinois - Urbana — Odd-even effects, the non-monicotonic dependency of physical properties on odd/even number of structural units, are widely observed in homologous series of crystalline materials. However, such alternation is not expected for amorphous molecular materials because of periodic packing. Herein, we report the synthesis and characterization of a class of stable network-forming ionic glasses with specific structure to frustrate crystallization. We performed incoherent elastic neutron scattering measurements of the nanosecond mean squared displacement and quasi-elastic neutron scattering measurements of the nanosecond relaxation time. The results indicated that the even-numbered cations showed much slower dynamics than neighboring odd-membered cations, i.e., one-methylene unit structural difference causes an abnormal difference (about five times) in cations’ diffusional dynamics. The observed difference in mobility exists both around Tg and extends to the liquid temperature regime well above Tg. The observed dynamic odd-even effect serves as another intriguing example of significant dynamic differences induced by insignificant structural changes, as is common in glass transition.

5:18PM Q43.00013 Glass formation behavior of an isolated polymer chain, WESTON MERLING, JACK MILESKI, DAVID SIMMONS, University of Akron — A single polymer chain in isolation logically represents the extreme limit of nanocoherence with respect to segmental dynamics and glass formation. Work in thin polymer films suggests that one should expect a large Tg suppression in such systems. However, recent dielectric relaxation measurements of isolated chains of P2VP in a silica substrate found bulk-like Tg in this system, apparently raising questions about the nature of observed nanocoherence effects on the glass transition. Here we describe simulations of glass formation in an isolated polymer chain, both free-floating and deposited on a substrate. Results indicate that free-floating isolated polymer chains exhibit a depression in the dynamic glass transition temperature equivalent to more than 100K in polystyrene units. However, when a chain is deposited on a substrate with sufficiently favorable surface interactions, bulk-like dynamics can be recovered due to competition between the free-surface and adsorbed interface. When this compensation effect is taken account, these results indicate that the observation of bulk-like dynamics in isolated P2VP chains on a silica substrate is consistent with observations of large Tg suppressions in polymer films supported by less attractive substrates.

This material is based upon work supported by the National Science Foundation under Grant No. DMR1310433

Wednesday, March 4, 2015 2:30PM - 5:18PM –
Session Q44 GSNP: Networks and their applications
2:30PM Q44.00001 Topological Phenotypes in Complex Leaf Venation Networks, HENRIK RONEL-LENFTITSCH, JANA LASSER, Max Planck Institute for Dynamics and Self-Organization, DOUGLAS DALY, New York Botanical Garden, ELENI KATIFORI, Max Planck Institute for Dynamics and Self-Organization — The leaves of vascular plants contain highly complex venation networks consisting of recursively nested, hierarchically organized loops. We analyze the topology of the venation of leaves from ca. 200 species belonging to ca. 10 families, defining topological metrics that quantify the hierarchical nestedness of the network cycles. We find that most of the venation variability can be described by two dimensional phenotypic space, where one dimension consists of a linear combination of geometrical metrics and the other dimension of topological, previously uncharacterized metrics. We show how this new topological dimension in the phenotypic space significantly improves identification of leaves from fragments, by calculating a “leaf fingerprint” from the topology and geometry of the higher order venation systems. Further, we present a simple model suggesting that the topological phenotypic traits can be explained by noise effects and variations in the timing of higher order venation developmental events. This work opens the path to (a) new quantitative identification techniques for leaves which go beyond simple geometric traits such as vein density and (b) topological quantification of other planar or almost planar networks such as arterial vasculature in the neocortex and lung tissue.
2:42PM Q44.00002 Nonlinear Dynamics and Control in Microfluidic Networks. DANIEL CASE, Northwestern University, JEAN-REGIS ANGILELLA, Universite de Caen et de Basse Normandie, ADILSON MOTTER, Northwestern University — Researchers currently use abundant external devices (e.g., pumps and computers) to achieve precise flow dynamics in microfluidic systems. Here, I show our use of network concepts and computational methods to design microfluidic systems that do not depend on external devices yet still exhibit a diverse range of flow dynamics. I present an example of a microfluidic channel described by a nonlinear pressure-flow relation and show that complex flow behavior can emerge in systems designed around a terminal. By controlling the flow into and out of this terminal in such a system, we demonstrate the propagation of fluid flow through intermediate channels not directly connected to the controlled terminal. I also show that adding (or removing) flow channels to a system can result in unexpected changes in the total mass flow rate, depending on the network structure of the system. We expect this work to both expand the applicability of microfluidics and promote scaling up of current experiments.

This research was funded by the National Science Foundation.

2:54PM Q44.00003 Independence of bond-level response in disordered networks. CARL GOODRICH, ANDREA LIU, University of Pennsylvania; SIDNEY NAGEL, University of Chicago — Many properties of spring networks, such as bulk elasticity, are a sum of contributions from individual bonds. For disordered systems, these contributions are often characterized by continuous distributions with tails that can be many times larger than the mean. Here, we show that these disordered networks are “stronger” or “weaker” than others. How the network responds to compression, for example, tells little about how it will respond to shear. This leads to a new principle for disordered solids: independence of bond-level response. We will show how this principle can be exploited to construct metamaterials with unique, textured, tunable and often extreme response.

3:06PM Q44.00004 ABSTRACT WITHDRAWN

3:18PM Q44.00005 Phase-space network structure of two-dimensional ±J spin glasses. XIN CAO, Hong Kong Univ of Sci & Tech, FENG WANG, Boston University, YI LONG HAN, Hong Kong Univ of Sci & Tech — We illustrate a complex-network approach to study the phase spaces of spin glasses. By exactly mapping the whole ground-state phase spaces of two-dimensional Edwards-Anderson bimodal (±J) spin glasses into networks, we discovered various phase-space properties via network analysis. The Gaussian connectivity distribution of the phase-space networks demonstrates that both the number of free spins and the visiting frequency of microstates follow Gaussian distributions. The spectra of phase-space networks are Gaussian, which is proved to be exact when the system is infinitely large. The phase-space networks exhibit community structures, which enables us to construct the entropy landscape of the ground state as a network and discover its scale-free property. The phase-space networks exhibit fractal structures, as a result of the rugged entropy landscape. Moreover, we show that the connectivity distribution, the community structure and the fractal structure drastically change at the ferromagnetic-glass transition. These quantitative measurements of the ground states provide new insight into the studies of spin glasses. On the other hand, the phase-space networks establish a new class of complex networks with unique topology.

The work was supported by RGCGrants GRF601613.

3:30PM Q44.00006 Thermal Transport in Cayley-Tree Networks. TSAMPIKOS KOTTOS, HUANAN LI, Wesleyan Univ; BORIS SHAPIRO, Technion — In recent years there has been a lot of attention in the microscopic derivation of the laws that dictate heat current in low dimensional systems. However, many real structures are not simple one or two-dimensional structures. Rather, they are characterized by a complex connectivity that can be easily designed and realized in the laboratory. It is therefore necessary to unveil the rules that dictate thermal transport in such networks. In this contribution we present analytical results on heat current and its thermal fluctuations for a Cayley tree consisting of two types of harmonic masses: vertex masses \( M \) where phonon scattering occurs and bond masses \( m \) where phonon propagation take place. The tree is coupled to thermal reservoirs consisting of one-dimensional harmonic chain of masses \( m \). We find that the heat current is a non-monotonic function of the mass-ratio \( \mu = M/m \). In particular, there are cases when the heat current is strictly zero below some critical value \( \mu^* \). The effects of imperfections (disorder) on the heat transport are also discussed and analyzed.

This work was partly sponsored by a NSF DMR-1306984 grant and AFOSR MURI FA9550-14-0037 grant.

3:42PM Q44.00007 Fragmentation of random trees. ZIYA KALAY, Kyoto University, ELLI BEN-NAIM, Los Alamos National Laboratory — We investigate the fragmentation of a random recursive tree by repeated removal of nodes, resulting in a forest of disjoint trees. The initial tree is generated by sequentially attaching new nodes to randomly chosen existing nodes until the tree contains \( N \) nodes. As nodes are removed, one at a time, the tree resolves into an ensemble of disjoint trees, like a forest. We study the statistical properties of trees and nodes in this heterogeneous forest. In the limit \( N \to \infty \), we find that the system is characterized by a single parameter: the fraction of remaining nodes \( m \). We obtain analytically the size density \( \phi \) of trees of size \( s \), which has a power-law tail \( \phi \sim s^{-\alpha} \), with exponent \( \alpha = 1 + 1/m \). Therefore, the tail becomes steeper as further nodes are removed, producing an unusual scaling exponent that increases continuously with time. Furthermore, we investigate the fragment size distribution in a growing tree, where nodes are added as well as removed, and find that the distribution for this case is much narrower.

3:54PM Q44.00008 Cascading Failures and Stochastic Analysis for Mitigation in Spatially-Embedded Random Networks. NOEMI DERZSY, XIN LIN, ALAA MOUSSAWI, BOLESŁAW K. SZYMANSKI, GYORGY KORNISS, Rensselaer Polytechnic Institute — In complex information or infrastructure networks, even small localized disruptions can give rise to congestion, large-scale correlated failures [1], or cascades, — a critical vulnerability of these systems. Recent studies have demonstrated that driven-cascading overload failures in spatial graphs, such as the power grid, are non-self-avoiding, hence predictability is poor and conventional mitigation strategies are largely ineffective [2]. In particular, we have shown that protecting all nodes (or edges) by the same additional capacity (tolerance) can actually lead to larger global failures, i.e., “paying more can result in less”, in terms of robustness [2]. Here, we explore stochastic methods for optimal heterogeneous distribution of resources (node or edge capacities) subject to a fixed total cost. In addition to random geometric graphs, we also investigate cascading failures on the UCTE European electrical power transmission network. [1] A. Bernstein, D. Bienstock, D. Hay, M. Uzunoglu, and G. Zussman, http://arxiv.org/abs/1206.1099 (2011). [2] A. Asztalos, S. Sreenivasan, B.K. Szymanski, and G. Korniss, PLOS One 9(1): e84563 (2014).

4:06PM Q44.00009 Cooperative SIS epidemics can lead to abrupt outbreaks. FAKHTEH GHANBARNE-JAD, Max Planck Institute for the Physics of Complex Systems, Germany, LI CHEN, Robert Koch-Institute, 13353 Berlin, Germany, WEIRAN CAI, Technische Universität Dresden, Germany, PETER GRASSBERGER, Forschungszentrum Jülich, Germany. In this paper, we study spreading of two cooperative SIS epidemics in mean field approximations and also within an agent based framework. Therefore we investigate dynamics on different topologies like Erdos-Renyi networks and regular lattices. We show that cooperativity of two diseases can lead to strongly first order outbreaks, while the dynamics still might present some scaling laws typical for second order phase transitions. We argue how topological network features might be related to this interesting hybrid behaviors.

3:54PM Q44.00008 Cascading Failures and Stochastic Analysis for Mitigation in Spatially-Embedded Random Networks. NOEMI DERZSY, XIN LIN, ALAA MOUSSAWI, BOLESŁAW K. SZYMANSKI, GYORGY KORNISS, Rensselaer Polytechnic Institute — In complex information or infrastructure networks, even small localized disruptions can give rise to congestion, large-scale correlated failures [1], or cascades, — a critical vulnerability of these systems. Recent studies have demonstrated that driven-cascading overload failures in spatial graphs, such as the power grid, are non-self-avoiding, hence predictability is poor and conventional mitigation strategies are largely ineffective [2]. In particular, we have shown that protecting all nodes (or edges) by the same additional capacity (tolerance) can actually lead to larger global failures, i.e., “paying more can result in less”, in terms of robustness [2]. Here, we explore stochastic methods for optimal heterogeneous distribution of resources (node or edge capacities) subject to a fixed total cost. In addition to random geometric graphs, we also investigate cascading failures on the UCTE European electrical power transmission network. [1] A. Bernstein, D. Bienstock, D. Hay, M. Uzunoglu, and G. Zussman, http://arxiv.org/abs/1206.1099 (2011). [2] A. Asztalos, S. Sreenivasan, B.K. Szymanski, and G. Korniss, PLOS One 9(1): e84563 (2014).

3Supported in part by DTRA, NSF, and ARL NS-CTA
4:18PM Q44.00010 Eigenvalue Separation in the Laplacian Spectra of Random Geometric Graphs¹, AMY NYBERG, KEVIN E. BASSLER, Department of Physics, University of Houston — The graph Laplacian spectra of networks are important for characterizing both their structural and dynamical properties. As a prototypical example of networks with strong correlations, we investigate the spectra of random geometric graphs (RGGs), which describe networks whose nodes have a random physical location and are connected to other nodes within a threshold distance r. RGGs model transportation grids, wireless networks, and biological processes. The spectrum consists of two parts, a discrete part consisting of a collection of integer valued delta function peaks centered about the average degree and a continuous part that exhibits the phenomenon of eigenvalue separation. We examine the behavior of eigenvalue separation for large network size N in several scaling regimes based on the parameter α such that \( N^{\alpha} = c \) is constant. We identify a transition at \( \alpha = 1/3 \), above which the separated peaks get closer together as N increases and separation is eventually lost, but below which the peaks get farther apart. Also, an approximation for the expected number of separated peaks is given in terms of N and the average degree and we show that the expected number of peaks scales as \( N^{\alpha} \).

¹This work was supported by the NSF through grant DMR-1206839 and by the AFOSR and DARPA through grant FA9550-12-1-0405.

4:30PM Q44.00011 Bounds for percolation thresholds on directed and undirected graphs¹, KATHLEEN HAMILTON, LEONID PRYADKO, University of California - Riverside — Percolation theory is an efficient approach to problems with strong disorder, e.g., in quantum or classical interest in graph theory as a tool for describing complex connections in various kinds of networks: social, biological, technological, etc. In particular, percolation on graphs has been used to describe internet stability, spread of contagious diseases and computer viruses; related models describe market crashes and viral spread in social networks. We consider site-dependent percolation on directed and undirected graphs, and present several exact bounds for location of the percolation transition in terms of the eigenvalues of matrices associated with graphs, including the adjacency matrix and the Hashimoto matrix used to enumerate non-backtracking walks. These bounds correspond to a mean field approximation and become asymptotically exact for graphs with no short cycles. We illustrate this convergence numerically by simulating percolation on several families of graphs with different cycle lengths.


¹This research was supported in part by the NSF grant PHY-1416578 and by the ARO grant W911NF-11-1-0027

4:42PM Q44.00012 Reconstructing Weighted Networks from Dynamics¹, EMILY S.C. CHING, Department of Physics, The Chinese University of Hong Kong, P.Y. LAI, Department of Physics, Graduate Institute of Biophysics, and Center for Complex Systems, National Central University, C.Y. LEUNG, Department of Physics, The Chinese University of Hong Kong — The knowledge of how the different nodes of a network interact or link with one another is crucial for the understanding of the collective behavior and the functionality of the network. We have recently developed a method that can reconstruct both the links and their relative coupling strength of bidirectional weighted networks. Our method requires only measurements of node dynamics as input and is based on a relation between the pseudo-inverse of the matrix of the correlation of the node dynamics and the Laplacian matrix of the weighted network. Using several examples of different dynamics, we demonstrate that our method can accurately reconstruct the connectivity as well as the weights of the links for weighted random and weighted scale-free networks with both linear and nonlinear dynamics.

¹The work of ESCC and CYL has been supported by the Hong Kong Research Grants Council under grant no. CUHK 14300914.

4:54PM Q44.00013 Identification of core-periphery structure in networks, XIAO ZHANG, TRAVIS MARTIN, MARK NEWSMAN, Univ of Michigan - Ann Arbor — Many networks can be decomposed into a dense core plus an outlying, loosely-connected periphery. In this talk I will describe a method for performing such a decomposition on empirical network data using methods of statistical inference. Our method fits a generative model of core-periphery structure to observed data using a combination of an expectation-maximization algorithm for calculating the parameters of the model and a belief propagation algorithm for calculating the decomposition itself. We find the method to be efficient, scaling easily to networks with a million or more nodes and we test it on a range of networks, including real-world examples as well as computer-generated benchmarks.

5:06PM Q44.00014 Small-World Propensity: A novel statistic to quantify weighted networks, DANIELLE BASSETT, SARAH MULDOON, Univ of Pennsylvania, ERIC BRIDGEFORD, John Hopkins University — Many real-world networks have been shown to display a small-world structure with high local clustering yet short average path length between any two nodes. However, characterization of small-world properties has generally relied on a binarized representation of such graphs, neglecting the important fact that, in reality, many real-world networks are actually composed of weighted connections spanning a wide range of strengths. Hence, we present a generalization of the Watts-Strogatz formalism for weighted networks along with a novel statistic called the Small-World Propensity that quantifies both binary and weighted small-world structure. We apply this measure to real-world brain networks and show that by retaining network weights, we are able to better understand the small-world structure of these systems.

Wednesday, March 4, 2015 2:30PM - 5:30PM – Session Q45 DPOLY: Transport in Charged and Ion-Containing Polymers 216AB - Christopher Soles, National Institute of Standards and Technology

2:30PM Q45.00001 Molecular Dynamics Simulations of Ion Transport and Mechanisms in Polymer Nanocomposites¹, SANTOSH MOGURAMPPELZY, VENKAT GANESAN, Department of Chemical Engineering, University of Texas at Austin, Austin, Texas 78712, United States — Using all atom molecular dynamics and trajectory-extending kinetic Monte Carlo simulations, we study the influence of Al₂O₃ nanoparticles on the transport properties of Li⁺ ions in polymer electrolytes consisting of polyethylene oxide (PEO) melt solvated with LiBF₄ salt. We observe that the nanoparticles have a strong influence on polymer segmental dynamics which in turn correlates with the mobility of Li⁺ ions. Explicitly, polymer segmental relaxation times and Li⁺ ion residence times around polymer were found to increase with the addition of nanoparticles. We also observe that increasing short range repulsive interactions between nanoparticles and polymer membrane leads to increasing polymer dynamics and ion mobility. Overall, our simulation results suggest that nanoparticle induced changes in conformational and dynamic properties of the polymer influences the ion mobilities in polymer electrolytes and suggests possible directions for using such findings to improve the polymer matrix conductivity.

¹The authors acknowledge the Texas Advanced Computing Center (TACC) at The University of Texas at Austin for providing computing resources that have contributed to the research.
2:42PM Q45.00002 Viscoelastic Nanomechanics of Ionomically Cross-linked Polyelectrolyte Networks

 BIAO HAN, Drexel University, DAEYEON LEE, University of Pennsylvania, LIN HAN, Drexel University

Understanding the mechanics of ionically cross-linked polyelectrolyte networks is critical for applications where nm-to-um mechanics is the key to success. This study aims to reveal the roles of ionic cross-links and fixed charges in the viscoelasticity of layer-by-layer poly(allylamine hydrochloride)/poly(acrylic acid) microfilms, PAH/PAA, a complex held by pH-sensitive amine-carboxyl links. AFM-nanoindentation and force relaxation (tip R=12.5um) was performed at ion strength(IS)=0.01-1.0M, pH=5.5-2.0 (pKa of PAA=2.3). When pH changes from 5.5 to 2.0, the films swell for 4x from densely linked, net neutral state to loosely linked, positively charged one. A >100x reduction in indentation modulus was observed at all IS, suggesting the dominance of decrease in cross-link density. In most states, more than 90% force relaxation was observed, where cross-link breaking/reformation likely dominates viscoelasticity. However, at pH=2.5 and IS=0.01M, when electrical double layer repulsion is important (Debye length≈3nm), relaxation was about 60%, highlighting the contribution of fixed charges. In summary, this study revealed unique viscoelastic behaviors of PAH/PAA due to the pH- and IS-dependent cross-link and charge densities.

2:54PM Q45.00003 Charge transport and glassy dynamics of poly(ethylene oxide)-based single-ion conductors under geometrical confinement

 JAMES RUNT, CIPRIAN IACOB, Materials Science and Engineering, Penn State University

Segmental and local dynamics as well as charge transport are investigated in a series of poly(ethylene oxide)-based single-ion conductors (ionomers) with varying counters (Li+, Na+) confined in unidirectional nanoporou silica membranes. The dynamics are explored over a wide high and low temperature range by broadband dielectric relaxation spectroscopy. Slowing of segmental dynamics and a decrease in dc conductivity (strongly coupled with segmental relaxation) of the confined ionomers are associated with surface effects — resulting from interfacial hydrogen bonding between the host nanoporous silica membrane and the guest ionomers. These effects are significantly reduced or eliminated upon pore surface modification through silanization. The primary transport properties for the confined ionomers decrease by about one decade compared to the bulk ionomer. A model assuming reduced mobility of an adsorbed layer at the pore wall/ionomer interface is shown to provide a quantitative explanation for the decrease in effective transport quantities in non-silanized porous silica membranes. Additionally, the effect of confinement on ion aggregation in ionomers by using X-ray scattering will also be discussed.

1Supported by the National Science Foundation, Polymers Program.

3:06PM Q45.00004 High Efficiency Conduction at High Ion Contents in Ionomeric Electrolytes

 KERAN LU, JANNA MARANAS, SCOTT MILNER, Pennsylvania State University

High conductivity solid polymer electrolytes (SPEs) can open the door to safer batteries with greater capacity. Current SPEs have low conductivity, which in part is due to collective motion losses from ions diffusing as clusters. Charge is “carried” by neutral ion clusters (i.e. pairs). Using an ion-only coarse-grained molecular dynamics simulation, we show that a high ion content ionomeric electrolyte shows negligible collective motion losses due to the passing nature of ion transport. Compared to carrying, passing randomizes cation-anion motion beyond their coordination distance, resulting in greater conduction efficiency in agreement with experiments. These results suggest that well designed ion networks at higher ion contents could potentially produce highly-conductive SPEs.

3:18PM Q45.00005 Effect of molecular weight on ion diffusion and transference number in poly(ethylene oxide)

 KSENIA TIMACHOVA, NITASH BALSARA, University of California - Berkeley

Solid polymer electrolytes are of great interest for their potential use in high specific energy, solid-state batteries, however, salt transport properties in polymer electrolytes have not been comprehensively addressed over a wide range of molecular weights. Poly(ethylene oxide) (PEO) has been the most widely studied polymer electrolyte due to its high solvency of lithium salts and low glass transition temperature. This study presents measurements of the transport properties of lithium bis(trifluoromethanesulfonimide)imidide (LiTFSI) in PEO at both the high concentration present in functional electrolytes and in the dilute limit for a large range of PEO molecular weights. Individual diffusion coefficients of the Li+ and TFSI- ions were measured using pulsed-field gradient nuclear magnetic resonance and the cation transfer number was calculated. The diffusion coefficients, concentration number, and conductivity as a function of molecular weight and salt concentration provide a complete set of transport properties for PEO.

3:30PM Q45.00006 ABSTRACT WITHDRAWN

3:42PM Q45.00007 Conductivity Scaling Relationships in Nanostructured Membranes based on Proton Polymerized Ionic Liquids

 GABRIEL SANOJA, University of California, Berkeley, NATHANIEL LYND, University of Texas, Austin, RACHEL SEGALMAN, University of California, Santa Barbara

Nanostructured membranes based on proton polymerized ionic liquids are of great interest for a variety of electrochemical applications. Understanding the relationship between composition, structure, and ionic conductivity for these materials is essential for designing novel membranes with improved properties. In this work, we explore the effect of volume fraction of ionic liquid on conductivity, α using a model system composed of poly(isoprene-block-ethylene oxide-stat-histamine) glycidyl ether diblock copolymers [Pi-b-P(EO-stat-HGE)] and the resulting [Pi-b-P(EO-stat-IL)] obtained after treatment with trifluoroacetic acid. These materials self-assemble into lamellar structures with volume fractions of ionic liquid ranging from 0.50 to 0.90 as demonstrated by SAXS. Pi-b-P(EO-stat-IL) membranes exhibit conductivities up to 4 x 10^{-3} S/cm at room temperature. In addition, Pi-b-P(EO-stat-IL) based membranes have lower water uptake (λ = 8-10) in comparison with most proton conducting membranes reported elsewhere. The low λ in these membranes might translate into a stronger effect of morphology on transport properties.

1Joint Center for Artificial Photosynthesis

3:54PM Q45.00008 Electrochemical Doping of poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene] using Polymerizable Ionic Liquids

 LAYLA MASRI, JANELLE LEGER, Western Washington University

A number of emerging organic electronic technologies utilize the mixed ionic/electronic conducting character of conjugated polymeric materials. We have developed a process by which fixed doping can be achieved in conjugated polymers through the formation of covalent bonds by replacing the salt used in traditional devices with polymerizable ionic liquids (PILs). It has previously been shown that poly[2-methoxy-5-(3,7-dimethyl-actoxy)-p-phenylenevinylene (MDMO-PPV) doped with alllyltrimethylammonium allylsulfonate (ATOAAS) will produce a fixed junction light-emitting electrochemical cell due to the dissociation and subsequent immobilization of ATOAAS. We will discuss electrochemical doping of poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene] (MEH-PPV) films with ATOAAS. We characterize these films via UV-Vis and cyclic voltammetry with emphasis on studying the formation of new mid-band gap energies associated with the color change observed when the film is electrochemically doped. We will discuss the mechanism for the formation of these mid-band gap energies and the applications of these films to developing technologies.
4:06PM Q45.00009 Structure and dynamics of single-ion conducting P(STFSI)-ran-P(EGMA) copolymer electrolytes, JENNIFER SCHAEFER, CHRISTOPHER SOLES, National Institute of Standards and Technology — Recently, PEO-based copolymers containing the lithiated STFSI monomer have been investigated for use as single-ion conducting electrolytes in lithium batteries. Single-ion conducting electrolytes eliminate ion concentration gradients that diminish cell performance. The low ionic conductivity of these electrolytes has limited their applicability thus far, but electrolytes based on the STFSI monomer have been shown to have sufficient conductivity to support cell operation at moderate temperatures. We will report on the characterization of the morphology and dynamics of P(STFSI)-ran-P(EGMA) copolymer electrolytes as a function of the monomer ratio (ion loading) and length of the polyethylene glycol comb. Copolymers containing sufficiently short PEG combs remain amorphous at ambient temperatures over a range of STFSI content.

4:18PM Q45.00010 Tuning the ionic conductivity in protic polymerized ionic liquid homo, random, and block copolymers, CHRISTOPHER EVANS, RACHEL SEGALMAN, University of California-Santa Barbara, UCSB TEAM — Proton conducting membranes are of interest for a number of energy applications including use in fuel cells and artificial photosynthesis systems. We have synthesized a new class of protic polymerized ionic liquids (PILs) based on imidazolium cations which exhibit high conductivities in the solid state. In contrast to previous imidazolium based PILs, the ionic liquid moity is attached via a carbon on the imidazole thus leaving the two nitrogens available to act as a proton donor/acceptor. The conductivities of these protic PILs, measured by dielectric spectroscopy, are orders of magnitude higher than the analogous non-protic PILs at a given distance above (Tg). These high conductivities are the result of a strong contribution from proton motion. A series of random and block copolymers containing the polymerized ionic liquid monomer and a non-ionic comonomer were also investigated to determine the role of comonomer on the conductivity of these materials. It was found that methyl acrylate, which has a low glass transition temperature and high dielectric constant, can result in improvements of ionic conductivity. Studies using solid state NMR are underway to understand the role of protons and mobile anions in controlling the overall conductivity of these materials.

4:30PM Q45.00011 Morphology-Conductivity Relationship in Salt-containing Diblock Copolymer/Homopolymer Mixtures, MATTHEW IRWIN, ROBERT HICKEY, TIMOTHY P. LODGE, Univ of Minn - Minneapolis — In order to unravel how ionic conductivity is affected by material morphology, a model system of polystyrene (PS), poly(ethylene oxide) (PEO), PS-block-PEO, and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) was fabricated and characterized. These pseudo-ternary polymer blends, in which the lithium salt associates nearly exclusively with the ethylene oxide, have the potential to form a variety of morphologies such as lamellae and the three-dimensionally interpenetrating bicontinuous microemulsion by simply changing blend composition. Similar to what has been observed in salt-containing diblock copolymers, both the order-disorder transition (ODT) temperature and the ODT temperature window of these blends increase sharply with salt loading. By modulating the relative volume fraction of the homopolymers in the blend, it was shown that although less than order-of-magnitude changes in the domain spacing do not appreciably affect ion conductivity, some morphologies can result in significantly better conductivity than others. These results outline what factors matter most when designing polymer electrolytes for applications such as rechargeable lithium metal batteries and proton exchange membranes.

4:42PM Q45.00012 The Effect of Structural Modifications on Ionic Conductivity in Newly-Designed Polyester Electrolytes, DANIELLE PESKO, Univ of California - Berkeley, YUKI JUNG, GEOFF COATES, Cornell University, NITASH BALSARA, Univ of California - Berkeley — Gaining a fundamental understanding of the relationship between molecular structure and ionic conductivity of polymer electrolytes is an essential step toward designing next generation materials for battery applications. In this study, we use a systematic set of newly-designed polymers with varying side-chain lengths and oxygen functional groups to elucidate the effects of structural modifications on the conductive properties of the corresponding electrolytes. Mixtures of polyesters and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) were characterized using ac impedance spectroscopy to measure the ionic conductivity at various temperatures and salt concentrations. The relative conductivities of these electrolytes in the dilute limit are directly comparable to results of molecular dynamics simulations performed using the same polymers. The simulations correspond well with the experimental results, and provide molecular level insight about the solvation environment of the lithium ions and how the ions transport through these polyesters.

4:54PM Q45.00013 Membranes with artificial free-volume enabled by block copolymer self-assembly, NIKOS PETZETAKIS, NITASH BALSARA, UC Berkeley — There has been considerable success towards the development of polymeric porous materials with pore sizes in the meso- or macro-scale regime. However, manipulation of polymer porosity in the micro-scale (pore diameter < 2nm) remains challenging. Previous studies relied on changes in the chemical composition and structure of the polymeric material in order to achieve the formation of larger fractional free volume. In the present report we demonstrate a methodology with which we can force a polymeric material away from structural equilibrium and then kinetically arrest it at this -out of equilibrium- state, ultimately, enabling the creation of a polymeric material with artificial free volume. Our methodology is based on block copolymer/homopolymer binary blend self-assembly where the membranes are made by first creating a heterogeneous film of a ABA type triblock copolymer containing a soluble homopolymer, B. Then in a second washing step the soluble homopolymer chains are dissolved away. The volume fraction of the composite membrane occupied initially by chains of homopolymer B is now converted to extra free volume in the microphase of block B. Key role of block A is to kinetically arrest the structure of the polymer during and after the washing step.

5:06PM Q45.00014 Noise and Ionic Conductivity in Glass Nanochannels1, BENJAMIN WIENER, Brown University, ALESSANDRO SIRIA, LYDÉRIC BOQUET, Ecole Normale Supérieure, Paris. DEREK STEIN, Brown University — Ion transport in nanochannels is relevant to processes in biology and has technological applications like batteries, fuel cells, and water desalination. We report experimental studies of the ionic conductance and noise characteristics of pulled glass capillaries with openings on the order of 50 nanometers. We employed an ac measurement technique to probe very low frequency fluctuations in the conductivity and to test a theory attributing these to chemical fluctuations in the surface charge density of the glass. We also investigate Hooge’s empirical description of the noise power spectrum and its relationship to current rectification observed in nanochannels in the surface dominated “Dukhin” regime. Finally, we test the effects of anion and cation mobility on the direction and magnitude of the observed rectification.

5:18PM Q45.00015 Structure of Nafion Thin Films on Gold1, ADAM WEBER, AHMET KUSOGLU, ALEXANDER HEXEMER, Lawrence Berkeley National Laboratory — Nafion is the prototypical ionomer in electrochemical energy devices due to its good ionic conductivity and permeselectivity. In most devices, ionomers are in contact with precious metal catalysts. When confined to nanometer-thick “thin” films (10 to 100 nm), Nafion’s morphology and associated transport properties deviate from the bulk. These changes are a function of the substrate and film thickness. In this talk, results from a systematic study of Nafion thin-film morphology on gold substrate using Grazing-incidence X-Ray Scattering (GISAXS) will be presented. GISAXS experiments carried out for a range of incident angles combined with the simulations of the electron density are used to demonstrate that the collected patterns are real and show an anisotropic long-range structural order that is strongest when the film thickness is around 50 nm and weakens for thicker and thinner films. Such ordering is not readily discernible on other substrates like carbon, nor with non-phase separated polymers like polystyrene. Results presented herein provide new insights into the key role of substrate/film interactions in inducing ordered structure in Nafion, which has implications for understanding ionomers interacting with various organic and inorganic materials in electrochemical devices.

1Supported by U. S. Department of Energy under contract number DE-AC02-05CH11231.
2:30PM Q46.00001 Dynamic force measurement of rearrangements in a 2D network of droplets, SOLOMON BARKLEY, MATILDA BACKHOLM, KARI DALNOKI-VERESS, McMaster University — The interaction between two liquid droplets in an immiscible liquid is well understood. However, the emulsions relevant to biological and industrial processes involve high concentrations of these droplets, and multi-body effects cannot be ignored. As droplets rearrange in response to a disturbance, the importance of individual pair-wise interactions between droplets changes with the geometry of neighbours. Here we report on an experimental setup consisting of a two-dimensional network of monodisperse droplets stabilized with a surfactant. The system is studied with micropipettes, which permits direct measurement of forces along with simultaneous imaging of the droplet network. One micropipette is used to apply a tensile or compressive force to the droplet cluster, while a second pipette acts as a force-transducing cantilever, deflecting in response to rearrangements of the droplets.

2:42PM Q46.00002 Precise measurements of droplet-droplet contact forces in quasi-2D emulsions, JANNA LOWENSOHN, CARLOS ORELLANA, ERIC WEEKS, Emory University — We use microscopy to visualize a quasi-2D oil-in-water emulsion confined between two parallel slides. We then use the droplet shapes to infer the forces they exert on each other. To calibrate our force law, we set up an emulsion in a tilted sample chamber so that the droplets feel a known buoyant force. By correlating the stress of the droplets and the strength of contacts with the buoyant forces, we validate our empirical force law. We improve upon prior work in our lab by using a high-resolution camera to image each droplet multiple times, thus providing sub-pixel resolution and reducing the noise. Our new technique identifies contact forces with only a 1% uncertainty, five times better than prior work. We demonstrate the utility of our technique by examining the normal modes of the droplet contact network in our samples.

2:54PM Q46.00003 Fluidization of a bubble raft under oscillatory compression, KLEBERT FEITOSA, NICHOLAS HAGANS, CHRISTINE O’DEA, James Madison University — Fluidization of two-dimensional foam is characterized by rearrangement events known as T1-events where clusters of four bubbles switch neighbors. We study rearrangement events in a bubble raft subject to periodic compression by an oscillating boundary. As the amplitude of oscillation increases, T1-events transition from being mostly reversible (elastic regime), to being increasingly irreversible (plastic regime). In addition, T1-events are found to occur most frequently right before the direction of oscillation reverses, where the stress is maximum. By contrast, the velocity field of the bubble raft shows strong dynamical heterogeneity after the direction of oscillation reverses and the stress relaxes.

3:06PM Q46.00004 Dynamical and structural transitions in periodically-driven emulsions: Reversibility loss and random hyperuniform organization, JOOST H. WEJJS, Ecole Normale Supérieure de Lyon, France, RAPHAËL JEANNERET, Warwick University, United Kingdom, REMI DREYFUS, Centre National de la Recherche Scientifique, DENIS BARTOLEO, Ecole Normale Supérieure de Lyon, France — We present experimental results and numerical simulations of a microfluidic echo process, in which a large number of droplets interact in a periodically driven viscous fluid [Jeanneret & Bartolo, Nature Comm. 5, 3474 (2013)]. Upon increasing the driving amplitude we demonstrate the collective reversibility loss of the droplet dynamics. In addition, the system undergoes a dynamical phase transition associated with a structural one: at the onset of irreversibility the droplet ensemble self-organises into a random hyperuniform state. Numerical simulations evidence that the purely reversible hydrodynamic interactions together with hard-core repulsion account for most of our experimental findings. Hyperuniformity is relevant for the production of large-band-gap materials, but are difficult to construct both numerically and experimentally. The hydrodynamic echo-process may provide a robust, fast, and simple way to produce hyper uniform structures over a wide range of packing fractions.

3:18PM Q46.00005 The Versatile Elastohydrodynamics of a Free Particle near a Thin Soft Wall, THOMAS SALEZ, PCT Lab, UMR CNRS 7083 Guillier, ESPCI ParisTech, PSL Research University, Paris, France, BAUDOUIN SAINTYVES, L. MAHADEVAN, SEAS, Harvard University, Cambridge, MA, USA — We address the free motion of a buoyant particle inside a viscous fluid, in the vicinity of a thin compressible elastic wall. After discussing the main scalings, we obtain analytically the dominant drag forces within the soft lubrication approximation. By including those into the equations of motion of the particle, we establish a general governing system of three coupled nonlinear and singular differential equations, that describe the three essential motions: sedimentation, hydroplaning, and hydrospinning, through four dimensionless control parameters. Numerical integration allows us to predict a wide zoology of exotic solutions – despite the low-Reynolds feature of the flow – including: spontaneous oscillation, Magnus-like effect, enhanced sedimentation, and boomerang-like effect. We compare these predictions to experiments. The presented elementary approach could be of interest in the description of a broad variety of elastohydrodynamical phenomena, including: landslides, ageing of cartilaginous joints, and motion of a cell in a microfluidic channel or in a blood vessel.

3:30PM Q46.00006 Dual-probe active microrheology, BENJAMIN DOLATA, ROSEANNA N. ZIA, Cornell University — Microrheology has revolutionized the study of microscopically small systems, whereby a Brownian probe particle is monitored as it travels through a complex fluid and its motion is tracked to infer properties of the embedding medium. A range of applications enables study of various materials and flow regimes: in passive microrheology probe diffusion is related to linear viscoelastic properties via a Stokes-Einstein relation, but precludes study of networked materials. Dual-probe passive microrheology overcomes this limitation in some cases. But these techniques are restricted to linear-response properties. In active microrheology a probe is driven through the medium, and reveals strongly non-equilibrium rheology, but is limited to dispersed systems. We have developed a new model for the microscale interogation of general complex fluids: Dual-probe Active Microrheology. Via a combination of asymptotic and numerical solutions to the Smoluchowski equation, we have computed the microstructural and rheological response of a colloidal dispersion to the motion of two probes driven with forces ranging from strong to weak, at arbitrary separations and orientations to their lines of centers. The interactive force between the probes and the colloids reveals a novel non-equilibrium repulsive interaction which we connect to nonlinear rheology.

3:42PM Q46.00007 The impact of hydrodynamics on stress formation, relaxation, and memory in colloidal dispersions: Transient, nonlinear microrheology, RITESH P. MOHANTY, ROSEANNA N. ZIA, Cornell University — In active microrheology, a probe is driven through a complex medium. Most work thus far has focused on steady behavior and established the relationship between the microstructure, probe speed, and rheology. But important information about structural development and relaxation are captured by startup and cessation of flows in the non-linear regime, where the structure is driven far from equilibrium. Here we study theoretically the rate of stress formation and relaxation under non-linear microrheological forcing of hydrodynamically interacting colloids. We study the behavior analytically in the double limits of weak and strong probe forcing and weak and strong hydrodynamic interactions and numerically in between. To elucidate the detailed role of hydrodynamic, Brownian, and interparticle forces in stress formation and relaxation, we employ an excluded annulus model to introduce each systematically, and study the rheological and structural response for arbitrary forcing and strength of hydrodynamic interactions. Hydrodynamics introduce an additional mode of dissipation, which manifests as a reduction in the rate of stress formation during startup. While this non-equilibrium contribution vanishes instantly upon flow shutoff, a delicate interplay between Brownian and interparticle forces influences relaxation, revealing multiple relaxation modes. The recovery of entropically stored energy is studied.
3:54PM Q46.00008 Rheology and Dynamics of Colloidal Superballs. JOHN ROYER, GEORGE BURTON, NIST, DANIEL BLAIRE, Georgetown University, STEVEN HUDSON, NIST — Relatively little is known about the role particle shape plays in the dynamics of colloidal suspensions, particularly at higher packing densities where particle interactions and changes in the microstructure become increasingly important. We examine the role of particle shape by characterizing both the bulk rheology and micro-scale diffusion in a suspension of pseudo-cubic silica superballs. Varying the packing density 0 ≤ φ ≤ 0.42, we compare the high-shear viscosity and long-time self-diffusion coefficient D2(φ) to established hard-sphere results. In dilute suspensions the superball viscosity is nearly indistinguishable from the that of hard spheres, indicating that the individual superball hydrodynamics are not dramatically different. However, there is a significant difference in the diffusion, with the superball D2(φ) decreasing faster with increasing φ. Looking at the suspension microstructure, we find that while the hard sphere pair distribution g(r) jumps to a finite value at contact r = 2a, the superball g(r) is shifted to higher distances. This suggests a simple rescaling φ → φ_{eff} defined by the minimal sphere needed to enclose the superballs, which roughly collapses the diffusion results.

4:06PM Q46.00009 Colloidal transport and diffusion over a tilted periodic energy landscape. XIAOGUANG MA, Hong Kong University of Science and Technology, PIK-YIN LAI, National Central University, Taiwan, BRUCE ACKERSON, Oklahoma State University, PENG TONG, Hong Kong University of Science and Technology — A tilted two-layer colloidal system is constructed to study force-assisted barrier-crossing dynamics over a periodic energy landscape. The energy landscape is provided by the bottom layer colloidal spheres forming a fixed crystalline pattern on a glass substrate. The corrugated surface of the bottom colloidal crystal provides a gravitational potential field for the top layer diffusing particles. By tilting the sample at an angle with respect to the direction of gravity, a tangential component of the gravitational force F is applied to the diffusing particles. The measured mean drift velocity v(F,E) and diffusion coefficient D(F,E) of the particles as a function of F and energy barrier height E agree well with the exact solution of the one-dimensional Langevin equation. From the exact solution we show analytically and verify experimentally that there exists a scaling region, in which v and D both scale as (F)_exp[E^*(F)/k_B T], where the Arrhenius pre-factor a(F) and effective barrier height E^*(F) are both modified by F. The experiment demonstrates the applications of this model system in evaluating different scaling forms of a(F) and E^*(F) and their accuracy, in order to extract useful energetic information.

3Work supported in part by the Research Grants Council of Hong Kong SAR.

4:18PM Q46.00010 Colloidal diffusion over a random landscape. YUN SU, XIAO-GUANG MA, Hong Kong University of Science and Technology, PIK-YIN LAI, National Central University, Taiwan, PENG TONG, Hong Kong University of Science and Technology — A two-dimension quenched random energy landscape is generated by using a randomly packed layer of colloidal spheres of two different sizes fixed on a glass substrate. A number of monodisperse particles diffuse on the top of the first layer particles. The diffusing particles in water feel the gravitational energy landscape U(x,y) generated by the modulated surface of the first layer particles. The trajectories of the particles are obtained by optical microscopy and particle tracking. The energy landscape U(x,y) is obtained from the measured population histogram P(x,y) of the diffusing particles via the Boltzmann distribution, P(x,y) = exp[-U(x,y)/k_B T], where k_B T is the thermal energy of the particles. The distribution of the energy barrier heights is obtained from the measured U(x,y). From the particles’ trajectories we determine the energy landscape parameters over the random landscape, such as the energy landscape over the escape energy. A quantitiative relationship between the long-time diffusion coefficient and the random energy landscape and the coordination number is good agreement with the theoretical prediction. ^Work supported in part by the Research Grants Council of Hong Kong SAR.

4:30PM Q46.00011 Inertial flow regimes of the suspension of finite size particles. IMAN LASHGARI, Linne FLOW Centre, KTH Mechanics, Stockholm, Sweden, FRANCESCO PICANO, Department of Industrial Engineering, University of Padova, Padova, Italy, LUCA BRANDT, Linne FLOW Centre, KTH Mechanics, Stockholm, Sweden — We study inertial flow regimes of the suspensions of finite size neutrally buoyant particles. These suspensions experience three different regimes by varying the Reynolds number, Re, and particle volume fraction, ϵ. At low values of Re and ϵ, flow is laminar-like where viscous stress is the dominating term in the stress budget. At high Re and relatively small ϵ, the flow is turbulent-like where Reynolds stress has the largest contribution to the total stress. At high ϵ, the flow regime is a form of inertial shear-thickening characterized by an significant enhancement in the wall shear stress not due to the increment of Reynolds stress but to the particle stress. We further analyze the local behavior of the suspension in the three different regimes by studying the particle dispersion and collisions. Turbulent cases shows higher level of particle dispersion and higher values of the collision kernel (the radial distribution function times the particle relative velocity as a function of the distance between the particles) than those of the inertial shear-thickening regimes providing additional evidence of two different transport mechanisms in the Bagnoldian regime.

1Support from the European Research Council (ERC) is acknowledged.


4:42PM Q46.00012 Flow mechanism of colloidal solutions under shear revealed by neutron scattering and simulation. XIN LI, WEI-REN CHEN, LUIS SANCHEZ-DIAZ, Oak Ridge National Laboratory, YUN LIU, National Institute of Standards and Technology, LIONEL POURCAR, Institut Laue-Langevin, WILLIAM HAMILTON, CHANGWOO DO, Oak Ridge National Laboratory, TAKUYA IWASHITA, TAKESHI EGAMI, KAO-HSIANG LIU, University of Tennessee — Using small angle neutron scattering technique and Brownian dynamics simulation we investigate the effect of external steady shear on the concentrated solutions of silica particles in the shear thinning regime. Three dimensional anisotropic structure factors are obtained as a function of shear rate. Accordingly the evolution of local topology, defined by the colloidal connectivity, is revealed by the variation of local strain. We further determine the elastic resistant length scale of the colloidal systems via characterizing the quantitative dependence of the correlation length on the strain rate.

1Research presented in this work is supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Energy Division.

1Supported by the Army Research Laboratory under Grant W911NF-12-2-0022

4:54PM Q46.00013 Steady-state flow properties of amorphous materials. VIKRAM JADHAO, THOMAS O’CONNOR, MARK ROBBINS, Johns Hopkins University — Molecular dynamics (MD) simulations are used to investigate the steady-state shear flow curves of a standard glass model: the bidisperse Lennard-Jones system. For a wide range of temperatures in the neighborhood of the glass transition temperature T_g predicted by the mode coupling theory, we compute the steady-state shear stress and viscosity as a function of the shear rate \dot{\gamma}. At temperatures near and above T_g the stress crosses over from linear Newtonian behavior at low rates to power law shear-thinning at high rates. As T decreases below T_g, the stress shows a plateau, becoming nearly rate-independent at low \dot{\gamma}. There is a weak increase in stress that is consistent with Eyring theory for activated flow of a solid. We find that when the strain rate is reduced to extremely low values, Newtonian behavior appears once more. Insights gained from these simulations are applied to the computation of flow curves of a well-established boundary lubricant: squalane. In the elastohydrodynamic regime, squalane responds like a glassy solid with an Eyring-like response, but at lower rates it has a relatively small Newtonian viscosity.
5:06PM Q46.00014 X-ray photon correlation spectroscopy studies of structural irreversibility in a colloidal gel subjected to oscillatory shear flow. MU SUNG KWEON, WESLEY BURGHARDT, Northwestern University, SUBRAMANIAN RAMAKRISHNAN, GOLDA LOUIS, DANICA THOMAS, Florida State University, SURESH NARAYANAN, Argonne National Laboratory — X-ray photon correlation spectroscopy (XPCS) is used to probe the microscopic structural reversibility in a colloidal gel subjected to oscillatory shear flow. Silicon dioxide particles in decalin aggregate into a gel structure as a result of depletion interactions associated with dissolved polystyrene molecules. XPCS studies on aged quiescent gels show negligible structural dynamics on time scales of tens of seconds. Such samples were subjected to oscillatory shear with varying strain amplitude using a rheometer installed in the XPCS beam line and x-ray capable polycarbonate fixtures; this enable simultaneous rheological measurements during the XPCS experiment. In the presence of unidirectional shear flow, the decay of the XPCS autocorrelation function is dominated by the convective motion induced by the applied deformation. In oscillatory shearing of samples in the absence of significant structural relaxation, the autocorrelation function becomes periodic, returning to its initial value once every oscillation period. At higher strains, irreversible motions at the microscopic level lead to decay in the ‘echoes’ of the autocorrelation function. Interestingly, structural irreversibility is detected by XPCS only at strains that are significantly higher than those at which nonlinearity.

Wednesday, March 4, 2015 2:30PM - 5:30PM –
Session Q47 DBIO: Physics of Bacteria and Viruses 217B – Guannan Liu, Princeton University

2:30PM Q47.00001 Using Fitness Landscapes for Rational Hepatitis C Immunogen Design. GREGORY HART, ANDREW FERGUSON, University of Illinois at Urbana-Champaign — Hepatitis C virus afflicts 170 million people worldwide, 2-3% of the global population. Prophylactic vaccination offers the most realistic and cost effective hope of controlling this epidemic, particularly in the developing world where expensive drug therapies are unavailable. Despite 20 years of research, the high mutability of the virus, and lack of knowledge of what constitutes effective immune responses, have impeded development of an effective vaccine. Coupling data mining of sequence databases with the Potts model, we have developed a computational approach to systematically identify viral vulnerabilities and perform rational design of vaccine immunogens. We applied our approach to the nonstructural proteins NS3, NSA, NS, and NSB which are crucial for viral replication. The predictions of our model are in good accord with experimental measurements and clinical observations, and we have used our model to design immunogen candidates to elicit T-cell responses against vulnerable regions of these viral proteins.

2:42PM Q47.00002 Impact of cell regeneration in human respiratory tract on simultaneous viral infections. LUBINA JAHAN RASHID PINKY, HANA DOBOROVLNY, Texas Christian University — Studies have found that ~40% of patients hospitalized with influenza-like illness are infected with at least two different viruses. In these longer infections, we need to consider the role of cell regeneration. Several mathematical models have been used to describe cell regeneration in infection models, though the effect of model choice on the predicted time course of simultaneous viral infections is not clear. We investigate a series of mathematical models of cell regeneration during simultaneous respiratory virus infections to determine the effect of cell regeneration on infection dynamics. We perform a nonlinear stability analysis for each model. The analysis suggests that coexistence of two viral species is not possible for any form of regeneration. We find that chronic illness is possible, but with only one viral species.

2:54PM Q47.00003 Basic Reproduction Number of a Gamma-Distributed Within-Host Infection Model. IRMA RODRIGUEZ, HANA DOBOROVLNY, Texas Christian University — In epidemiology, the basic reproduction number (R0) is used to measure the spread potential of a disease. It is defined as the number of secondary infections produced by a first infection in a homogeneous susceptible population. Traditional ordinary differential equation infection models assume exponential transitions between different stages of cell infection. This assumption is not biologically realistic, so non-exponential models are now being investigated. The basic reproduction number of non-exponential models has yet to be calculated. Here we present an analysis of a gamma-distributed model that has allowed us to calculate R0 for this model.

3:06PM Q47.00004 Observations of Bacterial Behavior during Infection Using the ARGOS Method. A.J. CHAREST, Wentworth Inst of Techn, S. ALGARNI, G.S. IANNACCHIONE, Worcester Polytech Inst — This research employed the Area Recorded Generalized Optical Scattering (ARGOS) approach which allowed for the observation of bacterial changes in terms of individual particles and population dynamics in real time. This new approach allows for an aqueous environment to be manipulated while conducting time-specific measurements over an indefinite time period. This current study provides a more time-specific method in which the bacteria remained within the initial conditions and allows for more time precision than provided by analyzing concentrations of plaque-forming units (PFU). This study involved the bacteria (F-amp) during infection by bacteriophage T4:18. We proposed a model for flagellation of P. aeruginosa.
4:30PM Q47.00006 Seeing is believing: Direct imaging of charge flow along pili proteins reveals new mechanism for antibacterial electron transfer

RIKHIL MALVANKAR, SIBEK EBRU YALCIN, RAMESH ADHIKARI, MARK TUOMINEN, DEREK LOVLEY, University of Massachusetts Amherst — Visualization of charge flow on the nanoscale in proteins is crucial for a fundamental understanding of several life processes. Here, we report direct visualization of charge propagation along native pili of Geobacter sulfurreducens at nanometer resolution using electrostatic force microscopy. Surprisingly, charges injected at a single point into individual, untreated pili, still attached to cells, propagate over the entire filament. The charges propagate despite a lack of cytochromes on the pilus, in contrast to the dominant biochemical model that proteins are electronically insulated and must incorporate redox-active cofactors in order to achieve electron transport functionality. The mobile charge density in pili is comparable to synthetic organic conductors, increasing with proton doping, and with temperature-dependence consistent with previously discovered metallic-like transport mechanism. Conductive pili enable syntrophic bacteria to share energy by directly exchanging electrons among each other. Measurements along individual pili using nanoelectrodes showed ohmic behavior strongly dependent on the amino acid composition of pili. Electron transfer rate measurement revealed that the pilus conductivity is the decisive factor in controlling the bacterial respiration rate.

1 Funded by Office of Naval Research, DOE Genomic Sciences, NSF-NSEC CHM (CMMI-1025020) and Burroughs Wellcome Fund.

3:42PM Q47.00007 Phase separation like dynamics during Myxococcus xanthus fruiting body formation

GUANNAN LIU, SHASHI THUTUPALLI, MANON WIGBERS, JOSHUA SHAEVITZ, Princeton Univ — Collective motion exists in many living organisms as an advantageous strategy to help the entire group with predation, forage, and survival. However, the principles of self-organization underlying such collective motions remain unclear. During various developmental stages of the soil-dwelling bacterium, Myxococcus xanthus, different types of collective motions are observed. In particular, when starved, M. xanthus cells eventually aggregate together to form 3-dimensional structures (fruiting bodies), inside which cells sporulate in response to the stress. We study the fruiting body formation process as an out of equilibrium phase separation process. As local cell density increases, the dynamics of the aggregation M. xanthus cells switch from a spatio-temporally random process, resembling nucleation and growth, to an emergent pattern formation process similar to a spinodal decomposition. By employing high-resolution microscopy and a video analysis system, we are able to track the motion of single cells within motile collective groups, while separately tuning local cell density, cell velocity and reversal frequency, probing the multi-dimensional phase space of M. xanthus development.

3:54PM Q47.00008 Cell size control and homeostasis in bacteria

SERENA BRADDE, GC CUNY, SATTAR TAHERI, JOHN SAULS, UCSD, NOBERT HILL, UC Berkeley, PETRA LEVINE, Washington University, JOHAN PAULSSON, Harvard, MASSIMO VESPOLA, SUCKJOON JUN, UCSD — How cells control their size is a fundamental question in biology. The mechanisms for sensing size, time, or a combination of the two are not supported by experimental evidence. By analysing distributions of size at division and generation time of hundreds of thousands of Gram-negative E. coli and Gram-positive B. subtilis cells under a wide range of tightly controlled steady-state growth conditions, we are now in the position to validate different theoretical models. In this talk I will present all possible models in details and present a general mechanism that quantitatively explains all measurable aspects of growth and cell division at both population and single-cell levels.

4:06PM Q47.00009 Population Dynamics of the Stationary Phase Utilizing the ARGOS Method

S. ALGARNI, Worcester Polytech Inst, A.J. CHAREST, Wentworth Inst Techn, G.S. IANNACCHIONE, Worcester Polytech Inst — The Area Recorded Generalized Optical Scattering (ARGOS) approach to light scattering employs large image capture array allowing for a well-defined geometry in which images may be manipulated to extract structure with intensity at a specific scattering wave vector (I(q)) and dynamics with intensity at a specific scattering wave vector over time (I(q,t)). The ARGOS method provides morphological dynamics noninvasively over a long time period and allows for a variety of aqueous conditions. This is important because traditional growth models do not provide for conditions similar to the natural environment. The present study found that the population dynamics of bacteria do not follow a traditional growth model and that the ARGOS method allowed for the observation of bacterial changes in terms of individual particles and population dynamics in real time. The observations of relative total intensity suggest that there is no stationary phase and that the bacterial population demonstrates sinusoidal type patterns consistently subsequent to the log phase growth. These observation were compared to shape changes by modeling fractal dimension and size changes by modeling effective radius.

4:18PM Q47.00010 Nanomechanical Response of Bacterial Cells to Antimicrobial Peptides

RICHARD PARG, JOHN DUTCHE, University of Guelph — The effectiveness of antimicrobial compounds can be easily screened, however their mechanism of action is much more difficult to determine. Many compounds act by compromising the mechanical integrity of the bacterial cell envelope, and we have developed an atomic force microscopy (AFM)-based creep deformation technique to evaluate changes in the time-dependent mechanical properties of bacterial cells upon exposure to antimicrobial peptides. Measurements performed before and after exposure, as well as time-resolved measurements and those performed at different antimicrobial concentrations, revealed large changes to the viscoelastic parameters including a distinctive signature for the loss of integrity of the bacterial cell envelope. Our previous experiments have focused on Pseudomonas aeruginosa PA01 bacterial cells in Milli-Q water, for which the cells can withstand the large osmotic pressure. In our present study we have focused on performing the measurements in buffer to obtain more biologically relevant results. The AFM creep deformation measurement provides new, unique insight into the kinetics and mechanism of action of antimicrobial peptides on bacteria.


4:30PM Q47.00011 Quantifying Spatiotemporal Patterns in the Expansion of Twitching Bacterial Colonies

ERIN SHELTON, MAXIMILIANO GIULIANI, University of Guelph, LORI BURROWS, McMaster University, JOHN DUTCHE, University of Guelph — Type IV pili (T4P) are very thin (5-8 nm in diameter) protein filaments that can be extended and retracted by certain classes of Gram-negative bacteria including P. aeruginosa [1]. These bacteria use T4P to move across viscous interfaces, referred to as twitching motility. Twitching can occur for isolated cells or in a collective manner [2]. We have developed experimental and data analysis techniques to quantify the expansion of P. aeruginosa PA01 bacterial colonies at the glass-agar interface under well-controlled environmental conditions. By using particle image velocimetry (PIV) and Fourier analysis techniques, we have characterized the evolution of the advancing front of expanding colonies for a range of agar concentrations. This has allowed us to observe a transition in the collective motion of the bacterial cells as the agar concentration is increased. [1] Burrows, L.L. (2012) Annu. Rev. Microbiol. 66: 493-520; [2] Semmler, A.B., Whitchurch, C.B., Mattick, J.S. (1999) Microbiology 145: 2863-2873.
4:42PM Q47.00012 Characterization of MreB polymers in E. coli and their correlations to cell shape. JEFFREY NGUYEN, Princeton University, Dept. of Physics, NIKOLAY OUZONOV, ZEMER GITAI, Princeton University, Dept. of Molecular Biology, JOSHUA SHAEVITZ, Princeton University, Dept. of Physics — Shape influences all facets of how bacteria interact with their environment. The size of E. coli is determined by the peptidoglycan cell wall and internal turgor pressure. The cell wall is patterned by MreB, an actin homolog that forms short polymers on the cytoplasmic membrane. MreB coordinates the breaking of old material and the insertion of new material for growth, but it is currently unknown what mechanism sets the absolute diameter of the cell. With new techniques in fluorescence microscopy and imaging, we are able to quantify cell shape in 3-dimensions and access previously unattainable data on the conformation of MreB polymers. To study how MreB affects the diameter of bacteria, we analyzed the shapes and polymers of cells that have had MreB perturbed by one of two methods. We first treated cells with the MreB polymerization-inhibiting drug A22. Secondly, we created point mutants in MreB that change MreB polymer conformation and the cell shape. By analyzing the correlations between different shape and polymer metrics, we find that under both treatments, the average helical pitch angle of the polymers correlates strongly with the cell diameter. This observation links the micron scale shape of the cell to the nanometer scale MreB cytoskeleton.

4:54PM Q47.00013 Mechanism of cell alignment in groups of Myxococcus xanthus bacteria\(^1\). RAJESH BALGAM, OLEG IGOSHIN, Rice University — Myxococcus xanthus is a model for studying self-organization in bacteria. These flexible cylindrical bacteria move along. In groups, M. xanthus cells align themselves into dynamic cell clusters but the mechanism underlying their formation is unknown. It has been shown that steric interactions can cause alignment in self-propelled hard rods [1] but it is not clear how flexibility and reversals affect the alignment and cluster formation. We have investigated cell alignment process using our biophysical model of M. xanthus cell [2] in an agent-based simulation framework under realistic cell flexibility values. We observed that flexible model cells can form aligned cell clusters when reversals are suppressed but these clusters disappeared when reversals frequency becomes similar to the observed value. However, M. xanthus cells follow slime (polysaccharide gel like material) trails left by other cells and we show that implementing this into our model rescues cell clustering for reversing cells. Our results show that slime following along with periodic cell reversals act as positive feedback to reinforce existing slime trails and recruit more cells. Furthermore, we have observed that mechanical cell alignment combined with slime following is sufficient to explain the distinct clustering patterns of reversing and non-reversing cells as observed in recent experiments [3].

References

5:06PM Q47.00014 Magnetically-Actuated Escherichia coli System for Micro Lithography. S. LAUBACK, E. BROWN, L. PÉREZ-GUZMAN, C. PEACE, C. PIERCE, B.H. LOWER, S.K. LOWER, R. SOORYAKUMAR, Ohio State Univ - Columbus — Technologies that control matter at the nano- and micro-scale are crucial for developing new engineered materials and devices. While the more traditional approaches for such manipulations often depend on lithographic fabrication, they can be expanded upon by taking advantage of the biological systems within a living cell which also operate on the nano- and micro-scale. In this study, a system is being developed to functionalize a targeted location on the surface of a chip with the protein AmCyan from transformed Escherichia coli cells. Using established methods in molecular biology where a plasmid with the amcyan gene sequence is inserted into the cell, E. coli are engineered to express the AmCyan protein on their outer surface. In order to transport the cells to the targeted location, the transformed E. coli are labeled with superparamagnetic micro-beads which exert directed forces on the cells in an external field. Preliminary results of the protein expression on E. coli, the transport of the cells through weak magnetic fields to targeted locations and the potential to transfer protein from the cell to the chip surface will be presented.

5:18PM Q47.00015 Bactericidal Effects of Charged Silver Nanoparticles in Methicillin-resistant Staphylococcus aureus\(^1\). DULCE ROMERO-URBINA, J. JESUS VELAZQUEZ-SALAZAR, HUMBERTO H. LARA, JOSEFINA ARELLANO-JIMENEZ, EDUARDO LARIOS, The University of Texas at San Antonio, TONY T. YUAN, YOON HWANG, MAURIS N. DESILVA, Naval Medical Research Unit, JBSA Fort Sam Houston, MIGUEL JOSE-YACAMAN, The University of Texas at San Antonio — The increased number of infections due to antibiotic-resistant bacteria is a major concern to society. The objective of this work is to determine the effect of positively charged AgNPs on methicillin-sensitive Staphylococcus aureus (MSSA) and methicillin-resistant Staphylococcus aureus (MRSA) cell wall using advanced electron microscopy techniques. Positively charged AgNPs suspensions were synthesized via a microwave heating technique. The suspensions were then characterized by Dynamic Light Scattering (DLS) and Transmission Electron Microscopy (TEM) showing AgNPs size range from 5 to 30 nm. MSSA and MRSA were treated with positively charged AgNPs concentrations ranging from 0.06 mM to 31 mM. The MIC\(_{50}\) studies showed that viability of MSSA and MRSA could be reduced by 50% at a positively charged AgNPs concentration of 0.12 mM supported by Scanning-TEM (STEM) images demonstrating bacteria cell wall disruption leading to lysis after treatment with AgNPs. The results provide insights into one mechanism in which positively charged AgNPs are able to reduce the viability of MSSA and MRSA.

This work is supported by NSF MCB 0845919 and 111780.

Wednesday, March 4, 2015 2:30PM - 5:30PM – Session Q48 DBIO: Focus Session: Physics of Proteins: Dynamics and Function III 217C - Dimitri Antoniou, University of Arizona

2:30PM Q48.00001 Investigation at the atomic level of homologous enzymes reveals distinct reaction paths.\(^1\) IOANNA ZOI, STEVEN D. SCHWARTZ, Univ of Arizona — Bacterial enzymes Escherichia coli and Vibrio cholerae 5’-Methylthioadenosine nucleosidases (MTANs) have different binding affinities for the same transition state analogue. This was surprising as these enzymes share 60% sequence identity, have almost identical active sites and act under the same mechanism. We performed Transition Path Sampling simulations of both enzymes to reveal the atomic details of the catalytic chemical step, to explain the inhibitor affinity differences. Unlike EcMTAN, VcMTAN has multiple distinct transition states, which is an indication that multiple sets of coordinated protein motions can reach a transition state. We also identified the important residues that participate in each enzyme’s reaction coordinate and explained their contribution. Subtle dynamic differences manifest in difference of reaction coordinate and transition state structure and also suggest that MTANs differ from most ribosyl transferases. As experimental approaches report averages regarding reaction coordinate information, this study offers, previously unavailable, detailed knowledge to the explanation of bacterial MTANs catalytic mechanism, and could have a significant impact on pharmaceutical design.

1We acknowledge the support of the National Institutes of Health through Grant GM068036.
2:42PM Q48.00002 Mechanistic model of sodium+/proton antiport based on X-ray crystal structures and molecular dynamics simulations, OLIVER BECKSTEIN, DAVID L DOTSON, Arizona State Univ, CHIARA LEE, SHOKO YASHIRO, Imperial College, London, POVIAS UZDAVYNYS, CHRISTOPH VON BALLMOOS, DAVID DREW, Stockholm University, Sweden, ALEXANDER D. CAMERON, University of Warwick — Na⁺/H⁺ antiporters are membrane proteins that are vital for cell homeostasis but the mechanistic details of their transport mechanism remain unclear, in particular, how Na⁺ and protons bind to the transporter. We recently solved X-ray crystal structures for two such antiporters (NhaA and NapA) in two different conformations of the transport cycle. All-atom molecular dynamics (MD) simulations (for a total simulated time > 10 µs) indicate that sodium binding is dependent on the charge states of two conserved aspartate residues. A conserved lysine forms a previously unidentified salt bridge with one of the aspartates. Under simulated physiological pH the presence of a Na⁺ ion disrupts and breaks the salt bridge in NhaA. To quantify proton binding, we then performed heuristic pKa calculations on our ensemble of simulations. The calculations support our novel hypothesis that the conserved lysine in these antiporter MD simulations protonates in a sodium-dependent manner and thus acts as part of the transport machinery. In conjunction with simulations of the conformational transition we propose a new mechanistic model of ion binding for the CPA2 class of antiporters within the larger framework of the alternating access mechanism of transmembrane transport.

2:54PM Q48.00003 Another Look at the Mechanisms of Hydride Transfer Enzymes from Quantum and Classical Transition Path Sampling¹, MICHAEL DZIERLENGA, DIMITRI ANTONIOU, STEVEN SCHWARTZ, Univ of Arizona — The mechanisms involved in enzymatic hydride transfer have been studied for years but questions remain about the participation of protein dynamics and quantum effects, especially hydrogen tunneling. In this study, we use transition path sampling (TPS) with normal mode centroid molecular dynamics (CMD) to calculate the barrier to hydride transfer in yeast alcohol dehydrogenase (YADH) and lactate dehydrogenase (LDH). Calculation of the work applied to the hydride during the reaction allows for observation of the change in barrier height due to inclusion of quantum effects. Additionally, the same calculations were performed using deuterium as the transferring particle to validate our methods with experimentally measured kinetic isotope effects. The change in barrier height in YADH upon inclusion of quantum effects is indicative of a zero-point energy contribution, and is evidence that the protein mediates a near-barrierless transfer of the rate-limiting hydride. Calculation of kinetic isotope effects using the average difference in barrier between hydride and deuteride agreed well with experimental results.

¹The authors acknowledge the support of the National Institutes of Health Grants GM068036 and GM102226.

3:06PM Q48.00004 Free energy landscape of the Michaelis complex of lactate dehydrogenase: A network analysis of atomistic simulations, XIAOLIANG PAN, STEVEN SCHWARTZ, University of Arizona — It has long been recognized that the structure of a protein is a hierarchy of conformations interconverting on multiple time scales. However, the conformational heterogeneity is rarely considered in the context of enzymatic catalysis in which the reactant is usually represented by a single conformation of the enzyme substrate complex. Lactate dehydrogenase (LDH) catalyzes the interconversion of pyruvate and lactate with concomitant interconversion of two forms of the cofactor nicotinamide adenine dinucleotide (NADH and NAD⁺). Recent experimental results suggest that multiple states exist within the Michaelis complex of LDH, and they are catalytically competent at different reaction rates. In this study, millisecond-scale all-atom molecular dynamics simulations were performed on LDH to explore the free energy landscape of the Michaelis complex, and network analysis was used to characterize the distribution of the conformations. Our results provide a detailed view of the kinetic network the Michaelis complex and the structures of the substrates at atomic scale. It also shed some light on understanding the complete picture of the catalytic mechanism of LDH.

3:18PM Q48.00005 Theory of relaxation dynamics within carotenoids via high frequency stretching modes, VYTAUTAS BALEVICIUS, DARIUS ABRAMAVICIUS, Vilnius University — Carotenoids are ubiquitous natural pigment molecules acting as light harvesters in the blue-green region of the spectrum, and at the same time ensuring the photoprotection against excessive light by quenching the triplet state of chlorophylls and singlet oxygen. However, their photophysics is still not fully understood, because the absorption takes place not into the optically dark lowest excited state S₁, but to the short-lived higher-lying state S₂. This leads to complicated intramolecular energy redistribution schemes within carotenoids. From the transient absorption experiments it is known that the S₁ state is populated shortly after the excitation of the S₂ state (on the time-scale of tens of femtoseconds). The corresponding excited state absorption signal is blue-shifting and narrowing at early times, which is attributed to the vibrational cooling of the S₁ state. We apply the secular density matrix theory to take into account both the internal conversion from the S₂ into the S₁ state and the subsequent relaxation within the manifold of high-frequency vibrational states corresponding to the carbon-carbon stretching modes (C-C and C=C). It allows us to obtain relevant pump-probe spectra in the time range from femto- to picoseconds.

3:30PM Q48.00006 Connecting thermal and mechanical protein (un)folding landscapes, LI SUN, JEFFREY NOEL, Rice University, JOANNA SULKOWSKA, University of Warsaw, HERBERT LEVINE, JOSE ONUCHIC, Rice University — Molecular dynamics simulations supplement single-molecule pulling experiments by providing the possibility of examining the full free energy landscape using many coordinates. Here, we use an all-atom structure-based model to study the force and temperature dependence of the unfolding of the protein filamin by applying force at both termini. The unfolding force-time relation τ(F) indicates that the unfolding behavior can be characterized into three regimes: barrier-limited low- and intermediate-force regimes, and a barrierless high-force regime. Slope changes of τ(F) separate the three regimes. We show that the behavior of τ(F) can be understood from a two-dimensional free energy landscape projected onto the extension X and the fraction of native contacts Q. In the low-force regime, the unfolding rate is roughly force-independent due to the small (even negative) separation in X between the native ensemble and transition state ensemble (TSE). In the intermediate-force regime, force sufficiently separates the TSE from the native ensemble such that τ(F) roughly follows an exponential relation. The TSE becomes increasingly structured with force. The high-force regime is characterized by barrierless unfolding, approaching a time limit of around 10 µs.

3:42PM Q48.00007 ABSTRACT WITHDRAWN —

3:54PM Q48.00008 Rhodopsin Photoactivation Dynamics Revealed by Quasi-Elastic Neutron Scattering, DEBSINDHU BHOWMIK, UTSAB SHRESTHA, Wayne State University, MI, SUCHHITHRANGA M. C. D. PERERA, UDEEP CHAWLA, University of Arizona, AZ, EUGENE MAMONTOV, Oak Ridge National Laboratory, TN, MICHAEL BROWN, University of Arizona, AZ, XIANG-QIANG CHU, Wayne State University, MI — Rhodopsin is a G-protein-coupled receptor (GPCR) responsible for vision. During photoactivation, the chromophore retinal dissociates from protein yielding the opsin apoprotein. What are the changes in protein dynamics that occur during the photoactivation process? Here, we studied the microscopic dynamics of state-1 rhodopsin and the ligand-free opsin using quasielastic neutron scattering (QENS). The QENS technique tracks individual hydrogen atom motion because of the much higher neutron scattering cross-section of hydrogen than other atoms. We used protein with CHAPS detergent hydrated with heavy water. The activation of proteins is confirmed at low temperature up to 300 K by mean-square displacement (MSD) analysis. The QENS experiments at temperatures ranging from 220 K to 300 K clearly indicate an increase in protein dynamic behavior with temperature. The relaxation time for the ligand-bound protein rhodopsin is faster compared to opsin, which can be correlated with the photoactivation. Moreover, the protein dynamics are orders of magnitude slower than the accompanying CHAPS detergent, which unlike protein, manifests localized motions.
4:06PM Q48.00009 Predicting side-chain conformational changes of methionine using a hard-sphere model with stereochemical constraints, A. VIRRUETA, J. GAINES, C. S. O’HERN, L. REGAN, Yale University — Current research in the O’Hern and Regan laboratories focuses on the development of hard-sphere models with stereochemical constraints for protein structure prediction as an alternative to molecular dynamics methods that utilize knowledge-based corrections in their force-fields. Beginning with simple hydrophobic dipeptides like valine, leucine, and isoleucine, we have shown that our model is able to reproduce the side-chain dihedral angle distributions derived from sets of high-resolution protein crystal structures. However, methionine remains an exception - our model yields a chi-3 side-chain dihedral angle distribution that is relatively uniform from 60 to 300 degrees, while the observed distribution displays peaks at 60, 180, and 300 degrees. Our ability to resolve this discrepancy by considering clashes with neighboring residues, and averaging the reduced distribution of allowable methionine structures taken from a set of crystallized proteins. We will also re-evaluate the electron density maps from which these protein structures are derived to ensure that the methionines and their local environments are correctly modeled. This work will ultimately serve as a tool for computing side-chain entropy and protein stability.

1 A. V. is supported by an NSF Graduate Research Fellowship and a Ford Foundation Fellowship. J. G. is supported by NIH training grant NIH-5T15LM07056-28.

4:18PM Q48.00010 How can we understand an entire (super)family of proteins?, WOUTER HOFF, Oklahoma State University — Understanding how the functional properties of a protein are encoded in its amino acid sequence remains a formidable challenge. We use photoactive yellow protein (PYP) to determine how structure-function relationships can be obtained for an entire (super)family of proteins. PYP is a model system to study fundamental processes in proteins and a prototype for the PAS domain superfamily. It consists of a 100-residue PAS domain with an additional 25-residue N-terminal extension. PYP exhibits a photocycle that is initiated by pCA photosomerization, followed by proton transfer from Glu46 to the pCA and a subsequent protein quacke during formation of the pB intermediate. These structural changes are driven by the electrostatic epicenter formed by the buried ionized Glu46 side chain and involve partial protein unfolding, including the release of the N-terminal region. Deletion of the N-terminal region slows down pB decay 1,000-fold. We report results on family-wide structure-function relationships in PYP. (i) Transplanting mutations into the N-terminus of a highly studied PYP to a different PYP homolog are only partially successful, implying sequence context dependence of functional properties. (ii) We find a direct correlation between the strength of the hydrogen bonding between the pCA and Glu46 and functional properties of PYPs. The role of Glu46 as the epicenter for driving large conformational changes during pB formation is conserved. (iii) Across the PYP family the N-terminal region is negatively charged while the PAS core is positively charged. The resulting charge-charge interactions are critical for the function of the N-terminal region. (iv) We find that residues conserved in the PAS domain superfamily exert their effects through conserved patterns of side chain interactions.

4:54PM Q48.00011 A coarse-grained model to study calcium activation of the cardiac thin filament, JING ZHANG, STEVEN SCHWARTZ, University of Arizona — Familial hypertrophic cardiomyopathy (FHC) is one of the most common heart disease caused by genetic mutations. Cardiac muscle contraction and relaxation involve regulation of crossbridge binding to the cardiac thin filament, which regulates actomyosin interactions through calcium-dependent interactions in the dynamics of cardiac troponin (cTn) and tropomyosin (Tm). An atomistic model of cTn complex interacting with Tm has been studied by our group. A more realistic model requires the inclusion of the dynamics of actin filament, which is almost 6 times larger than Tm and cTn in terms of atom numbers, and extensive sampling of the model becomes very resource-demanding. By using physics-based protein united-residue force field, we introduce a coarse-grained model to study the calcium activation of the thin filament resulting from cTn’s allosteric regulation of Tm dynamics on actin. The time scale is much longer than that of all-atom molecular dynamics simulation because of the reduction of the degrees of freedom. The coarse-grained model is a good template for studying cardiac thin filament mutations that cause FHC, and reduces the cost of computational resources.

5:06PM Q48.00012 Photoduced conformational changes to porphyrin-bound albumin reduces albumin binding to Osteonectin, SARAH ROZINEK, UTSA and Air Force Research Lab., ROBERT THOMAS, Air Force Research Lab., LORENZO BRANCLEON, UTSA — Much work has shown light-induced structural changes to proteins are possible. For instance, we have previously shown that small secondary and tertiary structural changes occur to albumin when it is bound (non-covalently) to meso-tetrakis(4-sulfonatophenyl)porphyrin (TSPP) and irradiated with a low intensity laser. Further study of this light-induced protein modification could advance the understanding of albumin’s structure/function relationship. Then, this structural modification technique might be implemented to deactivate unwanted protein functions or even to bestow non-native protein properties. A necessary step toward this goal is to determine if and how protein function is affected once its structure is modified. The current study aims to explore the light-induced conformational change to TSPP-bound albumin by testing its ability to bind the biologically relevant albumin receptor, Osteonectin. In this Affinity-Depletion experiment, Osteonectin has been covalently attached to magnetic beads, forming an affinity column. TSPP-albumin will non-covalently bind the column, and we predict that the light-induced change to albumin will cause a reduction in binding to Osteonectin. This loss of binding ability would mean a deactivation of albumin’s natural cellular functions.

5:18PM Q48.00013 Probing second hydration shell of ionic solutions using Gigahertz to Terahertz spectroscopy, DEEPU GEORGE, CHOLA REGMI, SHENGFENG CHENG, NGUYEN VINH, Virginia Tech — Understanding how the functional properties of a protein are encoded in its amino acid sequence remains a formidable challenge. We use photoactive yellow protein (PYP) to determine how structure-function relationships can be obtained for an entire (super)family of proteins. PYP is a model system to study fundamental processes in proteins and a prototype for the PAS domain superfamily. It consists of a 100-residue PAS domain with an additional 25-residue N-terminal extension. PYP exhibits a photocycle that is initiated by pCA photosomerization, followed by proton transfer from Glu46 to the pCA and a subsequent protein quacke during formation of the pB intermediate. These structural changes are driven by the electrostatic epicenter formed by the buried ionized Glu46 side chain and involve partial protein unfolding, including the release of the N-terminal region. Deletion of the N-terminal region slows down pB decay 1,000-fold. We report results on family-wide structure-function relationships in PYP. (i) Transplanting mutations into the N-terminus of a highly studied PYP to a different PYP homolog are only partially successful, implying sequence context dependence of functional properties. (ii) We find a direct correlation between the strength of the hydrogen bonding between the pCA and Glu46 and functional properties of PYPs. The role of Glu46 as the epicenter for driving large conformational changes during pB formation is conserved. (iii) Across the PYP family the N-terminal region is negatively charged while the PAS core is positively charged. The resulting charge-charge interactions are critical for the function of the N-terminal region. (iv) We find that residues conserved in the PAS domain superfamily exert their effects through conserved patterns of side chain interactions.

5:20PM Q49.00001 Suppression of E. coli tumbling and wobbling in dilute polymeric fluids, ALISON PATTESON, University of Pennsylvania, ARVIND GOPINATH, Haverford College, PAULO ARRATIA, University of Pennsylvania — Bacteria commonly utilize a run-and-tumble swimming behavior to navigate through complex environments, such as mucus in the lungs or digestive system. This swimming behavior has been extensively studied in water-like fluids; yet, studies on the role of particles/polymers on the run-and-tumble technique are limited. Here, we experimentally investigate the role of polymer concentration on the swimming dynamics of E. coli. We find that small amounts of polymer drastically change the run-and-tumble behavior of E. coli cells, significantly enhancing the translational diffusion. The average cell velocity increases with polymer concentration (and viscosity) and the mean run times are enhanced. By varying polymer molecular weight, we show that enhanced translation is a result of two mechanisms: (1) suppression of cell wobbling due to elasticity and (2) enhancement of run times due to viscosity. Our results show that the transport of chemotactic cells can be independently modified by viscosity and elasticity.
2:42PM Q49.00002 Differential dynamic behaviors of undulatory nematodes in liquid vs. soft gel environment1, JIN-SUNG PARK, JENNIFER H. SHIN, Dept. of Mechanical Engineering, KAIST — Caenorhabditis elegans (C. elegans) is an undulatory nematode which exhibits two distinct locomotion types of swimming and crawling. Although in its natural habitat C. elegans lives in complex fluidic environment, our current understanding has been limited to the behavior of C. elegans in a simple Newtonian fluid. Here, we present some experimental results on the penetrating behavior of C. elegans at the interface from liquid to solid environment. Once C. elegans, which otherwise swims freely in a liquid, makes a contact to the solid gel boundary, it begins to penetrate vertically to the surface by changing its stroke motion characterized by a stiffer body shape and a slower stroke frequency. The particle image velocimetry (PIV) analysis reveals the flow streamlines produced by the stroke of worm. For the worm that crawls on a solid surface, we utilize a technique of traction force microscopy (TFM) to find that the crawling nematode forms localized force islands along the body where makes direct contacts to the gel surface.

1This work was supported by the National Research Foundation (NRF) grant 2013R1A1A2012420 and 2010-0016886.

2:54PM Q49.00003 Directed Paramagnetic Colloidal Swimmers, SIBANI LISA BISWAL, DI DU, Rice University, DEPT. CHEMICAL AND BIOMOLECULAR ENGINEERING TEAM — A novel micoscale swimmer can be generated by placing two paramagnetic colloids of different sizes in a rotating magnetic field. For propulsion at the microscale, viscous forces dominate over inertial forces. This results in the scallop theorem, where reversible displacements does not lead to any net motion. To achieve controlled swimming at the microscale, the swimmer must be able to make a sequence of deformations that are cyclic but not time reversible. Two paramagnetic bodies in a circular eccentric rotating magnetic field influence each other and propel together in a directed manne. The motion of each body tracks a half-moon course, shown in the figure below. We will describe this method and show how Brownian motion enhances this propulsion.

3:06PM Q49.00004 Mechanics of swimming at the small scale in complex fluids, THOMAS POWERS, Brown University — Recent experiments with bacteria in liquid crystalline solutions have revealed that nematic order affects the swimming behavior of bacteria. Motivated by these observations, we study a simple model of low-Reynolds-number swimming in an anisotropic fluid, that of an infinitely long two-dimensional sheet deforming via propagating transverse or longitudinal waves and immersed in a hexatic or a nematic liquid crystal. The liquid crystal is categorized by the dimensionless Ericksen number Er, which compares viscous and elastic effects. Paying special attention to the anchoring strength at the interface of the liquid crystal and the swimmer, we calculate how swimming speed depends on Er for small amplitude waves. We study both the sinusoidal steady-state problem as well as the startup problem in which the swimmer starts from rest.

3:42PM Q49.00005 Anomalous swimming behavior of bacteria in nematic liquid crystals1, ANDREY SOKOLOV, Materials Science Division, Argonne National Laboratory, Illinois 60439, USA, SHUANG ZHOU, OLEG LAVRENTOVICH, Liquid Crystal Institute, Kent State University, Kent, Ohio 44242, USA, IGOR ARANSON, Materials Science Division, Argonne National Laboratory, Illinois 60439, USA — Flagellated bacteria stop swimming in isotropic media of viscosity higher than 0.066kgm m−1s−1. However, Bacillus Subtilis slows down by only about 30% in a nematic chonicom liquid crystal (CLC, 14wt% DSCG in water), where the anisotropic viscosity can be as high as 6kgm m−1s−1. The bacteria velocity (Vb) is linear with the flagella rotation frequency. The phase velocity of the flagella Vf ≈ 2Vb in CLC, as compared to Vf ≈ 1Vb in water. The flow generated by the bacteria is localized along the bacterial body axis, decaying slowly over tens of micrometers along, but rapidly over a few micrometers across this axis. The concentrated flow grants the bacteria new ability to carry cargo particles in CLC, ability not seen in their habitat isotropic media. We attribute these anomalous features to the anisotropy of viscosity of the CLC, namely, the viscosities of splay and twist is hundreds times higher than that of bend deformation, which provides extra boost of swimming efficiency and enables the bacteria swim at considerable speed in a viscous medium. Our findings can potentially lead to applications such as particle transportation in microfluidic devices.

1A.S and I.A are supported by the US DOE, Office of Science, BES, Materials Science and Engineering Division. S.Z. and O.D.L are supported by NSF DMR 1104850, DMS-1434185.

3:54PM Q49.00006 Propulsion and instability of flexible helical flagella, NOOR KHOURI, MOHAMMAD JAWED, Massachusetts Institute of Technology, FANG DA, EITAN GRINSPUN, Columbia University, PEDRO REIS, Massachusetts Institute of Technology — We consider a macroscopic analogue model for the locomotion of uni-flagellar bacteria in a viscous fluid. The rescaling from the original micron-scale onto the desktop-scale is made possible by the prominence of geometry in the deformation process. As a model for the flagellum, we fabricate elastomeric filaments with fully customizable geometric and material properties, and rotate them at low Reynolds number conditions in a glycerin bath. Using digital imaging, we analyze the dynamics of the geometrically nonlinear deformed configurations. Our precision experiments are compared against numerical simulations that employ the Discrete Elastic Rods (DER) method, with an emphasis on quantifying the generated propulsive force. A novel mechanical instability is uncovered, whereby the filament buckles above a critical rotation frequency and we quantify its dependence on the physical and control parameters of the system. A scaling analysis allows us to rationalize the underlying physical mechanism and informs the original biological system that motivated the study.

4:06PM Q49.00007 Does Helicobacter pylori exhibit corkscrew motion while swimming?, MAIRA CONSTANTINO, JOSEPH HARDCASTLE, RAMA Bansil, Boston University — Helicobacter pylori is a spiral shaped bacterium associated with ulcers, gastric cancer, gastritis among other diseases. In order to colonize the harsh acidic environment of the stomach H. pylori has to go across the viscoelastic mucus layer of the stomach. Many studies have been conducted on the swimming of H. pylori in viscous media however none have taken into account the influence of cell-body shape on the trajectory. We present an experimental study of the effects of body shape in the swimming trajectory of H. pylori in viscous media by a quantitative analysis of the bacterium rotation and translation in gels using phase contrast microscopy and particle tracking techniques. Preliminary microscopic tracking measurements show very well defined helical trajectories in the spiral-shaped wild type H. pylori. These helical trajectories are not seen in rod-shaped mutants which sometimes display whirling motions about one end acting as a hinge. We will present an analysis of the different trajectories for bacteria swimming in media with different viscoelastic parameters.

4:18PM Q49.00008 How does Vorticella utilize its stalk contraction-relaxation cycle?, JIAZHONG ZHOU, DAVID ADMIRAAL, SANGJIN RYU, University of Nebraska-Lincoln — Vorticella is a sessile ciliate living in water, and it coils its slender stalk to pull the cell body (zooid) towards the substrate at a maximum speed of ~ 1 cm/s. After stalk contraction is completed, the stalk slowly relaxes to its extended state. Although this ultrafast stalk contraction has been studied in terms of cell motility, it poorly understood how Vorticella utilizes its stalk contraction. Here we propose a hypothesis that Vorticella can augment transport of particles near the substrate relying on water flow induced by the stalk contraction-relaxation cycle. We investigated our hypothesis using a computational fluid dynamics (CFD) model which models Vorticella as a solid sphere moving normal to a solid surface in water. Having simulated water flow caused by Vorticella, we calculated motions of particles near Vorticella, and then quantified the transport effect of Vorticella’s stalk contraction using microfluidic mixing indices.

1Supported by Laymann Seed grant from UNL.
4:30PM Q49.00009 A steering mechanism for phototaxis in Chlamydomonas, RACHEL BENNETT, RAMIN GOLESTANIAN, University of Oxford — Chlamydomonas shows both positive and negative phototaxis. It has a single eyespot near its equator and as the cell rotates during forward motion the light signal received by the eyespot varies. We use a simple mechanical model of Chlamydomonas that couples the flagellar beat pattern to the light intensity at the eyespot to demonstrate a mechanism for phototactic steering that is consistent with observations. The direction of phototaxis is controlled by a parameter in our model and the steering mechanism is robust to noise. In the dark, our model shows emergent run-and-tumble behavior and we see switching between directed phototaxis and run-and-tumble when we switch the light on and off.

4:42PM Q49.00010 Sorting choanoflagellates, VERONICA I. MARCONI, IFEG-CONICET and FaMAF, Universidad Nacional de Cordoba, Cordoba, Argentina, GASTON L. MINO, Department of Civil and Environmental Engineering, Ralph M. Parsons Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, JAVIER SPARACINO, IFEG-CONICET and FaMAF, Universidad Nacional de Cordoba, Cordoba, Argentina, ADOLFO J. BANCHIO, CARLOS A. CONDAT, IFEG-CONICET and FaMAF, Universidad Nacional de Cordoba, Cordoba, Argentina, MIMI A.R. KOEHL, Integrative Biology, University of California, Berkeley, California 94720, USA, NICOLE KING, Department of Molecular and Cell Biology, University of California, Berkeley, California 94720, ROMAN STOCKER, Department of Civil and Environmental Engineering, Ralph M. Parsons Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139 — In freshwater environments, as well as in oceans, environmental conditions are in constant fluctuation. Some heterotrophic plankton must adapt their swimming behavior in order to survive under these conditions. In the case of the choanoflagellate, the closest animal ancestor, the ability to forage for food is given not only by its single flagellum, but also by its differentiation between fast and slow swimmers. The understanding of how these cells with different strategies to swim search for food can give us a better insight into how eukaryotes respond to different stimuli. In this work, we have designed a microfluidic device that sorts choanoflagellates by their speed. The optimal geometry was found by a numerical model using the experimentally determined motilities of each swimmer type.

5:06PM Q49.00012 Swimming of Vorticella in two-dimensional confinement, Luz Sotoelo, Young-Gil Park, University of Texas-Pan American, SungHwan Jung, Virginia Polytechnic Institute and State University, Sangjin Ryu, University of Nebraska-Lincoln — Vorticella is a ciliate observed in the stalked sessile form (trophont), which consists of an inverted bell-shaped cell body (zoid) and a slender stalk attaching the zoid to a substrate. Having circular cilia bands around the oral part, the stalkless zoid of Vorticella can serve as a model system for microorganism swimming. Here we present how the stalkless trophont zoid of Vorticella swims in two-dimensional confined geometries which are similar to the Hele-Shaw cell. Having harvested stalkless Vorticella zooids, we observed their swimming in water between two glass surfaces using video microscopy. Based on measured swimming trajectories and distributions of zooid orientation and swimming velocity, we analyzed how Vorticella’s swimming mobility was influenced by the geometry constraints.

Wednesday, March 4, 2015 2:30PM - 5:18PM

Session Q50 GSOFT: Focus Session: Reconfiguring and Actuating Soft Matter II: Tunable Interactions 218 - Zorana Zeravcic, Rockefeller University

2:30PM Q50.00001 Magnetic field detector consisting of magnetic and semiconducting nanoparticles co-assembled in a liquid crystalline matrix, JOSÉ AMARAL, ANDREA RODARTE, JACKY WAN, CHRISTOPHER FERRI, MAKIKO QUINT, RON PANDOLFI, MICHAEL SCHEIBNER, LINDA HIRST, SAYANTANI GHOSH, University of California, Merced — An exciting area of research is using nano-constituents to create artificial materials that are multifunctional and allow for modification post-fabrication and in situ. In this work, we present the ensemble behavior of iron-oxide magnetic nanoparticles (MNP) and CdSe/ZnS quantum dots (QDs) that dispersed in an electro-optically active liquid crystalline (LC) matrix. The directed assembly of MNP's in the matrix is driven by the temperature-induced transition of the LC from the isotropic to the nematic phase as the MNP are mostly expelled into the isotropic regions, finally ending up clustered around LC defect points when the transition is complete. Our results show a two-fold intensity increase of QD photoluminescence intensity with low magnetic fields (less than 100 mT). We speculate this increase is due to MNP rearrangement which produces a compaction of the clusters, resulting in the detection of increased QD emission. The individual components work together to act as a magnetic field detector and since they are direct assembled in a LC medium, they could potentially be used in a wide range of fluid-based applications. This work was funded by NSF grants DMR-1056860 and ECC-1227034.

3This work was funded by NSF grants DMR-1056860 and ECC-1227034.

2:42PM Q50.00002 Computational and experimental study of magnetic colloidal assembly and martensitic transition, LIN FU, YE YANG, CATHERINE MARCOUX, JOSHUA SOCOLAR, PATRICK CHARBONNEAU, BENJAMIN YELLEN, Duke Univ — Colloidal self-assembly in external fields offers new ways to build up complex structures. Here, we study the self-assembly of a quasi-2D mixture of magnetic and non-magnetic particles immersed in a ferrofluid and under an external magnetic field. We calculate the external field strength-density-tilt angle phase diagram for the system by specialized Monte Carlo methods and compare the results with experiments. By tilting the external field away from the vertical, the system first undergoes magnetostriction, and then a martensitic phase transition between a checkerboard and a striped crystal. We find that the out-of-equilibrium transformation pathway depends strongly on the initial crystal orientation, external field strength and degree of confinement in the third dimension. Our findings suggest the possibility for improving the design of functional materials by selecting the specific type of transformation pathway to optimize either the shape change or the heat exchange properties.
phenomena are needed to describe the observed dynamics. We are especially interested in the crossover region where both phenomena can be used as a switching mechanism in "smart" fluids, i.e. fluids where properties can be tuned rapidly and reversibly by changing external parameters. We use numerical simulations to investigate the rheological properties of MR fluids close to the jamming transition as a function of the applied field and volume fraction. We use anisotropic polarizable colloidal particles and stimulate their reversible aggregation by applying a static external electric field. Through molecular dynamics simulations with a self-consistent calculation of the induced dipole moments, we demonstrate that such particles form monolayers capable of eliminating defects and dislocations, and even self-healing. Potential applications, such as tube formation, are also discussed.

3:06PM Q50.00004 Field-induced growth of self-annealing suspended colloidal monolayers. MING HAN, Northwestern University, LUIJTEN RESEARCH GROUP TEAM — Due to their reduced dimensionality, flexible sheet-like materials have numerous applications, e.g. offering the potential to serve as functional coatings or as a system for encapsulation, akin to biologic membranes. Here we report the ability to generate large ordered, flexible, and suspended monolayers via field-induced self-assembly. We use numerical simulations to investigate the rheological properties of MR thinning viscosities. They are also tunable, which means that both phenomena can be used as a switching mechanism in "smart" fluids, i.e. fluids where properties can be tuned rapidly and reversibly by changing external parameters. We use numerical simulations to investigate the rheological properties of MR fluids close to the jamming transition as a function of the applied field and volume fraction. We are especially interested in the crossover region where both phenomena are needed to describe the observed dynamics.

3:18PM Q50.00005 Directing colloidal assembly and a metal-insulator transition using quenched-disordered polymeric networks. ANH PHAN, University of Illinois at Urbana-Champaign, RYAN JADRICH, The University of Texas at Austin, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — Replica integral equation and effective medium theory methods are employed to elucidate how to massively reconfigure a colloidal assembly and realize equilibrium states of high electrical conductivity at low physical volume fractions [1]. This is achieved by employing variable mesh size networks of rigid rod or semiflexible polymers as a templating internal field. By exploiting bulk phase separation frustration and the tunable competing processes of colloid adhesion on the low dimensional network and fluctuation-driven colloid clustering in the pore spaces, distinct spatial organizations of greatly enhanced particle contacts can be achieved. As a result, a continuous, but very abrupt, transition from an insulating to metallic-like state can be realized via a small change of either the colloid-template or colloid-colloid attraction strength. Polymer conformational fluctuations are found to significantly modify the physical adhesion process and hence the ability of colloids to organize along the filamentary network strands. Qualitatively new physical behavior can emerge as the pore size approaches the colloid diameter, reflecting strong frustrating constraints of the template on colloidal assembly.


3:30PM Q50.00006 Enhanced Mechanical Properties of Nanoparticle Networks Cross-Linked by Biomimetic Catch Bonds. BADEL L. MBANGA, BALAJI V.S. IYER, VICTOR V. YASHIN, ANNA C. BALAZS, Chemical Engineering Department, University of Pittsburgh, Pennsylvania 15261, USA — The tunable behavior of cross-linked networks of Polymer-Granted Nanoparticles (PGNs) makes them excellent candidates for designing novel materials with enhanced mechanical properties. The building block of a PGN network is a nanoparticle with grafted polymer chains whose free ends' reactive groups can form bonds with the end chains on the nearby particles. We use computer modeling to study the tensile behavior of 3D samples, in which some fraction of cross-links is formed through the biomimetic "catch" bonds. In contrast to conventional "slip" bonds, the catch bonds might become stronger under an applied force due to transitions between two conformational states. The mechanical properties of the PGN networks are shown to exhibit a drastic improvement upon introduction of the catch bonds into the network. We discuss how ductility, toughness, and rate of strain recovery of the network depend on the catch bond content.

3:42PM Q50.00007 Magnetic Nano- and Micro-Particles in Living Cells: Kinetics and Fluctuations. C. PEASE, N. CHIANG, C. PIERCE, N. MUTHUSAMY, R. SOORYAKUMAR, Ohio State Univ - Columbus — Functional nano and micro materials have recently been used not only as diagnostic tools for extracellular studies but also as intracellular drug delivery vehicles and as internal probes of the cell. To realize proper cellular applications, it is important not only to achieve efficient delivery of these materials to targeted cells, but also to control their movement and activity within the confines of the cell. In this presentation, superparamagnetic nano and micro particles are utilized as probes, with their responses to weak external magnetic fields enabling them to be maneuvered within a cell. In order to generate the required local magnetic fields needed for manipulation, the fields emanating from microscopic domain walls stabilized on patterned surface profiles are used in conjunction with weak external magnetic fields to create mobile traps that can localize and transport the internalized particle. Preliminary findings on creating the mobile traps suitable for applications to probe the interior of cells, and the responses, both Brownian fluctuations and directed motion, of particles ranging in size from 200 nm to 1 micron within HS-5 cells will be presented. Future applications to probe cellular behavior within the framework of emerging biomaterials will be discussed.

3:54PM Q50.00008 Programming Directed Motion on the Micron Scale by Thermal Ratcheting. EMILY W. GEHERLS, W. BENJAMIN ROGERS, Harvard University, ZORANA ZERAVCIC, Rockefeller University, VINOTHAN N. MANOHARAN, Harvard University — We present an experimental system of DNA-functionalized colloidal particles which exhibit directed motion (“dancing”) along patterned substrates in response to temperature cycling. We take advantage of toehold exchange in the design of the DNA sequences that mediate the colloidal interactions to produce broadened, flat, or even re-entrant binding and unbinding transitions between the particles and substrate. Using this new freedom of design, we devise systems where by thermal ratcheting, we can externally control the direction of motion and sequence of steps of the colloidal dancer. We determine the maximum work that the system can perform by measuring a maximum average velocity as a function of the thermal ratcheting rate.

4:06PM Q50.00009 Tunable Thermal Switching via DNA-Based Nano Devices. MICHAEL ZWOLAK, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, CHIH-CHUN CHIEN, School of Natural Sciences, University of California, Merced, KIRILL VELIZHANIN, Theoretical Division, Los Alamos National Laboratory, YONATAN DUBI, Department of Chemistry and the Ilse Katz Center for Nano-Science, Ben-Gurion University — DNA has a well-defined structural transition – the denaturation of its double-stranded form into two single strands – that strongly affects its thermal transport properties. We show that, according to a paradigmatic model of DNA denaturation, one can engineer DNA “heattronic” devices that have a rapidly increasing thermal conductance over a narrow temperature range across the denaturation transition (∼350 K). The origin of this rapid increase of conductance, or “switching,” is the softening of the lattice and suppression of nonlinear effects as the temperature crosses the transition temperature and DNA denatures. Most importantly, we demonstrate that DNA nanojunctions have a broad range of thermal tunability due to varying the sequence and length, and exploiting the underlying nonlinear behavior. We discuss the role of disorder in the base sequence, as well as the relation to genomic DNA. These results set the basis for developing thermal devices out of materials with nonlinear structural dynamics, as well as understanding the underlying mechanisms of DNA denaturation.
4:18PM Q50.00010 Modeling the rapid de-swelling of toroidal hydrogels, SVETOSLAV NIKOLOV, YAWEN CHANG, ALEXANDER ALEXEYEV, ALBERTO FERNANDEZ DE LAS NIEVES, Georgia Institute of Technology — The utilization of synthetic hydrogel networks as 3-D cell culture platforms has allowed researchers to more effectively study how epigenetic factors affect cell growth and physiology. As a whole, this has emphasized the biomechanical role of scaffold structures and led to a number of advances in tissue engineering. Our current research focuses on modeling temperature activated shape transformations of toroidal poly(N-isopropylacrylamide) pNIPAM gels. We use dissipative particle dynamics (DPD) to simulate the steady (slow heating rates) and unsteady (fast heating rates) de-swelling behavior of these thermo-sensitive gels. Our simulations show that for slow heating rates the aspect ratio of the tori remains constant during de-swelling. For rapid heating rates we observe buckling instabilities. Our simulations agree with the experimental observations. 

Financial support by NSF CAREER Award DMR-1255288 is gratefully acknowledged.

4:30PM Q50.00011 Renewable Interfaces: Surface Topography Actuation for Complex Biological Adhesion Control, LUKA POCIVAVSEK, University of Pittsburgh Medical Center, SANGHO YE, University of Pittsburgh, KATHLEEN CAO, KA YEE C. LEE, University of Chicago, SACHIN VELANKAR, WILLIAM WAGNER, University of Pittsburgh — Controlling adhesion at biological interfaces is a complex problem with great biomedical importance. We use dynamic wrinkling, generated with PDMS/UVO chemistry under different macroscopic strains ($\epsilon_{ij} \sim 0.3$), to create a mechanical interface term that frustrates particle adhesion. This device actuates surface topography between flat (zero surface confinement $\chi_{ij}$) and wrinkled surfaces ($\chi_{ij} \sim (A/\lambda)^2$, where $A$ and $\lambda$ are wrinkle amplitude and wavelength, respectively), with a maximum rate of 0.6 Hz. Un-actuated PDMS placed in contact with whole sheep blood shows near total surface coverage with adhered platelets over 90 min. Actuation showed a nearly 100-fold decrease in platelet adhesion. Interestingly, topographic actuation is four times as effective compared to flat surface actuation in controlling platelet adhesion. Our model explores the competition between surface tension terms ($U_s = \gamma \epsilon_{ij}$) and interfacial elastic terms ($U_i = E_i(t \cdot \epsilon_{ij}^2 + t^3 \cdot (\chi_{ij}/\lambda)^2$) generated because of actuation and wrinkling, where $E_i$ is platelet modulus and $t$ is characteristic platelet length scale. The condition for de-adhesion is $U_s > U_i$.

4:42PM Q50.00012 Underwater Reversible Adhesion Between Oppositely Charged Weak Polyelectrolytes, LATIFAH ALFHAID, MARK GEOGHEGAN, NICHOLAS WILLIAMS, WILLIAM SEDDON, University of Sheffield — Force-distance data has shown that the adhesion between two oppositely charged polyelectrolytes: poly(methacrylic acid) (PMAA, a polyacid) and poly[2-(diethylamino)ethyl methacrylate] (PDEAEMA, a polybase), was controllable by varying the pH level of their surrounding. Accordingly, adhesive force at the interface between these two polymers was higher inside basic surroundings at pH 6 and 7, and then it started to decrease at pH level below 3 and above 8. Stimulating adhesion between PMAA gel and PDEAEMA brushes by adding salt to their surrounded water has only a limited effect on the adhesive force between them, contradicting previous results. Increasing the molar concentration of sodium chloride (NaCl) in the surrounded water of these two polymers from 0.1 to 1M did not decrease these adhesion forces between a PMAA gel and a grafted PDEAEMA layer (brush). The JKR equation was used to evaluate the adhesion forces between the polymer gel and the brushes and it was observed that the adhesion increased with the elastic modulus of the gel decreased.

4:54PM Q50.00013 Observing polymersome dynamics in controlled microscale flows, SUBHAKSHI KUMAR, ANISH SHENOY, CHARLES SCHROEDER, University of Illinois, Urbana Champaign — Achieving an understanding of single particle rheology for large yet deformable particles with controlled membrane viscoelasticity is a major challenge in soft materials. In this work, we directly visualize the dynamics of single polymersomes ($\sim 10 \mu m$ in size) in an extensional flow using optical microscopy. We generate polymer vesicle structures composed of polybutadiene-block-polyethylene oxide (PB-b-PEO) copolymers. Single polymersomes are confined near the stagnation point of a planar extensional flow using poly(methacrylic acid) (PMAA, a polyacid) and poly[2-(diethylamino)ethyl methacrylate] (PDEAEMA, a polybase) was controllable by varying the pH level of their surrounding. Accordingly, adhesive force at the interface between these two polymers was higher inside basic surroundings at pH 6 and 7, and then it started to decrease at pH level below 3 and above 8. Stimulating adhesion between PMAA gel and PDEAEMA brushes by adding salt to their surrounded water has only a limited effect on the adhesive force between them, contradicting previous results. Increasing the molar concentration of sodium chloride (NaCl) in the surrounded water of these two polymers from 0.1 to 1M did not decrease these adhesion forces between a PMAA gel and a grafted PDEAEMA layer (brush). The JKR equation was used to evaluate the adhesion forces between the polymer gel and the brushes and it was observed that the adhesion increased with the elastic modulus of the gel decreased.

5:06PM Q50.00014 pH-induced structural changes in aqueous CTAB/NaSal solutions, CHINEDU UMEASIEGBU, RAMANAN KRISHNAMOORTI, VEMURI BALAKOTAIAH, Department of Chemical Engineering, University of Houston — Cationic surfactants in the presence of hydrotropic salts exhibit pH-sensitive changes to rheological properties and can thus be utilized in ensuring effective stimulation of heterogeneous carbonate reservoirs. In this study, we investigate the pH-induced changes in microstructure and viscoelasticity of aqueous solutions of cetyltrimethylammonium bromide (CTAB) and sodium salicylate (NaSal), and their dependence on temperature, NaSal-to-CTAB ratio (CS/CD) and CTAB concentration (CD). It was observed that the solutions can be switched between gel-like (viscoelastic) and fluid-like (non-viscoelastic) behavior over a narrow pH range, and that the transition pH and associated change in viscoelasticity were strongly dependent on CS/CD. Dynamic light scattering and small-angle neutron scattering results revealed a hitherto unseen re-entrant transition in which micelles transition from cylindrical to spherical micelles but revert to flexible cylindrical micelles on transition pH and associated change in viscoelasticity. Our observations suggest that in addition to the well described electrostatic and hydrophobic interactions in cationic surfactant - hydrotrope interactions, the pH-induced microstructural changes are governed by complementary cation-π interactions and hydrogen bonding.

Wednesday, March 4, 2015 5:45PM - 7:00PM – Session R3 APS: The Division of Materials Research at NSF - Mary Galvin-Donahue, Division Director, followed by discussion of Broader Impacts in Research 202AB -

5:45PM R3.00001 The Division of Materials Research at NSF - Mary Galvin-Donahue, Division Director, followed by discussion of Broader Impacts in Research –

Wednesday, March 4, 2015 6:45PM - 7:45PM – Session R6 DCMP: Transformational Opportunities for Energy Sciences 006A - George Crabtree, Argonne National Laboratory
6:45PM R6.00001 Community input and update from Basic Energy Sciences Advisory Committee's Directing Matter and Energy Subcommittee, JOHN SARRAO, Los Alamos National Laboratory — BESAC has been charged to update its 2007 report Directing Matter and Energy: Five Challenges for Science and the Imagination, which depicts the science of controlling materials at the electronic, atomic, and molecular levels and represents a revolutionary view of 21st century fundamental science serving the BES community. This report outlined five grand challenges for basic science. These grand challenges, as explicated in the 2007 report, have proven to be a superb prod for the scientific community in the U.S. and beyond. The 46 Energy Frontier Research Centers, created by the Department Of Energy after acceptance of the grand challenge report, as well as the advances of the broader research community, have very effectively pursued the high bar that the five original grand challenges set. From the published results of research that was generated by the original grand challenges, we suggest new opportunities to advance our understanding and mastering of nature. These themes suggest transformational opportunities for energy science of the next decade and beyond. In this town hall, we will present the current status of this study and solicit community input in support of the effort. Additional background information is available at www.besac2014.com.

Wednesday, March 4, 2015 6:30PM - 8:00PM — Session R20 APS: "App"y Hour Grand Hyatt San Antonio Republic B -

6:30PM R20.00001 “App”y Hour —

Wednesday, March 4, 2015 5:45PM - 6:45PM — Session R21 APS: Joint Task Force on Undergraduate Physics Programs 201 -

5:45PM R21.00001 Joint Task Force on Undergraduate Physics Programs —

Wednesday, March 4, 2015 6:30PM - 7:30PM — Session R47 DBIO: Review of Trends in Biological Physics 217B - Wolfgang Losert, University of Maryland

6:30PM R47.00001 Trends in Biological Physics: Neuroscience , SARA SOLLA, Northwestern University —

7:00PM R47.00002 Trends in Biological Physics: Synthetic Biology , WENDELL LIM, University of California, San Francisco — —

Wednesday, March 4, 2015 6:00PM - 7:00PM — Session R50 APS: NSBP & NSHP Receptions Grand Hyatt Travis B & Travis C -

6:00PM R50.00001 NSBP/NSHP Reception —

Wednesday, March 4, 2015 6:00PM - 7:00PM — Session R51 APS: LGBT Roundtable Discussion Grand Hyatt San Antonio Bonham B -

6:00PM R51.00001 LGBT Roundtable Discussion —

Wednesday, March 4, 2015 7:30PM - 9:30PM — Session R52 APS: Special Evening Event Hosted by the Editors of Physics Texas DE - Jessica Thomas, Editor, Physics

7:30PM R52.00001 Rise of the Colloidal Machines , SHARON C. GLOTZER, University of Michigan — Digital matter is a new approach in science, engineering, and medicine that uses powerful algorithms and fast computers to discover and design the materials of the future. The idea is to identify and program atoms, molecules, nanoparticles, and microparticles with the optimal shapes and interactions for forming new materials with unprecedented properties. In this talk, I’ll discuss the exciting possibilities of using nano- and micron-sized colloidal particles in the design and fabrication of functional elements for robot-like machines, such as colloidal muscles, digital colloidal bits, bionic colloidal assemblies, and colloidal swarms. These functional colloidal elements could allow researchers to make smart, shape-shifting materials, like those comprising the Terminator T-1000. I’ll also outline the fundamental physics challenges to realizing smart colloidal materials and machines.

Wednesday, March 4, 2015 7:00PM - 8:30PM — Session R53 APS: Diversity Networking Reception Grand Hyatt San Antonio Crockett CD -

7:00PM R53.00001 Diversity Networking Reception —

Wednesday, March 4, 2015 8:00PM - 10:00PM — Session R54 FHP: Staged Reading of the Play: Background Grand Hyatt Lone Star BC -
I. Gutiérrez Lezama et al. demonstrated the possibility to achieve gate-induced ambipolar transport at the surface [1]. 2H-MoTe$_2$ band gap of around 1.0 eV. This compound shows very high mobility at room temperature and strong absorption throughout the solar spectrum. Previous studies of 2H-MoTe$_2$'s layered structure and the indirect-to-direct band gap transition when approaching the single-layer limit. 2H-MoTe$_2$ shows unique advantages in probing the quasiparticle band structures of the TMD samples with a limited lateral size. However, the STS investigations thus far have not yet consistent results even for the measurement of the quasiparticle band gap. Here we present a new comprehensive methodology of scanning tunneling spectroscopy, which contains the ability not only to probe electronic structures, but also to extract the information on their origins in the Brillouin zone. Thus, we map out, for first time, the quasiparticle energy locations in both the valence and conduction bands of TMD compounds. This capability also allows us to unravel the systematic trend in the critical point energy locations as a function of the cation-anion orbital coupling, the spin-orbital coupling, as well as the interlayer coupling. Such knowledge is critical for understanding the optical properties of TMDs emerging at the atomic scale.

8:12AM S.1.0002 Real-space methods for calculating the electronic response of 2D materials$^1$, BENJAMIN GARRETT, JAMES CHELIKOWSKY, University of Texas at Austin — We study the effects of applied fields on several 2D materials including graphene and metal dichalcogenides. We use a real space density functional method with 2D periodic boundary conditions. This negates the need for a supercell and allows us to directly simulate a transverse electric field. The dielectric properties can be calculated without layer-layer interactions. Changes in band structure in response to imposed fields are also discussed.

1This work is supported by DOE grant DE-FG02-06ER46286. Computational resources were provided by NERSC.

8:24AM S.1.0003 Scanning tunneling microscopy/spectroscopy study of graphene – MoS$_2$ heterojunction$^1$, SHIVANI RAJPUT, YAOYI LI, DUSHYANT TOMER, LIAN LI, University of Wisconsin, Milwaukee — Atomic scale topographic fluctuations are relevant to a number of graphene applications including graphene / semiconductor Schottky diodes [1,2]. In this work, we investigate the atomic structures and electronic properties of graphene-MoS$_2$ heterojunction fabricated by transferring chemical vapor deposited monolayer graphene onto mechanically exfoliated multilayer MoS$_2$. Scanning tunneling microscopy reveals the formation of Moiré patterns with corrugations $\sim 0.03$ nm, but no ripples, in contrast to graphene-SiC junctions [1,2]. Scanning tunneling spectroscopy further indicates that the periodic modulations of the Moiré pattern do not influence the electronic properties of the junction. Additional states near the Fermi level are also observed, likely due to impurities trapped at the interface during graphene transfer. These results and their impact on the properties of the van der Waals graphene-MoS$_2$ heterojunction will be discussed at the meeting.

1Supported by U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-07ER46228.

8:36AM S.1.0004 Imaging and Manipulating Defects in Insulating Hexagonal Boron Nitride Using Scanning Tunneling Microscopy, DILLON WONG, JAIRO VELASCO, LONG JU, JIUNW LEE, SALMAN KAHN, HSINZON TSAI, CHAD GERMANY, University of California, Berkeley, TAKASHI TANIGUCHI, CHIH-KANG SHIH, Univ of Texas, Austin, KENJI WATANABE, National Institute for Material Science, ALEX ZETTL, KAUST, CHIH-KANG SHIH, Univ of Texas, Austin, MING-YANG LI, JING-KAI HUANG, IAMS, Academia Sinica, LAIN-JONG LI, IAMS, Academia Sinica; TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Material Science, ALEX ZETTL, CHIH-KANG SHIH, Univ of Texas, Austin, MING-YANG LI, JING-KAI HUANG, IAMS, Academia Sinica, LAIN-JONG LI, IAMS, Academia Sinica; KAUST, CHIH-KANG SHIH, Univ of Texas, Austin — Accurate knowledge of the electronic structures of materials is the key enabler for the advancement of science and technology based on such materials. Recent emergence of transition metal dichalcogenides (TMDs) as potentially transformative 2D electronic and photonic materials has triggered intensive research activities to investigate their electronic structures. Compared with the previous experimental efforts such as optical spectroscopies and angle resolved photoemission, the scanning tunneling spectroscopy (STS) has the unique advantages in probing the quasiparticle band structures of the TMD samples with a limited lateral size. However, the STS investigations thus far have not yielded consistent results even for the measurement of the quasiparticle band gap. Here we present a new comprehensive methodology of scanning tunneling spectroscopy, which contains the ability not only to probe electronic structures, but also to extract the information on their origins in the Brillouin zone. Thus, we map out, for first time, the critical point energy locations in both the valence and conduction bands of TMD compounds. This capability also allows us to unravel the systematic trend in the critical point energy locations as a function of the cation-anion orbital coupling, the spin-orbital coupling, as well as the interlayer coupling. Such knowledge is critical for understanding the optical properties of TMDs emerging at the atomic scale.

8:48AM S.1.0005 Electronics and atomic scale properties of defects and dopants in 2H-MoTe$_2$, MARIA LONGOBAIRDI, ALBERTO UBALDINI, ENRICO GIANNINI, University of Geneva, DPMC, DAVID R. BOWLER, London Centre for Nanotechnology and Department of Physics and Astronomy, University of London, CHRISTOPH RENNER, University of Geneva, DPMC — We present a detailed STM/STS investigation and corresponding DFT modeling of native dopants and atomic scale defects and their influence on the local electron density of states of 2H-MoTe$_2$. Semiconducting transition metal dichalcogenides (TMDs) are attracting increasing interest in the field of electronics and optoelectronics owing to their layered structure and the indirect-to-direct band gap transition when approaching the single-layer limit. 2H-MoTe$_2$ is a semiconducting TMD with a bulk band gap of around 1.0 eV. This compound shows very high mobility at room temperature and strong absorption throughout the solar spectrum. Previous studies demonstrated the possibility to achieve gate-induced ambipolar transport at the surface [1]. 2H-MoTe$_2$ is thus an attractive candidate for novel optoelectronic devices such as light-emitting diodes, photo detectors and solar cell technology. Controlling the atomic nature and density of defects and dopants is crucial for the development of the aforementioned applications and devices.

9:00AM S1.00006 Simulated scanning tunneling microscopy of few-layer phosphorus allotropes through hexagonal boron nitride, PABLO RIVERO, CEDRIC HORBATH, Univ of Arkansas-Fayetteville, ZHEN ZHU, JIE GUAN, DAVID TOMANEK, Michigan State University, SALVADOR BARRAZA-LOPEZ, Univ of Arkansas-Fayetteville — Four stable layered phosphorus allotropes that are almost degenerated in their configuration energy have been recently discussed [1]. Due to their high reactivity under ambient conditions, their exposed surfaces must be protected [2]. Here, we address the influence of a capping monolayer of hexagonal boron nitride on the scanning tunneling microscopy images of few-layered phosphorus.


9:12AM S1.00007 Scanning Tunneling Spectroscopy of Transition Metal Dichalcogenides: Quasiparticle Gap, Critical Point Energies and Heterojunction Band Offsets, CHIH-KANG SHIH, The University of Texas at Austin — As an emergent atomically thin electronic and photonic materials material, transition metal dichalcogenides (TMDs) has triggered intensive research activities toward understanding of their electronic structures. Here I will introduce a comprehensive form of scanning tunneling spectroscopy (STS) which allows us to probe details quasi-particle electronic structures of TMDs. More specifically, we show that not only the quasi-particle band gaps but also the critical point energy locations and their origins in the Brillouin Zone (BZ) can be revealed using this comprehensive form of STS. By using this new method, we unravel the systematic trend of the critical point energies for TMDs due to atomic orbital couplings, spin-orbital coupling and the interlayer coupling. Moreover, by combining the micro-beam X-ray photoelectron spectroscopy (micro-XPS) and STS, we determine the band offsets in planar heterostructures formed between dissimilar single layer TMDs (MoS2, WSe2, and WS2). We show that both commutativity and transitivity of heterojunction band off hold within the experimental uncertainty.

Other Contributors: (i) Chendong Zhang, Yuxuan Chen, and Amber Johnson at the University of Texas at Austin; (ii) Ming-Yang Li, Jing-Kai Huang, Lain-Jong Li, Chih-Piao Chuu and Mei-Yin Chou at the Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan.

9:48AM S1.00008 Structural phase transitions in monolayer molybdenum dichalcogenides, DUK-HYUN CHOE, HA JUNE SUNG, KEE JOO CHANG, Department of Physics, KAIST — The recent discovery of two-dimensional materials such as graphene and transition metal dichalcogenides (TMDs) has provided opportunities to develop ultimate thin channel devices. In contrast to graphene, the existence of moderate band gap and strong spin-orbit coupling gives rise to exotic electronic properties which vary with layer thickness, lattice structure, and symmetry. TMDs commonly appear in two structures with distinct symmetries, trigonal prismatic 2H and octahedral 1T phases which are semiconducting and metallic, respectively. In this work, we investigate the structural and electronic properties of monolayer molybdenum dichalcogenides (MoX2, where X = S, Se, Te) through first-principles density functional calculations. We find a tendency that the semiconducting 2H phase is more stable than the metallic 1T phase. We show that a spontaneous symmetry breaking of 1T phase leads to various distorted octahedral (1T') phases, thus inducing a metal-to-semiconductor transition. We discuss the effects of carrier doping on the structural stability and the modification of the electronic structure.

10:00AM S1.00009 Scanning Tunneling Microscopy study on exfoliated single-layer MoSe2, XIADONG ZHOU, ALI DADGAR, Department of Physics, Columbia University, New York, New York 10027, USA, FRANCES M. ROSS, IBM T.J.Watson Research Center, Yorktown Heights, New York 10598, USA, ABHAY N. PASUPATHY, Department of Physics, Columbia University, New York, New York 10027, USA — Monolayer transitional metal dichalcogenides (TMDs) MX2 (M = Mo, W, Ti etc; X = S, Se, Te) are a new platform for exploring new electronic and optical phenomena and functionality. However, much remains to be understood about their chemical and local electronic properties when taken to the monolayer limit. We will discuss a scanning tunneling microscopy (STM) study on exfoliated single-layer MoSe2 using a 4-probe STM system. The ability to carry out scanning electron microscopy (SEM) in our system allows us to easily locate and measure single-layer MoSe2 flakes that are mechanically exfoliated on a SiO2/Si substrate and are only a few micrometers in lateral size. Using a combination of imaging and spectroscopy, we will discuss the chemical purity and nature of defect states in this monolayer material. Using an electrostatic back gate, we will describe measurements of the single-particle electronic bandgap as a function of the chemical potential.

10:12AM S1.00010 Defect states in monolayer transition metal dichalcogenides, MAHTAB KHAN, University of Central Florida — Monolayer transition metal dichalcogenides (TMDC) have attracted considerable attention in the past few years. They are direct bandgap semiconductors, with the conduction and valence band edges at the doubly degenerate corners (± K points) of the hexagonal Brillouin zone. Recently, by using novel etching techniques, it was possible to remove a controlled number of atoms from monolayer MoS2, thereby creating a hexagonally shaped pit. By solving the Dirac equation analytically, we show that a pit gives rise to bound states with interesting properties. In particular, the optical selection rules turn out to be very strict. We confirm our analytical results by means of numerical density functional theory (DFT) calculations.

10:24AM S1.00011 Thermoelectric imaging of grain boundaries in monolayer MoS2 on the atomic scale, SANGHEE CHO, HO-KI LYEO, Korea Research Institute of Standards and Science, LAIN-JONG LI, King Abdullah University of Science and Technology, YONG-HYUN KIM, Korea Advanced Institute of Science and Technology, CHENDONG ZHANG, CHIH-KANG SHIH, The University of Texas at Austin — We used scanning thermoelectric microscopy to investigate structural defects such as point defects, edge and grain boundary in ultrathin films of MoS2 grown on graphite. Such structural changes cause the variation in local electronic states, which can be detected by thermoelectric measurement that is differentially sensitive to the Fermi electronic states. Measured thermoelectric power increased with increasing thickness of MoS2 from monolayer to multilayer, which makes a different contrast in the images of thermoelectric measurements. The changes in thermoelectric power with varying thickness can be accounted for by the changes in energy band structure. This imaging method enabled us to identify the metallic edge states, which is similar to prior measurements from tunneling spectroscopy, at the boundaries between MoS2 and graphite. Moreover, grain boundaries appear with distinct contrast in thermoelectric measurements from micrometer to atomic scale, whereas the boundaries were subtle in topographic measurements. Simultaneous measurements of topographic and thermoelectric signal revealed the structural and electronic properties of grain boundaries on the atomic scale.
10:36AM S1.00012 Occupied and Unoccupied Electronic Structure of Na doped MoS\(_2\) (0001). T. KOMESU, University of Nebraska, Lincoln, D. LE, University of Central Florida, X. ZHANG, University of Nebraska, Lincoln, Q. MA, University of California - Riverside, E. F. SCHWIER, Y. KOJIMA, M. ZHENG, H. IWASAWA, K. SHIMADA, M. TANIGUCHI, Hiroshima University, Japan, L. BARTELS, University of California - Riverside, T. S. RAHMAN, University of Central Florida, P. A. DOWBEN, University of Nebraska, Lincoln — The influence of sodium on the band structure of MoS\(_2\) (0001) and the comparison of the experimental band dispersion with density functional theory (DFT) shows excellent agreement for the occupied states (angle-resolved photoemission), and qualitative agreement for the unoccupied states (inverse photoemission spectroscopy). We will show that Na adsorption leads to charge transfer to the MoS\(_2\) surface causing an effect similar to n-type doping of a semiconductor. Moreover, results of our simulations and measurements clearly indicate that the MoS\(_2\) occupied valence band structure shifts rigidly to greater binding with little change in the occupied state dispersion and that the unoccupied states shift downward, approaching the Fermi level, yet the amount of the shift for the unoccupied states is greater than that of the occupied states, effectively causing a narrowing of the bandgap. At higher Na coverages MoS\(_2\) surface becomes metallic. Details of electronic band structure of Na/MoS\(_2\) (0001) will be discussed in light of the role of the frontier orbitals in facilitating chemical reactivity of the system.

10:48AM S1.00013 Effects of spatial averaging on the ARPES spectra of graphene. FREDERIC JOUCKEN, NICOLAS RECKINGER, University of Namur. JOSE AVILA, MARIA CARMEN ASENSIO, Soleil Synchrotron, JÉRÔME LAGOUTE, Université Paris 7 - Paris Diderot, JEAN-FRANÇOIS COLOMÉ, JACQUES GHJESSEN, ROBERT SPOKEN, University of Namur, PHYSICS DEPARTMENT, UNIVERSITY OF NAMUR COLLABORATION, ANATES BEAMLINE, SOLEIL SYNCHROTRON COLLABORATION, STM LAB, MPQ, UNIVERSITÉ PARIS 7 - PARIS DIDEROT COLLABORATION — We report on an ARPES nanoscope investigation (nano-ARPES) and demonstrate that spatial averaging of ARPES data, even on a single graphene domain, lead to apparent kinks in the dispersion relation as well as variations of the MDC widths with binding energy that do not appear in the spectra acquired on a very small spot (below 100nm X 100nm). At the same time, we show that the electronic dispersion relation of our graphene sample is perfectly linear while the MDC widths do not display a simple dependence with the binding energy.

Thursday, March 5, 2015 8:00AM - 11:00AM — Session S2 DMP: Focus Session: Beyond Graphene - Optics in 2D Semiconductors V 001B - Bernhard Urbanzek, INSA Toulouse (France)

8:00AM S2.00001 Optical and electrical responses of optically excited single layer MoS\(_2\) depending on the carrier concentration. SEONG CHU LIM, JINHEE LEE, JUNGHO KIM, HOMIN CHOI, JAESOO KIM, JUNGJOON BAE, MOHAN KUMAR, Department of Energy Science, Center for Integrated Nanostructure Physics, Sungkyunkwan University, Suwon, Republic of Korea — In this work, we study both optical and electrical responses of a single layer molybdenum disulfide (MoS\(_2\)) connecting source and drain electrodes deposited on SiO\(_2\) layer. Depending on the gate bias, the incremental rate of the photocurrent is different, implying the carrier concentration is closely involved with the observations. In semiconducting state at high negative gate bias, the increase of the number of carriers is more influential on electrical conductivity of MoS\(_2\), whereas in metallic state at high positive gate bias, the electron-electron scattering is more dominant. In addition, the photoluminescence (PL) is significantly affected by the carrier concentration as well. At low concentration, PL is stronger than that of higher carrier concentration and PL is weakened Coulomb interaction between electron-hole pairs.

8:12AM S2.00002 Electronic and optoelectronic properties of Few Layer MoS\(_2\) Flake. JIE ZHANG, SUJOY GHOSH, MILINDA WASALA, SAIKAT TALAPATRA, Department of Physics, Southern Illinois University Carbondale IL-62901, USA — We will report on the electronic and optoelectronic properties of few-layers flakes of MoS\(_2\) obtained by mechanical exfoliation of bulk MoS\(_2\) crystal. Measurements performed in field effect transistor (FET) geometry show a room temperature mobility \(\mu_{FET} \sim 40\text{cm}^2\text{V}^{-1}\text{s}^{-1}\). Temperature dependent (50K \textless T \textless 300K) photococonductivity measurements investigated using continuous laser of \(\lambda = 658\text{nm} (E=1.88eV)\), over a broad range of illuminating laser intensity, \(P (0.1\mu W < P < 2\mu W)\) indicate a fractional power dependence of steady state photocurrent on P. Room temperature responsivity obtained in these samples were found to be \(\sim 1 \text{A W}^{-1}\). Variation and/or dependence of these measured properties with respect to temperature will be presented and compared with similar measurements performed other layered 2D Transition Metal Dichalcogenides. This work is supported by the U.S. Army Research Office through a MURI grant # W911NF-11-1-0362.

8:24AM S2.00003 Optical properties of two dimensional gallium selenide. ALARIC BERGERON, Polytechnique Montreal, RICHARD LEONELLI, Université de Montréal, SEBASTIEN FRANCOEUR, Polytechnique Montreal, COPL TEAM — Gallium selenide is a layered metal chalcogenide compound with peculiar but attractive optical properties. Its very high \(d_{2g}\) coefficient, along with its optical transparency from 0.65 to 18 \(\mu m\) and high optical damage threshold, makes it an ideal material for non-linear optical applications. The band structure of GaSe presents a pseudo-direct bandgap, with the direct transition sitting \(-20\text{meV}\) above the indirect one, allowing for efficient photoconductivity and photoluminescence. This could be very interesting for various optoelectronic applications. In this study, we have analyzed the angular and polarization dependence of photoluminescence and second harmonic generation of 2D GaSe flakes of varying thicknesses, down to the monolayer. These results are examined in the light of the few-layer structure symmetry and the unusual optical selection rules forbidding light emission perpendicularly to the basal plane.

8:36AM S2.00004 Optoelectronics of Transition Metal Dichalcogenide Monolayers and Heterostructures. JOHN SCHABLEY, University of Washington — Monolayer transition metal dichalcogenides (TMDs) contain 2D valley excitons which reside in two degenerate momentum space valleys at the edges of the Brillouin zone. It is crucially important to understand fundamental 2D exciton properties in TMD monolayers and van der Waals heterostructures. By performing coherent nonlinear optical spectroscopy with high spectral resolution, we observe nanosecond decay dynamics in single monolayers of MoSe\(_2\), implying the presence of a previously unreported long-lived state that appears to trap the exciton population. In MoSe\(_2\)-WSe\(_2\) vertical heterostructures, we observe intralayer excitons, where the electron and hole are confined to different monolayers, and show evidence of strong exciton-exciton interaction effects and long lifetimes. Based on TMD monolayer excitons, we have also investigated a variety of fundamental quantum devices, including a nano-cavity laser and a second-harmonic generation transistor. Finally, we report a new type of single quantum emitter, based on single localized excitons spatially confined to defects in monolayer of WSe\(_2\). The photoluminescence from these localized excitons is spectrally narrow and shows strong anti-bunching, demonstrating the single photon nature of the emission.
9:12AM S2.00005 Strong in-plane anisotropic optical properties of monolayer, few-layer and bulk ReSe$_2$\textsuperscript{1}. HUAN ZHAO, Univ of Southern California, QIUSHI GUO, Yale University, LUHAO WANG, Univ of Southern California, FENGNIAN XIA, Yale University, HAN WANG, Univ of Southern California — Recently, there has been growing interest in the anisotropic properties of certain two-dimensional (2D) materials with reduced lattice symmetry, such as black phosphorus, for developing novel applications in nanoelectronics and infrared optoelectronics. In this work, we report the strong anisotropic optical and electronic properties of monolayer, few-layer and bulk ReSe$_2$, an emerging member of the 2D transition metal dichalcogenides (TMDs) family. With its bandgap around 1.1 eV and potentially tunable with layer number and strain, ReSe$_2$ may complement black phosphorus for optoelectronic applications utilizing its anisotropic properties in the near-infrared and visible range. Through careful investigations of the polarization-resolved Raman spectroscopy, photoluminescence (PL), polarization-resolved optical extinction spectrum, angle-resolved DC conductance and first principles calculations, we observed and explained the consistent dependence of phonon, optical and electrical properties of ReSe$_2$ on its in-plane crystal orientation. Our results reveal the interesting anisotropic properties of 2D ReSe$_2$ and shed light on its potential applications in electronics and optoelectronics.

\textsuperscript{1}This work was supported by the Army Research Laboratory.

9:24AM S2.00006 Electronic and photo-electronic transport in sputter deposited MoS$_2$ film , MILINDA WASALA, SUJOY GHOSH, JIE ZHANG, JULIANNA RICHIE, DIPANJAN MAZUMDAR, Department of Physics, Southern Illinois University Carbondale IL-62901, USA, SWASTIK KAR, Department of Physics, Northeastern University, Boston, MA-02115, USA, SAIKAIT TALAPATRA, Department of Physics, Southern Illinois University Carbondale IL-62901, USA — Here we report on the electrical transport as well as photo response of large area sputter deposited few-layers of thin MoS$_2$. Temperature dependent (55 K -275K) electronic conductivity measured on these samples show evidence of 2D Variable Range Hopping (2D-VRH) mechanism within 100K-275K. Photoconductivity measurements investigated using a continuous laser of $\lambda$ =658nm ($E=1.88eV$), over a broad range of illuminating laser intensity, P ($0.19\mu W < P < 11\mu W$). The steady state photocurrent $(I_{ph})$ indicates a fractional power dependence on laser intensity. The highest responsivities obtained in these films are found to be $\sim 0.2A/W$. The frequency (with Laser pulse frequency range 1Hz-200Hz) dependent photocurrent will be presented and discussed. This work is supported by the U.S. Army Research Office through a MURI grant # W911NF-11-1-0362 and NSF-PIRE OISE-0968405.

9:36AM S2.00007 Unusual Electrooptic Response of Colloidal 2D Transition Metal Dichalcogenide Nanodiscs , DANIEL ROSSI, Texas A&M University, DONG HEE SON, Texas A&M Univ, JINWOO CHEON, JAE HYO HANN, WONIL JUNG, Yonsei University — We have characterized an unusual electrooptic response in colloidal solutions of TiS$_2$, WSe$_2$, and ZrS$_2$ layered transition metal dichalcogenide (TMD) nanodiscs, where transient orientation order is induced by the time varying component of a square-wave electric field, giving rise to linear dichroism which decays even in the presence of the aligning field. Interestingly, identical electrooptic response were seen from both the rising and falling edges of the field, indicating that particle alignment responds to the absolute value of $\Delta E$, regardless of the DC field offset, essentially performing the optical electric field edge detection. Both the magnitude and decay time of the electrooptic response were sensitive to solvent polarity, which we believe is related to the polarity dependent interparticle interactions previously observed in colloidal TiS$_2$ nanodisc solutions. This unusual behavior appears to be a general property of colloidal TMD nanodiscs, potentially resulting from the time varying anisotropy of the induced dipole moment, in contrast to other anisotropic nanostructures with little to no dipole moment anisotropy, where the electrooptic response is dictated by the magnitude of the electric field.

9:48AM S2.00008 Biaxial Strain Engineering in Suspended MoS$_2$, DAVID LLOYD, Boston University, XINGHUI LIU, University of Colorado at Boulder, LAUREN CANTLEY, ERIC KOCH, GUANG YANG, Boston University, NARASIMHA BODDETI, University of Colorado at Boulder, MARTIN L. DUNN, Singapore University of Technology and Design, J. SCOTT BUNCH, Boston University, BUNCH TEAM — Monolayer MoS$_2$ is a direct gap semiconductor and has attracted significant interest for its potential uses in electronics and optoelectronics. It has also been shown to have a highly strain-sensitive bandgap and can sustain strains of up to 11 percent, making it ideally suited for using strain engineering to tune it’s electrical and optical properties. Herein, we fabricate pressurized MoS$_2$ blisters using single and few layer MoS$_2$ membranes suspended over cylindrical microcavities. By applying a pressure difference across the membrane and measuring the changes to its photoluminescence spectrum we study the effect of elastic biaxial strain engineering on the bandgap of MoS$_2$.

10:00AM S2.00009 Pronounced photovoltaic response from PN-junctions of multi-layered MoSe$_2$ on h-BN\textsuperscript{1}. SHAHRIAR MEMARAN\textsuperscript{2}, NIHAR PRADHAN*, ZHENGGUANG LU, DANIEL RHODES, JONATHAN LUDWIG, QIONG ZHOU, NHMF, Florida State Univ, PULICKEL AJAYAN, Rice Univ., DMITRY SMIRNOV, LUIS BALICAS, NHMF, Florida State Univ — Transition metal dichalcogenides (TMDs) such as MoS$_2$, WSe$_2$, etc., are semiconducting van der Waals bonded solids which are exfoliable down to single atomic layers. Monolayers display unique optical as well as optoelectronic properties, while heterostructures incorporating graphene and multi-layered TMDs display pronounced photovoltaic behaviour. Here, we report the observation of rectification and enhanced photocurrents as well as photovoltaic, in lateral PN junctions based on multi-layered ambipolar MoSe$_2$ crystals stacked onto h-BN. Our PN junctions composed of $\sim$10 atom layers are translucent enough to yield photoresponsivities of 1 A/W, external quantum efficiencies exceeding 30 %, short circuit currents exceeding 10$^{-3}$ A/cm$^2$, and photovoltaic efficiencies surpassing 5 % with fill factors of $\sim$70 %. These values compare favourably with those of transparent photovoltaic cells. Given that TMDs can be grown in large area, that their band gap(s) can be tuned by varying composition, and the available strategies for increasing their efficiency, our results suggest a remarkable potential for semi-transparent photovoltaic cells composed of just a few layers of TMDs.

\textsuperscript{1}This work is supported by the U.S. Army Research Office MURI grant W911NF-11-1-0362

\textsuperscript{2}These authors contributed equally to this work

10:12AM S2.00010 Temperature dependent photoconduction in atomically thin Layers of Indium Selenide , SUJOY GHOSH, MILINDA WASALA, JIE ZHANG, Department of Physics, Southern Illinois University Carbondale IL-62901, USA, SIDONG LEI, ROBERT VAJTAI, PULICKEL M. AJAYAN, Department of Materials Science and Nano Engineering, Rice University, Houston, Texas 77005, United States, SAIKAIT TALAPATRA, Department of Physics, Southern Illinois University Carbondale IL-62901, USA — We will report on the photo response in few-layers of thin Indium Selenide (InSe) flakes exfoliated from crystals grown using chemical vapor transport technique. Temperature dependent (20 K -300K) photoconductivity measurements investigated using a continuous laser of $\lambda$ =658nm ($E=1.88eV$), over a broad range of illuminating laser power, P ($0.1\mu W < P < 4\mu W$) indicate a power dependence of steady state photocurrent $(I_{ph})$ on P ($I \sim P^\beta$ with $\beta \sim 1$). The highest responsivity obtained in these samples were $\sim 0.5A/W$. Variation and/or dependence of these measured properties with respect to temperature will be presented. The frequency (with Laser pulse frequency range 1Hz-200Hz) dependent photocurrent will be presented and discussed. This work is supported by the U.S. Army Research Office through a MURI grant # W911NF-11-1-0362.
it through to publication. Those based at undergoing a period of rapid change, these core principles remain largely unchanged. In this talk, I will endeavour to explain how Nature editors – in particular fostering a greater appreciation of these great works of science amongst the wider public. Although the publishing landscape for scientific research is currently two-fold: facilitating the prompt communication of the most important scientific developments to the relevant research communities, while at the same time authors and the research community, the underlying principles of managing the process for journals published by IOP Publishing remain unchanged and yet the UK — Online publishing is challenging, and potentially changing, the role of publishers in both managing the peer-review process and disseminating the work communities they interact with, adapting? In this context, are alternatives to peer review on the horizon? Are these challenges unique to physics journals, or have been transformed by the internet. In particular, increasingly their role appears to be to validate research, not to disseminate it. How are journals, and the duty of scientists in the scientific community, because all scientists take turns serving either as authors, referees, and editors in the peer review process. We lack the themes of trust, where the trust is in institutions and procedures that emerge from expert communities. The practice of peer review is viewed as a citizenly objectivity by the community. The way in which this tends to be done is by peer review conducted by journals. Peer review as currently practiced touches on must be verified by someone who is not the maker of those claims, and who furthermore has no stake in the matter. In other words, claims need to be evaluated objectively, by the community. The way in which this tends to be done is by peer review conducted by journals. Peer review as currently practiced touches on the themes of trust, where the trust is in institutions and procedures that emerge from expert communities. The practice of peer review is viewed as a citizenly duty of scientists in the scientific community, because all scientists take turns serving either as authors, referees, and editors in the peer review process. We lack the resources to have a work evaluated by the entire community, so we substitute with a representative. Yet, in most examples of scientific review, the referee or referees are anonymous. This question is particularly important when the peer review process is brought to bear in order to evaluate matters beyond scientific validity, more "subjective" criteria such as relative importance, breadth of interest – criteria that do not appear to have an objective standard of comparison and validation. I will show that the anonymity of referees, far from endangering this trust, actually strengthens it. I will show that this anonymity is crucial in order to maintain any objectivity in scientific peer review, and why authors should not try to unmask the referee.

Previously, it has been recognized that scientific claims must be verified by someone who is not the maker of those claims, and who furthermore has no stake in the matter. In other words, claims need to be evaluated objectively, by the community. The way in which this tends to be done is by peer review conducted by journals. Peer review as currently practiced touches on the themes of trust, where the trust is in institutions and procedures that emerge from expert communities. The practice of peer review is viewed as a citizenly duty of scientists in the scientific community, because all scientists take turns serving either as authors, referees, and editors in the peer review process. We lack the resources to have a work evaluated by the entire community, so we substitute with a representative. Yet, in most examples of scientific review, the referee or referees are anonymous. This question is particularly important when the peer review process is brought to bear in order to evaluate matters beyond scientific validity, more "subjective" criteria such as relative importance, breadth of interest – criteria that do not appear to have an objective standard of comparison and validation. I will show that the anonymity of referees, far from endangering this trust, actually strengthens it. I will show that this anonymity is crucial in order to maintain any objectivity in scientific peer review, and why authors should not try to unmask the referee.

1 The Authors thank FAPESP for financial support

Thursday, March 5, 2015 8:00AM - 10:00AM —
Session S4 FEd: Physics Education Research: Course Transformation and Outreach

8:00AM S3.00001 There is no “I” in referee: Why referees should be anonymous DANIEL UCKO 1
Department of Philosophy, Stony Brook University, Stony Brook, NY — From the early days of modern science, it has been recognized that scientific claims must be verified by someone who is not the maker of those claims, and who furthermore has no stake in the matter. In other words, claims need to be evaluated objectively, by the community. The way in which this tends to be done is by peer review conducted by journals. Peer review as currently practiced touches on the themes of trust, where the trust is in institutions and procedures that emerge from expert communities. The practice of peer review is viewed as a citizenly duty of scientists in the scientific community, because all scientists take turns serving either as authors, referees, and editors in the peer review process. We lack the resources to have a work evaluated by the entire community, so we substitute with a representative. Yet, in most examples of scientific review, the referee or referees are anonymous. This question is particularly important when the peer review process is brought to bear in order to evaluate matters beyond scientific validity, more "subjective" criteria such as relative importance, breadth of interest – criteria that do not appear to have an objective standard of comparison and validation. I will show that the anonymity of referees, far from endangering this trust, actually strengthens it. I will show that this anonymity is crucial in order to maintain any objectivity in scientific peer review, and why authors should not try to unmask the referee.

1 Also at The American Physical Society (APS).

8:36AM S3.00002 Validity, not Dissemination SAMINDRANATH MITRA, American Physical Society APS — Science journals have been transformed by the internet. In particular, increasingly their role appears to be to validate research, not to disseminate it. How are journals, and the communities they interact with, adapting? In this context, are alternatives to peer review on the horizon? Are these challenges unique to physics journals, or also seen in other publication scenarios?

9:12AM S3.00003 Peer-review: An IOP Publishing Perspective TIMOTHY SMITH, IOP Publishing, Bristol, UK — Online publishing is challenging, and potentially changing, the role of publishers in both managing the peer-review process and disseminating the work that they publish in meeting contrasting needs from diverse groups of research communities. Recognizing the value of peer-review as a fundamental service to authors and the research community, the underlying principles of managing the process for journals published by IOP Publishing remain unchanged and yet the potential and demand for alternative models exists. This talk will discuss the traditional approach to peer-review placed in the context of this changing demand.

9:48AM S3.00004 Inside Nature ANDREA TARONI, Nature Physics — Since its launch in 1869, Nature has seen its mission as two-fold: facilitating the prompt communication of the most important scientific developments to the relevant research communities, while at the same time fostering a greater appreciation of these great works of science amongst the wider public. Although the publishing landscape for scientific research is currently undergoing a period of rapid change, these core principles remain largely unchanged. In this talk, I will endeavour to explain how Nature editors — in particular those based at Nature Physics — apply these principles in practice, and so determine which few of the many excellent research submissions that we receive make it through to publication.

Thursday, March 5, 2015 8:00AM - 10:00AM —
Session S3 FHP: Invited Session: Why Peer Review? 002AB - Robert Crease, Stony Brook University
8:00AM S4.00001 Assessing the Impacts of a Hybrid “Flipped” Approach to University Physics.  
CHRIS HUGHES, SCOTT PAULSON, James Madison University — Over the course of several years, the physics faculty at James Madison University has been gradually reforming the introductory calculus-based physics sequence to a hybrid model using a ‘flipped classroom’ approach. The content traditionally delivered during lecture was divided into approximately 150 short (5-10 minute) videos. For homework, students are assigned 3-5 videos to watch before each class session. These assignments are combined with in-class activities including gouger problem solving and the tutorials developed by the University of Washington group to provide the students with focused guidance on concepts and skills that students traditionally have left our classes not having mastered. For the fall semester course on mechanics, the Force Concept Inventory (FCI) was used to evaluate student outcomes. For the spring semester course on E&M and optics, the Conceptual Survey of Electricity and Magnetism (CSEM) was used. Student reaction to the course structure was generally positive though there were some complaints in the student evaluations at the end of each semester. However, a positive impact on student outcomes was observed based on the Hake gains on the FCI.

8:12AM S4.00002 Lecture capturing assisted teaching and learning experience.  
LI CHEN, MCPHS University — When it comes to learning, a deep understanding of the material and a broadband of knowledge are equally important. However, provided limited amount of semester time, instructors often find themselves struggling to reach both aspects at the same time and are often forced to make a choice between the two. On one hand, we would like to spend much time to train our students, with demonstrations, step by step guidance and practice, to develop strong critical thinking skills and problem-solving skills. On the other hand, we also would like to cover a wide range of content topics to broaden our students’ understanding. In this presentation, we propose a working scheme that may assist to achieve these two goals at the same time without sacrificing either one. With the help of recorded and pre-recorded lectures and other class materials, it allows instructors to spend more class time to focus on developing critical thinking skills and problem-solving skills, and to apply and connect principle knowledge with real life phenomena. It also allows our students to digest the material at a pace they are comfortable with by watching the recorded lectures over and over. Students now have something as a backup to refer to when they have random mistakes and/or missing spots on their notes, and hence take more ownership of their learning. Advanced technology have offered flexibility of how/when the content can be delivered, and have been assisting towards better teaching and learning strategies.

LEIGH SMITH, Dept of Physics, Univ of Cincinnati — I will describe methods used at the University of Cincinnati to enhance student success in an algebra-based physics course. The first method is to use ALEKS, an adaptive online mathematics tutorial engine, before the term begins. Approximately three to four weeks before the beginning of the term, the professor in the course emails all of the students in the course informing them of the possibility of improving their math proficiency by using ALEKS. Using only a minimal reward on homework, we have achieved a 70% response rate with students spending an average of 8 hours working on their math skills before classes start. The second method is to use a flipped classroom approach. The class of 135 meets in a tiered classroom twice per week for two hours. Over the previous weekend students spend approximately 2 hours reading the book, taking short multiple choice conceptual quizzes, and viewing videos covering the material. In class, students use Learning Catalytics to work through homework problems in groups, guided by the instructor and one learning assistant. Using these interventions, we have reduced the student DWF rate (the fraction of students receiving a D or lower in the class) from an historical average of 35 to 40% to less than 20%.

8:36AM S4.00004 Developing a Standard Based Advanced Lab Course that Fulfills COM3 Requirements.  
RUDI MICHALAK, University of Wyoming — An advanced physics lab has been developed into a course that fulfills the requirements for a university studies program ‘COM3’ course using Standard Teaching (ST) methods. The COM3 course is a capstone course under the new USP2015 study requirements for all majors. It replaces the WC writing requirement, typically filled in the English Dept., and adds the teaching of oral and digital communication skills. ST is a method that replaces typical assessments (homework / exam grades) with new assessments that measure certain specified learning outcomes. In combination with oral assessments and an oral final exam, the ST proves an efficient tool to implement the USP Learning Outcomes into a physics course. COM3 requires an unprecedented seven learning outcomes in a single course. Variety of learning outcomes: interdisciplinary goals, levels of writing (with drafting steps), organizational structure, standard language metrics, research and presentation deliverance skills, appropriate addressing of a variety of audiences, etc. With other assessment approaches than ST this variety would be difficult to meet in a physics course. An extended ST rubric has been developed for this course and will be presented and discussed in some detail.

8:48AM S4.00005 Enhancing Faculty Engagement and Student Learning in Foundational STEM Courses at a Large Public University1.  
HOWARD JACKSON, KATHLEEN KOENIG, Department of Physics, University of Cincinnati, Cincinnati, OH 45221-0011 — Enhancing student learning requires both the strong involvement of the faculty member and the student. We present preliminary efforts of an NSF-supported multi-disciplinary program to enhance learning in foundational STEM courses. A central theme, supported by evidenced-based research across the STEM disciplines, is that active learning engages students in ways that enhance student learning. A secondary theme is that sustained use of active learning techniques by faculty needs a supportive local culture. We describe our initial efforts with the use of Teaching and Learning Liaisons, faculty members trained in research-based instructional strategies in order to lower the barriers for faculty to try new (to them) active learning strategies, and to increase the probability that these faculty carry out the strategies with fidelity. We have assembled a collection of faculty across the STEM disciplines of Biology, Chemistry, and Physics to participate and will compare initial activities by these departments. Efforts to create a supportive culture for these faculty was also provided by tangible department head efforts.

1We acknowledge support from the National Science Foundation (DUE-1022563).

9:00AM S4.00006 Understanding the Spread of Research-Based Instructional Strategies: A Case Study of SCALE-UP.  
ALEXIS KNAUB, CHARLES HENDERSON, Western Michigan University, ROBERT BEICHNER, North Carolina State University, MELISSA DANCY, University of Colorado- Boulder, KATHLEEN FOOTE, North Carolina State University — Secondary implementations of research-based instructional strategies are often non-trivial and can be met with challenges. This talk will focus on lessons learned from a case study of the secondary implementations of Student-Centered Active Learning Environment with Upside-Down Pedagogies (SCALE-UP). SCALE-UP, which started in the physics department of North Carolina State University, is now used across disciplines and at institutes throughout the world. We have examined how SCALE-UP has spread within departments, between departments, and across universities. Both qualitative and quantitative data provide explanation on what has helped and hindered the spread of SCALE-UP at these various levels. We will focus on implications for faculty interested in introducing new instructional strategies at their institution.
9:12AM S4.00007 Lessons from Girl Scout Physics Outreach Day at the University of Michigan, J.T. BOURJ, J.C. WALRATH, C.A. AIDALA, University of Michigan, Ann Arbor, MI — The University of Michigan Society of Women in Physics (SWIP) has been actively collaborating in and coordinating community outreach activities since its founding in 2004. These events range from public demonstration days to high school Physics Olympiad competitions. In 2012, SWIP started an interactive demonstration day for local Girl Scout troops to specifically target an elementary and middle-school aged audience. Girl Scout Day became an annual event, and SWIP interacted with the same set of girls as they matured from 4th-6th graders to 6th-8th graders. At each event, SWIP conducted informal verbal and written surveys on their perceptions of Physics. While in all events girls of all ages asked questions regarding the experience of being a physicist and physics careers, the first event received a significant number of gendered questions. For example, “What percentage of women are physicists?” or “Are there lots of cool girls studying physics?” In following events, these questions were replaced with more technical questions about experiments from the day and questions like “Do you like your choice in jobs?” In this talk we will share our experiences from this outreach project and propose ideas on how to shape events for these age groups in the future.

9:24AM S4.00008 Rare Isotopes At Your Fingertips: a game for introducing students to nuclear science1. ZACHARY CONSTAN, National Superconducting Cyclotron Laboratory, BRIAN WINN, ANDREW DENNIS, Michigan State University, CHRIS WREDE, REMCO ZEGERS, HENDRIK SCHATZ, ALEX BROWN, National Superconducting Cyclotron Laboratory, NICHOLAS THURSTON, CHRISTOPHER BENOIT, SAHIL TANDON, WILLIAM JEFFERY, TYLER SUMMERS, ANDREW BAGDADY, PETER BURROUGHS, JOSEPH DYKSTRA, JOSHUA SHADIK, AMANDA KRUEGER, Michigan State University, MICHAEL BOWRY, CHARLES LOELIUS, MICHAEL BENNETT, National Superconducting Cyclotron Laboratory — Two units at Michigan State University, the Games for Entertainment and Learning (GEL) Lab and National Superconducting Cyclotron Laboratory (NSCL), are developing a touch-based digital game for physics outreach. Players will be able to explore the chart of the nuclides, accelerate stable nuclei, fragment them on a target, and handcraft rare isotopes from the excited protons and neutrons. Gameplay will lead them to the discovery of new isotopes, highlighting stability/instability, nucleosynthesis, radioactive decay, etc. The goal of this game is to bring an awareness and appreciation of nuclear science to a broader audience. Future funding sources will be used to further develop the game into a tool for the classroom, where students will learn about potential career paths in nuclear research.

1Work supported by grants from the American Physical Society and Michigan State University

9:36AM S4.00009 Mitchell Institute Physics Enhancement Program for High School Teachers (MIPEP)1. TATIANA ERIKHIMOVA, ALEXEY BELYANIN, BHASKAR DUTTA, Texas A&M University — The MIPEP is a two-week summer boarding school for physics teachers who had limited training in physics: usually 0-2 credit hours of college-level courses. The school was organized by the Mitchell Institute and Texas A&M Department of Physics and Astronomy during summers 2012-2014. Two weeks of intense training included lectures, physics labs, hands-on demos, tours of various campus research facilities, telescope observations, discussions and meetings with top researchers, and many other physics-related activities. Detailed assessment of the program was performed each year. We will review the results of the first three years of the school and plans for the future.

1The MIPEP has been generously supported by the Mitchell Foundation.

9:48AM S4.00010 Engaging undergraduates in interdisciplinary science during a pre-orientation camp1. JENNIFER HEATH, CATHERINE REINKE, MICHAEL CROSSER, ANNE KRUCHTEN, Linfield College — The Interdisciplinary First-Year Orientation Camp for Undergraduate Sciences (iFOCUS) was created three years ago at Linfield College. Foremost, we looked to create a supportive community to enhance the recruitment, retention, and success of science students— all students, and especially students from non-traditional backgrounds. We saw the close knit community of athletes that came together during pre-orientation practices. Could a community of science students come together with similar enthusiasm and energy? And, we were also looking for a way to expose first year students to a scientific way of thinking, embracing open-ended, research oriented, interdisciplinary problems. After the camp is over, iFOCUS students frequently join faculty research laboratories, they draw in additional students to ongoing learning communities, and a seminar series brings in outside speakers. I will discuss the program initiatives and outcomes, which have been especially useful to physics—where building an enthusiastic peer network and addressing misconceptions about science in general, and physics in particular, seem to be especially useful.

1Supported by the Hearst Foundation

Thursday, March 5, 2015 8:00AM - 10:48AM
Session S5 DMP DCOMP: Focus Session: Spin Fluctuations and Pairing Symmetry in Fe-based Superconductors
Juan Gorman Room 005 - Wei-Cheng Lee, Binghamton University

8:00AM S5.00001 Study on the correlation between s± pairing and intra-orbital spin fluctuations in 1111 iron based superconductors with isovalent doping. HIDE TOMO USUI, KATSUHIRO SUZUKI, KAZUHIKO KUROKI, Department of Physics, Osaka University — Recently, 1111 iron based superconductors with isovalent doping have been experimentally investigated in LnFeAsO1−xFx (Ln=La, Nd, Pr) [1-4]. Interestingly, it was found that Tc takes its local maximum in the intermediate regime of arsenic/phosphorous ratio, which indicates that the superconductivity is locally optimized at a certain Fe-Pn-Fe (Pn=Pnictogen) bond angle larger than 109 deg. Given this background, we study the correlation between the local lattice structure, the orbital character of the Fermi surface, and Tc in 1111 system with isovalent doping. We calculate the band structure of LnFeAsO1−xFx and construct effective five orbital models. To our surprise, it is found that superconductivity is indeed locally optimized in the intermediate arsenic doping regime. The origin of this local optimization is traced back to the gradual variation of the orbital character and the density of states of the hole Fermi surfaces around the Γ point, which is controlled by the bond angle. The consistency with the experiment strongly indicates the importance of the spin fluctuation played in this series of superconductors.

8:12AM S5.00002 Observation of Momentum-Confined In-Gap Impurity State in Ba$_2$K$_2$Fe$_{2}As_2$: Evidence for Antiphase $s^\pm$ Pairing. PENG ZHANG, PIERRE RICHARD, TIAN QIAN, XUX SHI, JUN MA, LINGKUN ZENG, XIAOPING WANG, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, EMILE RIENKELS, Helmholtz-Zentrum Berlin, BESSY, CHENGLIN ZHANG, Department of Physics and Astronomy, Rice University, PENGCHENG DAI, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, YIZHUANG YOU, ZHENGYU WENG, Institute for Advanced Study, Tsinghua University, XIANXIN WU, JIANGPING HU, HONG DING, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences — We report the observation by angle-resolved photoemission spectroscopy of an impurity state located inside the superconducting gap of Ba$_2$K$_2$Fe$_{2}As_2$ and vanishing above the superconducting critical temperature, for which the spectral weight is confined in momentum space near the Fermi wave-vector positions. We demonstrate, supported by theoretical simulations, that this in-gap state originates from weak scattering between bands with opposite sign of the superconducting-gap phase. This weak scattering, likely due to off-plane nonmagnetic (Ba, K) disorder, occurs mostly among neighboring Fermi surfaces, suggesting that the superconducting-gap phase changes sign within holelike (and electronlike) bands. Our results impose severe restrictions on the models promoted to explain high-temperature superconductivity in these materials.

8:24AM S5.00003 Anisotropic staggered magnetization in electron-doped Fe-based superconductors , HONG-YI CHEN. National Taiwan Normal University, C.S. TING, University of Houston — Based upon a two-orbital model with competing collinear antiferromagnetism and $s^\pm$ pairing superconductivity, the electronic structures are investigated by solving Bogoliubov-de Gennes equations. Our results for the optimally electron-doped compound exhibit the anisotropic staggered magnetization. The Fourier transformation of the staggered magnetization shows two uneven peaks at $Q_1 = (\pi, 0)$ and $Q_2 = (0, \pi)$. The spatial variation of the $s^\pm$ pairing superconductivity and the electronic charge distribution show a checkerboard-like pattern with $C_2$ symmetry. Finally, in the calculation of the local density of states, we found that the anisotropic staggered magnetization does not open a gap. Our results are good in agreement with the recently reported experimental results.

8:36AM S5.00004 Enhanced spin fluctuations and $s^\pm$ pairing by diagonal electron hopping in Fe-based superconductors , KAZUHIKO KUROIKA, Dept. of Physics, Osaka University — In the itinerant spin picture of the iron-based superconductors, the nesting between electron and hole Fermi surfaces is usually considered to be the origin of the spin fluctuation and thus the pairing glue. However, there have appeared some experimental observations suggesting absence of Fermi surface nesting. For instance, in the 1111 materials $Ln$FeAsO$_{1-x}$F$_x$ (Ln=La,Sm, etc.) [1], electron doping rate $x$ reaches up to 0.5, which in a rigid band picture would wipe out the hole Fermi surfaces. Still, superconductivity not only survives, but is even enhanced in the largely doped regime, in contradiction to the expectation from the bad nesting. Another example is $K_xFe_{2−y}Se_y$, where the ARPES experiments show the absence of hole Fermi surfaces[2-5]. In the present talk, we first focus on $Ln$FeAsO$_{1-x}$F$_x$, where the band structure is actually not rigid against doping, and the hole Fermi surface originating from the d$_{xy}$ orbital remains unchanged. The origin of this can be traced back to real space, where the nearest neighbor hopping $t_1$ within the d$_{xy}$ orbital is found to be strongly suppressed with doping [6]. Although the nesting itself is degraded, the spin fluctuation in the largely electron doped regime is enhanced due to $t_2 > t_1$, where $t_2$ is the second neighbor diagonal hopping. This re-enhances $s^\pm$ pairing superconductivity, and explains the double dome $\Delta T_c$ phase diagram of LaFeAsO$_{1−x}$F$_x$ [1]. From this viewpoint, it is also interesting to look into the relation between $t_1$ and $t_2$ in other materials. For instance, our first principles estimation for $K_xFe_{2−y}Se_y$ gives $t_1 = −0.008$ eV and $t_2 = 0.056$ eV, and from this strong reduction of $t_1$, both electron and hole Fermi surfaces are expected to be present around the $\Gamma$ point, in contradiction to previous experimental observations. Results of a recent ARPES experiment will be discussed from this viewpoint. References [1] S. Iimura et al., Nat. Commun. 3, 943 (2012). [2] T. Qian et al., Phys. Rev. Lett. 106, 187001 (2011). [3] Y. Zhang et al., Nature Mat. 10, 273 (2011). [4] D. Mou et al., Phys. Rev. Lett. 106, 107001 (2011). [5] M. Yi et al., Phys. Rev. Lett. 110, 067003 (2013). [6] K. Suzuki et al., Phys. Rev. Lett. 113, 027002 (2014).

9:12AM S5.00005 Anomalous scaling behavior of the Specific Heat jump $\Delta C$ vs. $T_c$ in the Fe-based superconductors , YUNKYU BANG, Department of Physics, Chonnam National University, Kwangju 500-757, Korea, G.R. STEWART, Physics Department, University of Florida, Gainesville, FL 32611-8440 — So called BNC scaling ($\Delta C \propto T_c$) has been observed in a wide range of the Fe-based superconducting compounds such as Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$, Ba(Fe$_{1-x}$Ni$_x$)$_2$As$_2$, BaFe$_2$As$_2$ and Ba$_2$Fe$_4$As$_2$. More recently, however, Canfield and coworkers reported that the Ba$_2$K$_2$Fe$_{2}As_2$ compound severely deviates from this scaling when $x>0.7$ and argued that this is an indication of the Lifshitz transition in the Ba$_2$K$_2$Fe$_{2}As_2$ compound at higher hole doping. In this presentation, we propose a theory that the BNC scaling as well as its strong deviation, as observed in Ba$_2$K$_2$Fe$_{2}As_2$, is an intrinsic property of the multiband superconductor mediated by a dominant interband pairing potential as realized in the sign-changing S-wave state.

9:24AM S5.00006 The effects of Coulomb interactions on the superconducting gaps in iron-based superconductors , ZHIDONG LEONG, PHILIP PHILLIPS, University of Illinois at Urbana-Champaign — Recent ARPES measurements on Co-doped LiFeAs report a large and robust superconducting gap on a band below the chemical potential. We will show that, unlike a conventional BCS theory, a multiband system with strong interband Coulomb interactions can explain the observations. We use a two-band model consisting of a superconducting electron band and a hole band that is below the chemical potential. The two bands are coupled via interband Coulomb interactions. Using Eliashberg theory, we found that superconductivity in the electron band induces a large superconducting gap in the hole band. Furthermore, the repulsive nature of the Coulomb interactions gives the induced gap an opposite sign, corresponding to an $s^\pm$ gap symmetry. Unlike other families of iron pnictides, the gap symmetry of LiFeAs has not been ascertained experimentally. The implications for the mechanism of pinning in iron pnictides will be discussed.

Z. Leong is supported by a scholarship from the Agency of Science, Technology and Research. P. Phillips is supported by the Center for Emergent Superconductivity, a DOE Energy Frontier Research Center, Grant No. DE-AC0298CH1088.

9:36AM S5.00007 Doping-induced crossover of the pairing symmetry in iron- pnictide superconductors , MAHMoud ABDEL-HAFIEZ, ZHENG HE, Center for High Pressure Science and Technology Advanced Research, Shanghai, 201203, China, XINGYE LU, HUIQIAN LUO, PENGCHENG DAI, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, XIAO-JIA CHEN, Center for High Pressure Science and Technology Advanced Research, Shanghai, 201203, China, HPSTAR TEAM, CHINESE ACADEMY OF SCIENCES TEAM — Iron pnictides present a rich phase diagram and superconductivity coexists and competes with the spin density wave and the nematic order, giving unconventional pairing mechanisms. Although various efforts have put forth to clarify pairing symmetry of the Cooper pair, experimental confirmations of the precise symmetry of the superconducting (SC) order parameter and its evolution with doping remains highly controversial. Here we present the investigation results of the low-temperature specific heat down to 70 mK for high-quality BaFe$_{2−x}$Ni$_x$As$_2$ single crystals. For $x \leq 0.12$, the temperature dependence of the SC-state specific heat provides strong evidence for a two-band $s$-wave order parameter. Upon doping for $x \geq 0.15$, we find the temperature and magnetic field contributions to the specific heat in $T^2$ and $H^2$ respectively, which strongly indicate the nodes in the SC gap.
9:48AM S5.00008 Leggett modes and vortex dynamics in time-reversal symmetry breaking multiband superconductors , MIKHAIL SILAEV, EGOR BABAЕV, The Royal Institute of Technology, Stockholm, Sweden — In the framework of quasiclassical kinetic theory we study the spectrum of collective excitations and vortex dynamics in multiband superconductors. We show that the existence of mixed phase-density modes in multiband superconductors with broken time-reversal symmetry generates a new contribution to the viscosity of magnetic flux flow. Near the time reversal symmetry breaking phase transition this new contribution dominates over the usual Tinkham and Bardeen-Stephen mechanisms and provides a peculiar temperature dependence of the vortex viscosity. The results could be relevant for three band superconductor Ba$_{1-x}$K$_x$Fe$_2$As$_2$.

10:00AM S5.00009 Spontaneous currents in a superconductor with s+is symmetry , MANFRED SIGRIST, Institut fur Theoretische Physik, ETH Zurich, SAURABH MAITI, University of Florida and NHMFL, ANDREY CHUBUKOV, William I. Fine Theoretical Physics Institute, and School of Physics and Astronomy, University of Minnesota — We analyze s+ıs state proposed as a candidate superconducting state for strongly hole-doped Ba-122. Such a state breaks time-reversal symmetry (TRS) but does not break any other discrete symmetry. We address the issue whether TRS breaking alone can generate spontaneous currents near impurity sites, which could be detected in, e.g., 7SR experiments. We argue that there are no spontaneous currents if only TRS is broken. However, supercurrents do emerge if the system is put under external strain and C4 lattice rotation symmetry is externally broken.

10:12AM S5.00010 Gap structure in Fe-based superconductors with accidental nodes , ALBERTO HINOJOSA ALVARADO, ANDREY CHUBUKOV, University of Minnesota Twin Cities — We study Fe-based superconductors with s-symmetry and accidental gap nodes on electron pockets. We consider ellipticity, hybridization and an additional inter-pocket pairing interaction and analyze their effect on the gap structure and on the existence of nodal points in the quasiparticle dispersions. Depending on these parameters the gap functions at the Fermi surface may be uniform, have nodal points, or vary their phase continuously. In the quasiparticle dispersions, there exist nodal points only if the phase difference between the hybridization and inter-pocket pairing parameters is a multiple of $\pi/2$. The two parameters tend to shift the position of the nodes in the same or in opposite directions depending on their relative phases. When the parameters reach a critical value the nodes disappear.

10:24AM S5.00011 Glide plane symmetry and gap structure in the iron-based superconductors , YAN WANG, Department of Physics, University of Florida, TOM BERLJIN, Oak Ridge National Laboratory, PETER HIRSCHFELD, Department of Physics, University of Florida, DOUGLAS SCALAPINO, Department of Physics, University of California, Santa Barbara, THOMAS MAIER, Oak Ridge National Laboratory — We consider the effect of glide plane symmetry of the Fe-pnictogen/chalcogen layer in Fe-based superconductors for pairing in spin fluctuation models. Recent theories have proposed that so-called $\eta$-pairing states with nonzero total momentum can be realized and possess exotic properties such as odd parity spin singlet symmetry and time-reversal symmetry breaking. Here we show that $\eta$-pairing is inevitable when the orbital level from orbitals with even and odd mirror reflection symmetry in $z$; however, by explicit calculation, we conclude that the gap function that appears in observable quantities is identical to that found in earlier, 1 Fe per unit cell pseudo-crystal momentum calculations. P.J.H. and Y.W. were supported by Grant No. DOE DE-FG02-05ER46236 and T.B. was supported as a Wigner Fellow at the Oak Ridge National Laboratory. A portion of this research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, US Department of Energy.

10:36AM S5.00012 Enhanced $s^\pm$ pairing due to prioritized diagonal motion of electrons in the iron-based superconductors , KAZUHIKO KUROKI, KATSUHIRO SUZUKI, HIDETOMO USUI, Osaka University — In the itinerant spin picture of the iron-based superconductors, the nesting between electron and hole Fermi surfaces is usually considered to be the origin of the spin fluctuation. However, there are now some experimental results suggesting that the nesting is not important for superconductivity. An example is the 1111 materials LnFeAsO$_{1-x}$F$_x$ (Ln=La,Sm etc.), where over 50% of electron doping can be accomplished. Superconductivity not only survives, but is even enhanced in the largely electron-doped regime, in contradiction to the expectation from the bad nesting. In La$_2$FeAsO$_{1-x}$F$_x$ in particular, the $x$ vs. $T_c$ phase diagram exhibits a double dome feature, suggesting a possible difference in the pairing mechanism between the lightly doped and the heavily doped regimes. In the present study, we analyze the five orbital model of this system, and show that a peculiar relation among the real space hoppings is realized in the largely electron-doped regime, namely, the next nearest neighbor hopping dominates over the nearest one within the $d_{xy}$ orbitals. We argue that this enhances the $s^\pm$ pairing, which is a next nearest neighbor pairing in real space, despite the degraded nesting. We also discuss about some other materials having similar real space hoppings.
8:36AM S6.00002 Surface plasmon decay dynamics in nanostructured systems: A Feynman diagram approach1, PRINEHA NARANG, RAVISHANKAR SUNDARARAMAN, ADAM S. JERMYN, WILLIAM A. GODDARD III, HARRY A. ATWATER, California Institute of Technology, (Caltech) — The decay of surface plasmon resonances is usually a detriment in the field of plasmonics, but the possibility to capture the energy normally lost to heat would open new opportunities in photon sensors and energy conversion devices. In the context of hot-electron devices, the large extinction cross-section at a surface plasmon resonance enables nanostructures to absorb a significant fraction of the solar spectrum in very thin films. Despite the significant experimental work in this direction, a complete theoretical understanding of plasmon-driven hot carrier generation with electronic structure details has been evasive. Recently we analyzed the quantum decay of surface plasmon polaritons and found that the prompt distribution of generated carriers is extremely sensitive to the energy band structure of the plasmonic material. In this context, we use a Feynman diagram approach to describe processes involving plasmons, electrons and phonons in plasmonic hot carrier generation. Built upon this general theoretical and computational framework, we present results on higher order processes such as multi-plasmon decays in metals which are critical for plasmon-driven upconversion.

3Join Center for Artificial Photosynthesis, California Institute of Technology

8:48AM S6.00003 Photonic pulling force in one-way waveguides, DANLU WANG, Univ of Texas, Austin, Department of Physics, CHENGWEI QIU, National University of Singapore, Department of Electrical and Computer Engineering, PETER RAKICH, Yale University, Department of Applied Physics, ZHENG WANG, Univ of Texas, Austin, Department of Electrical and Computer Engineering — Light can apply pulling force on dielectric particles through forward scattering, i.e., scattering that increases photon momentum. The forward scattering typically requires conditions in free space, e.g., large incident angle, excitation of dipole-quadrupole interaction on spherically shaped particles. Here we demonstrate photonic pulling forces on dielectric particles in photonic crystal defect waveguides supporting one-way chiral edge modes. Intuitively, momentum discrepancy between two co-existing one-way modes facilitate forward scattering on arbitrarily configured particles inside the waveguide, over a broad frequency range, upon proper choice of incident mode. The pulling forces are also topologically protected against bending of the waveguide. Moreover, we rigorously relates the direction and amplitude of photonic forces to the phase response of output modes versus the particle’s displacement. While the phase response of output modes is determined by wave functions of the involved modes.

9:00AM S6.00004 PT symmetry in optics, DEMETRIOS CHRISTODOUIDES, CREOL, The College of Optics and Photonics, University of Central Florida — Interest in complex Hamiltonians has been rekindled after the realization that a wide class of non-Hermitian Hamiltonians can have entirely real spectra as long as they simultaneously respect parity and time reversal operators. In non-relativistic quantum mechanics, governed by the Schrödinger equation, a necessary but not sufficient condition for PT symmetry to hold is that the complex potential should involve real and imaginary parts which are even and odd functions of position respectively. As recently indicated, optical systems observe the same conditions in free space, e.g., large incident angle, excitation of dipole-quadrupole interaction on spherically shaped particles. Here we demonstrate photonic pulling forces on dielectric particles in photonic crystal defect waveguides supporting one-way chiral edge modes. Intuitively, momentum discrepancy between two co-existing one-way modes facilitate forward scattering on arbitrarily configured particles inside the waveguide, over a broad frequency range, upon proper choice of incident mode. The pulling forces are also topologically protected against bending of the waveguide. Moreover, we rigorously relates the direction and amplitude of photonic forces to the phase response of output modes versus the particle’s displacement. While the phase response of output modes is determined by wave functions of the involved modes.

9:36AM S6.00005 Parity-Time Symmetric Nonlocal Metamaterials for Focusing and Image Processing, FRANCESCO MONTICONE, The University of Texas at Austin, CONSTANTINOS VALAGIANOPoulos, Aalto University, Finland, SILVIO SAVOIA, University of Sannio, Italy, ROMAIN FLEURY, ANDREA ALU, The University of Texas at Austin — Parity-Time (PT) symmetry refers to the invariance of a physical system upon reflection of space and time. An intriguing property of PT-symmetric quantum systems is the fact that they can have entirely real eigenvalue spectra, despite being non-Hermitian. Although the application of these concepts in quantum mechanics remains speculative, in classical optics non-Hermitian PT-symmetric systems can be readily realized with spatially balanced gain and loss. These systems have been shown to exhibit exotic responses, e.g., unidirectional invisibility, or anomalous scattering. Recently, negative refraction and planar focusing have been achieved by pairing a perfectly coherent absorbing metasurface with its time-reversed counterpart, i.e., a coherently lasing metasurface. Here, we generalize this idea to any pair of PT-symmetric structures, characterized by their scattering matrix, to put forward a realistic venue to PT-symmetric metamaterials for imaging. This approach allows us to design realistic structures based, e.g., on multilayered slabs, which implement the necessary nonlocality and spatial dispersion to achieve ideal all-angle negative refraction and planar focusing. We will also discuss how these concepts may realize arbitrary magnifying, focusing and image processing systems.

9:48AM S6.00006 Single-mode laser by parity-time symmetry breaking, LIANG FENG, NSF Nanoscale Science and Engineering Center, UC Berkeley and Department of Electrical Engineering, SUNY Buffalo, ZI JING WONG, NSF Nanoscale Science and Engineering Center, UC Berkeley, REN-MIN MA, NSF Nanoscale Science and Engineering Center, UC Berkeley and Department of Physics, Peking University, YUAN WANG, XIANG ZHANG, NSF Nanoscale Science and Engineering Center, UC Berkeley — Effective manipulation of cavity resonant modes is crucial for emission control in laser physics and applications. Using the concept of parity-time symmetry to exploit the interplay between gain and loss (i.e. light amplification and absorption), we demonstrate a parity-time synthetic laser with resonant modes that can be controlled at will. In contrast to conventional ring cavity lasers with multiple competing modes, our parity-time microring lasers exhibit robust broadband single-mode lasing regardless of the gain spectral bandwidth. Thresholdless parity-time symmetry breaking due to the rotationally symmetric structure leads to stable single-mode operation with the selective whispering-gallery mode order. Exploration of parity-time symmetry in laser physics may develop a new paradigm of strategically utilizing optical losses and open a door to next-generation optoelectronic devices for optical communications and computing.

1Support by the Office of Naval Research (ONR) MURI program under grant no. N00014-13-1-0649.

10:00AM S6.00007 Hybrid chiral metamaterials by dynamic shadowing growth, JOHN GIBBS, Northern Arizona University, PEER FISCHER, ANDREW MARK, SAHAND ESLAMI, TUNG-CHUN LEE, Max Planck Institute for Intelligent Systems — Coupling optical and magnetic properties is possible in hybrid and in higher-order magnetic field induced optical activities. Here, we show that these two mechanisms can be combined in nanostructures that are simultaneously ferromagnetic, chiral, and plasmonically resonant. In this talk, a short description of the fabrication of optically active helical metamaterials will first be given, followed by the highlighting of the materials’ enhanced optical properties. Giant circular dichroism (CD) and optical rotatory dispersion (ORD) in the visible arise from helical plasmonic modes within the individual structures and can be tuned by altering the material composition, i.e. nanolayers or nanocomposites, and/or by changing the structures’ morphologies. By fabricating metamaterials which exhibit both strong CD and are ferromagnetic at room temperature, higher order terms in the generalized dielectric function in the presence of a B-field can be measured easily. In particular, magnetochiral dichroism (MChD) is a cross-term between chirality and an applied external B-field which has only been measured in crystals and molecules, but never in a metamaterial. We show that arrays of helical Ni nanostructures, due to the plasmonic nature of Ni, their chirality, as well as the fact they retain their ferromagnetism even at scales comparable to the average ferromagnetic domain size, exhibit an MChD signal that is much more pronounced in a metamaterial and can therefore be easily measured in the laboratory.
10:12AM S6.00008 Chiral Quantum Dots¹, MILAN BALAZ, University of Wyoming, Department of Chemistry, Laramie, WY, USA — Chiral optically active semiconductor quantum dots (chiral QDs) represent appealing building blocks for assembly of nanomaterials with modular structural, electronic and optical properties. Chirality in QDs can originate from several distinct phenomena that can concurrently modulate the observed chiroptical and optical properties (e.g. chiral surface, orbital hybridization). We will use our experimental and theoretical data to elaborate on the origin of capping ligand induced chirality in achiral colloidal QDs [1]. We will present a simple method to prepare chiral QDs by post-synthetic chiral ligand functionalization of achiral QDs. Importantly, capping ligands can be used not only to induce but also to control chiroptical activity of QDs. Enantiomers of chiral ligands induce mirror-image chirality in QDs, and chiroptical properties of QDs can be further modulated by the chemical structure of capping ligands as well as the size of QDs.


¹This work was supported by U.S. Department of Energy (award DE-FG02-10ER46728), National Science Foundation (awards CBET-1403947 and DGE-0948027) and University of Wyoming.

10:24AM S6.00009 Generating Optical Vortex Arrays with Rectangular Hole Arrays¹, MIAO JIANG, Liquid Crystal Institute, Kent State Univ, Kent, OH, YU-BING GUO, Kent State Univ - Kent, QI-HUO WEI, Liquid Crystal Institute, Kent State Univ, Kent, OH — Paraxial optical beams are known to carry angular momentums which contain both spin and orbital components. Light carrying orbital angular momentum promise applications in information transfer and new spinoptic devices. In this paper we study optical transmission through rectangular hole arrays in metal films, and discuss their interactions with the angular momentum of light and applications in the generations of optical vortex arrays with different topological charges.

¹Work supported by NSF CMMI-1436565

10:36AM S6.00010 Manipulating the polarization state of light with a metallic stereostructured layer, XIANG XIONG, SHANG-CHI JIANG, YUAN-SHENG HU, MU WANG, RU-WEN PENG, Nanjing University — Without introducing dielectric material, we report here for the first time a wave plate constructed merely by metallic stereostructured layer. With an assembly of metallic L-shaped stereostructures (LSSs), the polarization state of the reflected light can be freely manipulated within a broad frequency band. The amplitude ratio of light in two orthogonal directions and the phase difference in these two directions can be tuned accurately and independently. We suggest that our design provides a new approach in realizing broadband wave plate device to manipulate the polarization state of light.

10:48AM S6.00011 Polarisation singularities in photonic crystals for an on-chip spin-photon interface, DARYL M. BEGGS, ANDREW B. YOUNG, ARTHUR C. T. THIJSSEN, RUTH OULTON, University of Bristol — Integrated quantum photonic chips are a leading contender for future quantum technologies, which aim to use the entanglement and superposition properties of quantum physics to speed up the manipulation of data. Quantum information may be stored and transmitted in photons, which make excellent flying qubits. Photons suffer little from decoherence, and single qubit gates performed by changing photon phase, are straightforward. Less straightforward is the ability to create two qubit gates, where one photon is used to switch another’s state; inherently difficult due to the extremely small interaction cross-section between photons. The required deterministic two-qubit interactions will likely need a hybrid scheme with the “flying” photonic qubit interacting with a “static” matter qubit. Here we present the design of a photonic crystal waveguide structure that can couple electron-spin to photon path, thus providing an interface between a static and a flying qubit. We will show that the complex polarization properties inherent in the photonic crystal eigenmodes supports polarization singularities – positions in the electric field vector where one of the parameters describing the local polarization ellipse is singular – and that these singularities are ideal for a range of quantum information applications. In particular, we will show that by placing a quantum dot at one of these singularities, the electron-spin becomes correlated with the photon emission direction, creating an in-plane spin-photon interface that can transfer quantum information from static to flying qubits.

Thursday, March 5, 2015 8:00AM - 11:00AM – Session S7 DMP DCMP: Focus Session: Dirac & Weyl Semimetals 006B - Madhab Neupane, Princeton University

8:00AM S7.00001 Prediction of a strain-tunable 2D Topological Dirac semimetal in monolayers of black phosphorus, XIUWEN ZHANG, QIHANG LIU, ALEX ZUNGER, University of Colorado, Boulder, THEORY TEAM — N-dimensional Topological Nonmetals (TMN) such as N = 2D HgTe/CdTe quantum wells or N = 3D Bi2Se3 have a finite (often tiny) band gap between occupied and unoccupied bands, and show conductive Dirac cones in their N-1 dimensional geometric boundaries. On the other hand, examples of topological semimetals (TSM) are known for 3D solids (Cd3As2) where they have Dirac cones in the 3D system itself. Using density functional calculation of bands and the topological invariant Z2, we predict the existence of 2D topological Dirac semimetal in few monolayers of strain tuned black phosphorus (BP), with Dirac cones induced by band inversion. The band structures of few monolayers and bulk crystal of BP under a few percent biaxial and uniaxial strains were calculated using state-of-art electronic structure methods. The critical strain of the transition to TSM was found to decrease as the layer thickness increases. We will discuss the protection of the Dirac cones by the crystalline symmetry in the 2D TSM and the manipulation of crystalline symmetry, which induces further topological phase transitions. Supported by the NSF-DMREF-13-34170.

8:12AM S7.00002 Interaction effects of a topological Dirac semimetal Na3Bi, RUIXING ZHANG, The Pennsylvania State University, JIMMY HUTASOIT, Leiden University, CHAOXING LIU, The Pennsylvania State University — We study the interaction effects of a topological Dirac semimetal Na3Bi based on the mean field theory. The phase diagram can be classified by two kinds of chiral-symmetry-breaking order parameters: nematic orders that break rotational symmetry and charge-density-wave (CDW) order that break translational symmetry. Under strong magnetic field, gapless Landau levels will be formed and result in stabilities due to the above order parameters. These order parameters are generally complex, and are identified as complex mass terms, which introduce axioms into the low energy theory. The possible experimental consequence is also studied.
8:24AM S7.00003 Density of states and transport in Weyl semimetals with long-range disorder1
, DMYTRO PESIN, University of Utah, Salt Lake City, UT, ALEX LEVCHENKO, Michigan State University, East Lansing, MI — We consider the density of states in a Weyl semimetal with long-range Coulomb impurities. We show that at energies close to the nodal point the motion of electrons is essentially classical, and compute the density of states at low energies for the cases of self-consistent screening, and screening by non-Weyl bands. As an alternative to the recent renormalization-group calculations, we develop a diagrammatic technique that is capable of capturing quantum corrections to the classical result, and determine the applicability range of the classical treatment, as well as the energy dependence of the density of states away from the nodal points. Finally, the obtained results are contrasted with those obtained from the self-consistent Born approximation, and the implications for the electrical, thermal and thermomagnetic transport properties of the Weyl semimetal are discussed.

1The work at the University of Utah is supported by NSF Grant No. DMR-1409089, the work at MSU is supported by NSF Grant No. DMR-1401908

8:36AM S7.00004 Theory of Symmetry Protected 2D Dirac Semimetals and Derivative Topological States , STEVE YOUNG, Center for Computational Materials Science, Naval Research Laboratory, CHARLES KANE, Department of Physics, University of Pennsylvania — We present the theory of symmetry-protected 2D Dirac semimetals. These systems are distinguished from graphene by the presence of spin-orbit coupling, under which the latter becomes a quantum spin hall insulator. 2D Dirac semimetals exhibit behavior distinct from both graphene and their three-dimensional counterparts. We discuss the symmetry requirements for such systems, and using the simplest tight-binding model satisfying them, describe their properties, as well as the states that result from relaxing various constraints, including Weyl semimetal and topological insulator states. Additionally, we provide suggestions for realizing these systems based on Density Functional Theory calculations.

8:48AM S7.00005 Thermoelectric properties of Weyl and Dirac semimetals , PONTUS LAURELL, REX LUNDGREN, GREGORY FIETE, University of Texas at Austin — We study the electronic contribution to the thermal conductivity and the thermopower of Weyl and Dirac semimetals using a semiclassical Boltzmann approach. We investigate the effect of various relaxation processes including disorder and interactions on the thermoelectric properties, and also consider doping away from the Weyl or Dirac point. We find that the thermal conductivity and thermopower have a dependence on the chemical potential that is characteristic of the linear electronic dispersion, and the electron-electron interactions modify the Lorenz number. For the interacting system, we also use the Kubo formalism to obtain the transport coefficients, finding exact agreement with the Boltzmann approach at high temperatures. We also consider the effect of electric and magnetic fields on the thermal conductivity in various orientations with respect to the temperature gradient. Notably, when the temperature gradient and magnetic field are parallel, we find a large contribution to the longitudinal thermal conductivity that is quadratic in the magnetic field strength, similar to the magnetic field dependence of the longitudinal electrical conductivity due to the presence of the chiral anomaly when no thermal gradient is present.

9:00AM S7.00006 Kondo effect and non-Fermi liquid behavior in Dirac and Weyl semimetals , E. ROSSI, Physics Department, College of William and Mary, ALESSANDRO PRINCIPI, GIOVANNI VIGNALE, Physics Department, University of Missouri — We study the Kondo effect in three-dimensional (3D) Dirac materials and Weyl semimetals [1]. We find the scaling of the Kondo temperature with respect to the doping n and the coupling J between the moment of the magnetic impurity and the carriers of the semimetal. We find that when the temperature is much smaller than the Kondo temperature the resistivity due to the Kondo effect scales as the n to the -4/3. We also study the effect of the interplay of long-range scalar disorder and Kondo effect. In the presence of disorder-induced long-range carrier density inhomogeneities the Kondo effect is not characterized by a Kondo temperature but by a distribution of Kondo temperatures. We obtain the expression of such distribution and show that its features cause the appearance of strong non-Fermi liquid behavior. Finally we compare the properties of the Kondo effect in 3D Dirac materials and 2D Dirac systems like graphene and topological insulators.

Work supported by ONR-N00014-13-1-0321.

9:12AM S7.00007 Visualizing the Electronic Structure of Topological Dirac Semimetals , YULIN CHEN, Oxford University — Three-dimensional (3D) topological Dirac semimetals (TDSs) represent an unusual state of quantum matter that can be viewed as “3D graphene.” In contrast to 2D Dirac fermions in graphene or on the surface of 3D topological insulators, TDSs possess 3D Dirac fermions in the bulk. Moreover, a TDS can potentially be driven into other exotic phases (such as Weyl semimetals, axion insulators or topological superconductors), making it a unique parent compound for the study of these states and the phase transitions between them. By investigating the electronic structure of Na3Bi and Cd3As2 with angle-resolved photoemission spectroscopy including kz information, we discovered bulk (3D) Dirac fermions with linear dispersions along all three momentum directions in both materials. Furthermore, we can demonstrate the robustness of these 3D Dirac fermions against in situ surface doping, showing the protection of the bulk crystal symmetry. These findings establish both materials as model systems of 3D TDSs, which can also serve as ideal platforms for exploring exotic physical phenomena and novel applications.

9:48AM S7.00008 Tendency to Localization in Interacting Weyl Semimetals1, HAIZHOU LU, SHUNQING SHEN, The Univ of Hong Kong — Weyl semimetals are novel topological states of quantum matter, in which electrons or Weyl fermions are robust against impurity or disorder, and tend to be delocalized. In a weak external magnetic field, a negative magnetoconductivity is found to be proportional to the square root of magnetic field at low temperatures, giving the signature of the delocalization. However, here we demonstrate that the metallic and delocalization behavior of Weyl semimetals can be sabotaged by electron-electron interaction and inter-valley effects. An “insulating” tendency is therefore illustrated in disordered and interacting Weyl semimetals. Reference: Hai-Zhou Lu and Shun-Qing Shen, arXiv:1411.2686

1This work was supported by Research Grants Council, University Grants Committee, Hong Kong, under Grant No. 17303714.

10:00AM S7.00009 Topological Imbert-Fedorov shift in Weyl semimetals , QING-DONG JIANG, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China, HUA JIANG, College of Physics, Optoelectronics and Energy, Soochow University, Suzhou 215006, China, HAIWEN LIU, QING-FENG SUN, X.C. XIE, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China — When a beam of light (photons) is reflected at an interface, the wave nature of photons can result in spatial shifts at the interface in the plane of incidence (longitudinal shift) and normal to the plane (transverse shift), which are referred as Goos-Hänchen (GH) shift and Imbert-Fedorov (IF) shift, respectively. As the massless fermionic cousin of photons, Weyl fermions are expected to share certain similar characteristics as photons. Here, we report the GH and IF effects in Weyl semimetals—a promising material harboring low energy Weyl fermions. Our results show that GH effect in WSMs is analogous to that discovered in a 2D relativistic material—graphene; however, the IF effect has no 2D counterpart, since it is genuinely a 3D effect. We emphasize that the IF shift actually originates from the topological effect of the systems, and can further lead to valley-dependent anomalous velocities. Experimentally, topological related IF shift can be utilized to characterize the Weyl semimetals and further to measure the Berry curvature. The valley-dependent anomalous velocities provide new ways for designing valleytronic devices of high efficiency.
10:12AM S7.00010 Chiral Anomaly and Diffusive Magnetotransport in Weyl Metals

ANTON BURKOV, University of Waterloo — We present a microscopic theory of diffusive magnetotransport in Weyl metals and clarify its relation to chiral anomaly. We derive coupled diffusion equations for the total and axial charge densities and show that chiral anomaly manifests as a magnetic-field-induced coupling between them. We demonstrate that a universal experimentally-observable consequence of this coupling in magnetotransport in Weyl metals is a quadratic negative magnetoresistance, which will dominate all other contributions to magnetoresistance under certain conditions.

10:24AM S7.00011 Plasmon mode as a detection of the chiral anomaly in 3D Weyl semimetals

JIANHUI ZHOU, Carnegie Mellon Univ, HAORAN CHANG, Sichuan Normal University, Chengdu, China, DI XIAO, Carnegie Mellon Univ — Weyl semimetals (WSMs) are one kind of three-dimensional gapless SMs with nontrivial topology in the momentum space. The chiral anomaly in Weyl SMs manifests as a charge imbalance between the Weyl modes of opposite chiralities induced by parallel electric and magnetic fields. We investigate the chiral anomaly effect on the plasmon mode in Weyl SMs within the RPA. We prove that the chiral anomaly gives rise to a new plasmon mode in intrinsic Weyl SMs. The chiral anomaly leads to some exotic properties in the plasmon dispersion in doped Weyl SMs. Consequently, the unconventional plasmon mode acts as a signature of the chiral anomaly in Weyl SMs, by which the spectrum of plasmon provides a proper way to detect the Lifshitz transition. Our work sheds light on the probing of the chiral anomaly in 3D Weyl SMs via the plasmon mode. The tunability of plasmons due to the chiral anomaly also makes Weyl SMs promising candidates for plasmonics. Reference: arXiv:1408.4876

1 NSF EFRI (No. 1434946), SRF of the Education Department of Sichuan Province under Grant No. 13ZB0157, the NSFC (Nos. 11074234, 11274286).

10:36AM S7.00012 Terahertz conductivity study of predicted Weyl semimetal Nd$_3$Ir$_2$O$_7$ and Eu$_2$Ir$_2$O$_7$ thin films

MATTHEW T. WARREN, J.C. GALLAGHER, T.T. MAI, J. BRANCHAM, F. YANG, Center for Emergent Materials, Department of Physics. The Ohio State University. Columbus, OH 43210, C.M. MORRIS, N.P. ARMITAGE, Department of Physics & Astronomy, The Johns Hopkins University, R. VALDES AGUILAR, Center for Emergent Materials, Department of Physics. The Ohio State University. Columbus, OH 43210 — There is currently a growing interest in identifying materials with novel topological properties outside of the s- or p-orbital based bismuth chalcogenide topological insulators. One such proposal is the pyrochlore iridate materials $R$$_2$Ir$_2$O$_7$, where $R$ is a lanthanide series atom or yttrium. These have been predicted to be Weyl semimetals, containing exotic Fermi arc surface states and also an anomalous Hall effect. We have studied the temperature dependent terahertz conductivity of thin films of Nd$_3$Ir$_2$O$_7$ and Eu$_2$Ir$_2$O$_7$ grown by a novel off-axis sputtering technique. We find a close correspondence between DC transport properties and the extracted Drude parameters from fits to the THz conductivity. We will discuss these results in light of the predicted Weyl semimetal state of these materials.

1 Work at OSU supported by the NSF MRSEC Center for Emergent Materials under grant DMR-1420451. Work at JHU supported by the Gordon and Betty Moore Foundation (GBMF2628).

10:48AM S7.00013 Coulomb disorder in three-dimensional Dirac materials

BRIAN SKINNER, Argonne National Laboratory — In three-dimensional materials with a Dirac spectrum, weak short-ranged disorder is essentially irrelevant near the Dirac point. This is manifestly not the case for Coulomb disorder, where the long-ranged nature of the potential produced by charged impurities implies large fluctuations of the disorder potential even when impurities are sparse, and these fluctuations are screened by the formation of electron/hole puddles. Here I outline a theory of such nonlinear screening of Coulomb disorder in three-dimensional Dirac systems, and present results for the typical magnitude of the disorder potential, the corresponding density of states, and the size and density of electron/hole puddles. The resulting conductivity is also discussed.

Thursday, March 5, 2015 8:00AM - 11:00AM –
Session S8 GSOFT: Disordered and Glassy Systems

8:00AM S8.00001 Network structure of the mussel plaque and its significance for load bearing and adhesion

EMMANOUELA FILIPPIDI, JUNTAE KIM, J. HERBERT WAITE, MATTHEW HELGESON, MEGAN T. VALENTINE, University of California, Santa Barbara — Marine mussels attach to rocks, each other, and a variety of surfaces via a flat, wide plaque that is interpenetrated by the collagen fibers of a thin, long thread that connects the plaque to the mussel body. The unusually strong adhesion of the plaque has long been attributed to the molecular design of its adhesive proteins that can form a variety of strong chemical bonds. However, the molecular energies for de-adhesion are orders of magnitude smaller than the macroscopic energies measured. We propose that the mesoscopic design of the plaque is critical in enhancing load bearing and eventually adhesion. We present new results on the structure of the plaque studied via electron microscopy and neutron scattering that exhibit a plaque geometry reminiscent of structural foams. Our studies reveal a collection of pores with an inner network, further connected with an outer network. The final structure can be described by two length scales. A synthetic soft system is constructed in an effort to mimic the two-lengthscale structure of the natural plaques. The structure of the native and synthetic systems is compared with the ultimate goal of evaluating the importance of the mesoscopic structure to mechanics and adhesion.

1 NSF MRSEC IRG-1

8:12AM S8.00002 Collapse dynamics of bubble raft under compression

CHIN-CHANG KUO, Department of Physics and Astronomy, University of California, Irvine, DEVIN KACHAN, ALEXANDER LEVINE, Department of Physics and Astronomy, University of California, Los Angeles, MICHAEL DENNIN, Department of Physics and Astronomy, University of California, Irvine, DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF CALIFORNIA, IRVINE COLLABORATION, DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF CALIFORNIA, LOS ANGELES COLLABORATION — We report on the collapse of bubble rafts under compression in a closed rectangular geometry. A bubble raft is a single layer of bubbles at the air-water interface. A collapse event occurs when bubbles submerge beneath the neighboring bubbles under applied compression causing the structure of the bubble raft to go from single-layer to multi-layer. We studied the collapse dynamics as a function of compression velocity. At higher compression velocity we observe a more uniform distribution of collapse events, whereas at lower compression velocities, the collapse events accumulate at the system boundaries. We will present results that compare the distribution of collapse probability in the experiments to simulations based on a one-dimensional Ising model with elastic coupling between spin elements. Both the experimental system and simulations are excellent models for collapse in a number of complex systems. By comparing the two systems, we can tune the simulation to better understand the role of the Ising and elastic couplings in determining the collapse dynamics.

1 We acknowledge DMR-1309102
The glass-forming ability of patchy repulsive spheres requires a repulsive sphere model that includes attractive interactions between patches on each sphere to study the glass-forming ability of alloys that include non-metallic components (e.g. metal-metalloid alloys). Using molecular dynamics simulations, we quantify the GFA by measuring the critical cooling rate below which crystallization occurs as a function of the size and spacing of the patches, as well as the symmetry of the crystalline state that competes with the glass. We find that the glasses can arrest no more than 20-30% solute nonmetallic atoms (such as B, Si, and P), which explains why non-metallic elements occur at low number fractions in BMGs.

1 National Science Foundation (NSF) MRSEC Grant No. DMR-1119826

8:36AM S8.00004 Some observations on hyperuniform disordered photonic bandgap materials, from microwave scale study to infrared scale study1, SAM TSITRIN, GEEV NAHAL, San Francisco State University, MARIAN FLORESCU, University of Surrey, UK, WEINING MAN, San Francisco State University, SAN FRANCISCO STATE UNIVERSITY TEAM, UNIVERSITY OF SURREY TEAM — A novel class of disordered photonic materials, hyperuniform disordered solids (HUDDS), attracted more attention. Recently they have been experimentally proven to provide complete photonic band gap (PBG) when made with Alumina or Si; as well as single-polarization PBG when made with plastic with refract index of 1.6. These PBGs were shown to be real energy gaps with zero density of photonic states, instead of mobility gaps of low transmission due to scattering, etc. Using cm-scale samples and microwave experiments, we reveal the nature of photonic modes existing in these disordered materials by analyzing phase delay and mapping field distribution profile inside them. We also show how to extend the proof-of-concept microwave studies of these materials to proof-of-scale studies for real applications, by designing and fabricating these disordered photonic materials at submicron-scale with functional devices for 1.55 micron wavelength. The intrinsic isotropy of the disordered structure is an inherent advantage associated with the absence of limitations of orientational order, which is shown to provide valuable freedom in defect architecture design impossible in periodic structures.

1 NSF Award DMR-1308084, the University of Surrey’s FRSF and Santander awards.
10:00AM S8.00011 Disordered surface vibrations in jammed sphere packings, DANIEL SUSSMAN, ANDREA LIU, University of Pennsylvania, SIDNEY NAGEL, University of Chicago — We study the vibrational properties of networks derived from jammed packings near a free surface. We find that, in addition to the usual surface modes predicted by continuum elasticity, these systems have a surface density of disordered vibrational modes extending to arbitrarily low frequencies. The spatial profile of the surface modes shows a two-length-scale decay. The length scales diverge at the jamming transition as \( \Delta z^{-1/2} \) and \( \Delta z^{-1} \), respectively, where \( \Delta z \) is the excess coordination number above isostaticity. We speculate that these findings have implications for thin-film Lennard-Jones systems, and argue that the low-temperature jamming perspective may shed light on the physics of mobile surface layers observed in small molecule and polymeric thin films.

10:12AM S8.00012 On the Marginal Stability of Glassy Systems, LE YAN, New York University, MARCO BAITY-JESI, La Sapienza Università di Roma, MARKUS MÜLLER, The Abdus Salam International Center for Theoretical Physics, MATTHIEU WYART, New York University — In various glassy systems that are out of equilibrium, like spin glasses and granular packings, the dynamics appears to be critical: avalanches involving almost the whole system could happen. A recent conceptual breakthrough argues that such glassy systems sample the ensemble of marginal stable states, which inevitably results into critical dynamics. However, it is unclear how the marginal stability is dynamically guaranteed. We investigate this marginal stability assumption by studying specifically the critical athermal dynamics of the Sherrington-Kirkpatrick model. We discuss how a pseudo-gap in the density distribution of local fields characterizing the marginal stability arises dynamically.

10:24AM S8.00013 Critical scaling of stresses and correlations with strain rate in overdamped sheared disordered solids, JOEL CLEMMER, Johns Hopkins University, KENNETH SALERNO, Sandia National Laboratories, MARK ROBBINS, Johns Hopkins University — Like many nonequilibrium systems, disordered solids exhibit a power-law distribution of avalanches and other critical behavior when driven slowly. We extend molecular dynamics studies of quasistatic shear of 2D and 3D overdamped binary LJ glasses to finite strain rate. Finite-size scaling is used to determine the critical behavior of the shear stress and several measures of temporal and spatial correlations in non-affine displacements. With increasing strain rate, there is a power-law rise in the shear stress with exponent \( \beta \) extending to lower rates in larger systems. This behavior is governed by the rise in the dynamic correlation length with decreasing stress with exponent \( \nu \). The correlation function of non-affine displacements exhibits novel anisotropic power law scaling with \( q \), the magnitude of the wave vector. Its strain rate dependence is used to determine the scaling of the dynamic correlation length in various angular directions. In the quasistatic limit, particle diffusion in 2D is proportional to strain with a system-size dependent diffusion constant. Increasing strain rate, the dynamic correlation length drops below the system-size and the diffusion constant begins to fall.

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

10:36AM S8.00014 Polyamorphism in tetrahedral substances: similarities between silicon and ice, ALEX ANTONELLI, Universidade Estadual de Campinas, KARL GARCEZ, Universidade Federal do Maranhão — Tetrahedral substances, such as silicon, water, germanium, and silica, share several thermodynamical anomalies. Among them, the so-called polyamorphism, i.e., the existence of more than one amorphous state, is, perhaps, the most studied one. In this work, we study the transformations between amorphs of silicon using Monte Carlo simulations. The simulations indicate that by compressing the low density amorphous state (LDA), which is obtained by quenching the liquid at high temperature, a new denser amorphous state is formed [1]. The transformation between these two forms of amorphous silicon displays clear hysteresis, similar to the experiment reported by McMillan et al. [2]. However, analogously to the case of ice, our simulations indicate that upon annealing the unannealed high density amorphous silicon (uHDA) evolves to more stable forms. The annealing of uHDA at pressures on the order of 20 GPa gives rise to an even denser form, the very high density amorphous silicon (VHDA), while at much lower pressures, about 5 GPa, the uHDA transforms into a lower density form, the expanded high density amorphous silicon (eHDA).

2 Work supported by FAPESP, CNPq, CAPES, and FAEPESP/UNICAMP

10:48AM S8.00015 Thermal Transport in C60 Molecular Crystals Above Room Temperature, CAROLINE S. GORHAM, ALAN J. H. MCGAUGHEY, Department of Mechanical Engineering, Carnegie Mellon University — The thermal conductivity of solid fullerene molecular systems has garnered significant interest as an example of materials whose thermal transport is dominated by Einstein-type oscillators. Using classical molecular dynamics simulations, this study isolates the roles of intramolecular and intermolecular vibrational degrees of freedom on the bulk thermal conductivity of the face-centered cubic \( C_{60} \) molecular crystal. The Green-Kubo method is used to predict the bulk thermal conductivity. The contributions to thermal transport resulting from collective motions of the molecules, molecular rotations, and intramolecular vibrations are isolated using non-equilibrium methods. These contributions are interpreted using a Debye model, a nearest-neighbor resistance network, and Allen-Feldman theory.

1 C.S.G. is grateful for funding from the NASA Office of Graduate Research through the Space Technology Research Fellowship.

Thursday, March 5, 2015 8:00AM - 11:00AM – Session S9 FIAP: Vanadium Oxides, Resistive Switching, and Interfaces with Oxides 006D - Rick Mengyan, Texas Tech University

8:00AM S9.00001 Vanadium Dioxide Phase Change Switches, MARK FIELD, CHRISTOPHER HILLMAN, PHILIP STUPAR, JONATHAN HACKER, ZACHARY GRIFFITH, KANG-JIN LEE, Teledyne Scientific & Imaging LLC — We have built RF switches using vanadium dioxide thin films fabricated within a section of inverted transmission line with integrated on chip heaters to provide local thermal control. On heating the films above the metal insulator transition we obtain record low switch insertion loss of -0.13 dB at 50 GHz and -0.5 dB at 110 GHz. We investigate the device physics of these switches including the effect of a deposited insulator on the VO2 switching characteristics, the self-latching of the devices under high RF powers and the effect of resistance change with temperature on the device linearity. Finally we show how these devices can be integrated with silicon germanium RF circuits to produce a field programmable device where the RF signal routing can be selected under external control.

1Supported under the DARPA RF-FPGA Program, Contract HR0011-12-C-0092
2Supported under the DARPA RF-FPGA Program, Contract HR0011-12-C-0092
8:12AM S9.00002 Interstitial hydrogen in vanadium dioxide\(^1\) —  W. B. FOWLER, M. STAVOLA, WEIKAI YIN, YING QIN, Lehigh University, L. A. BOATNER, Oak Ridge National Laboratory — It has long been recognized that VO\(_2\) has a monoclinic-to-rutile phase transition as the temperature increases through 340K, accompanied by a remarkable increase in conductivity from insulator to metal\(^{1,2}\). Recently it has been found that interstitial hydrogen can modify both the structural and the electronic phase transition\(^3\). The way hydrogen does this has only recently begun to be studied\(^4\). We are using infrared spectroscopy to study the properties of H\(_i\), and are also using the CRYSTAL06 code\(^5\) with hybridized DFT Hamiltonian to determine equilibrium positions and vibrational frequencies. IR spectroscopy finds several OH vibrational lines in hydrogenated VO\(_2\) samples. Within the monoclinic structure of VO\(_2\) there exist two non-inequivalent sites for H\(_i\), which may lead to distinct spectroscopic signatures. \(^{[1]}\) F. J. Morin, Phys. Rev. Lett. 3, 34 (1959). \(^{[2]}\) A. Zybersztejn and N. F. Mott, Phys. Rev. B 11, 4383 (1975). \(^{[3]}\) J. Wei et al., Nature Nanotechnology 7, 357 (2012). \(^{[4]}\) K. H. Wannick et al., Appl. Phys. Lett. 104, 101913 (2014). \(^{[5]}\) R. Dovesi et al., Crystal06 User’s Manual (University of Torino, Torino, 2006).

8:24AM S9.00003 Magnetism in Bulk Vanadium Dioxide Compounds —  P. W. MENGYAN, R. L. LUCHI, B. B. BAKER, G. JAYARTHNA, Texas Tech University — Vanadium dioxide (VO\(_2\)) compounds show a metal-semiconductor transition (MST) near room temperature (stoichiometric VO\(_2\) is metallic T > \(T_{\text{MST}}\) ≈ 340 K and semiconducting T < \(T_{\text{MST}}\)) that is accompanied by a structural transition; both can be triggered by thermal, optical, electrical or barometric means. This ultrafast (sub ms) transition has been studied extensively and there is still considerable disagreement regarding the mechanism responsible for these transitions. Incorporation of a few atomic percent of H in VO\(_2\) stabilizes the metallic phase down to 200 K. Impurities such as W, Ti, Au, Cr or F lower or raise \(T_{\text{MST}}\) without significantly modifying other properties. Some effects that dopants have on the material are well known, however, the role dopants play in modifying them is far from understood. This contribution presents results of the first muon spin rotation and relaxation (MuSR) measurements on bulk VO\(_2\) compounds where we find and characterize a low temperature magnetic phase that has not yet been reported. The introduction of 2.4 at\% of W or 5 at\% of Ti raise the onset of the magnetic phase from 35 K to nearly 170 K. MuSR probes the local magnetic environment and hence provides a direct measure of the local field properties.

8:36AM S9.00004 Voltage switching of a VO\(_2\) memory metasurface using ionic gel —  M.D. GODFLAM, M.K. LIU, B.C. CHAPLER, H.T. STINSON, A.J. STERNBACH, A.S. MCLEOD, Univ of California – San Diego, M. ROYAL, Duke University, BONG-JUN KIM, ETRI, D.N. BASOV, Univ of California - San Diego. We have demonstrated large area, low voltage, non-volatile tuning of an electrolyte-based vanadium dioxide (VO\(_2\)) THz memory metasurface. Using ionic gel gating, voltage is applied to drive the insulator-to-metal transition in an underlying VO\(_2\) layer. Through application of positive and negative voltages, the metasurface resonance can be switched into the "off" or "on" state by driving VO\(_2\) into a more conductive or insulating regime, respectively. As compared to our graphene-based control devices, the longer saturation time of resonance modification in VO\(_2\)-based devices suggests that this voltage-induced switching originates primarily from electrochemical effects resulting from oxygen migration across the electrolyte-VO\(_2\) interface.

8:48AM S9.00005 Effect of doping and chemical ordering on the optoelectronic properties of complex oxide semiconductors —  IFIAT NAYYAR, CHAMBERLIN SARA, TIFFANY KASPAR. Physical Sciences Division, Pacific Northwestern National Laboratory, Pacific Northwest National Laboratory, PACIFIC NORTHWEST NATIONAL LABORATORY — It has long been recognized that VO\(_2\) has a monoclinic-to-rutile phase transition near room temperature (stoichiometric VO\(_2\) is metallic T > \(T_{\text{MST}}\) ≈ 340 K and semiconducting T < \(T_{\text{MST}}\)) that is accompanied by a structural transition; both can be triggered by thermal, optical, electrical or barometric means. This ultrafast (sub ms) transition has been studied extensively and there is still considerable disagreement regarding the mechanism responsible for these transitions. Incorporation of a few atomic percent of H in VO\(_2\) stabilizes the metallic phase down to 200 K. Impurities such as W, Ti, Au, Cr or F lower or raise \(T_{\text{MST}}\) without significantly modifying other properties. Some effects that dopants have on the material are well known, however, the role dopants play in modifying them is far from understood. This contribution presents results of the first muon spin rotation and relaxation (MuSR) measurements on bulk VO\(_2\) compounds where we find and characterize a low temperature magnetic phase that has not yet been reported. The introduction of 2.4 at\% of W or 5 at\% of Ti raise the onset of the magnetic phase from 35 K to nearly 170 K. MuSR probes the local magnetic environment and hence provides a direct measure of the local field properties.

9:00AM S9.00006 ABSTRACT WITHDRAWN —

9:12AM S9.00007 Oxygen controlled bipolar switching in NiO memristor —  ZHONG SUN, YONGGANG ZHAO, DIYANG ZHAO. Tsinghua Univ, DEPARTMENT OF PHYSICS, TSINGHUA UNIVERSITY, BEIJING 100084, CHINA TEAM — As Leon Chua demonstrated, both unipolar and bipolar resistance switching devices are memristors. Over the past decade, metal/oxide/metal structure with NiO as a ReRAM functional layer has been investigated widely and in depth, due to its intrinsic unipolar resistance switching, which is attributed to the connection and rupture of nickel filament in NiO. Recently, several papers studying NiO nanowires or NiO films with C-AFM infer that bipolar switching mechanism may govern the NiO memristors on the nanoscale. However, a systematic research on the mechanism of bipolar switching in NiO memristor on the nanoscale is still lacking. Especially, the role of oxygen in a NiO memristor has never been explored. Here we carry out a comprehensive study of the mechanism of bipolar switching in NiO memristor, and uncover the dominant role of oxygen. NiO/Pt structures were measured by C-AFM equipped with 20 nm conductive tips. By controlling the inherent oxygen concentration of NiO film, film thickness, and chamber oxygen pressure, we demonstrate that it is the inner oxygen distribution, related to electric field-induced ion drift and oxygen exchange between NiO film and ambient, that acts as the state variable, whose response to applied bias results in the bipolar switching in NiO memristor.

9:24AM S9.00008 Understanding Electroforming and Resistive Switching in Silicon Dioxide Resistive Memory Devices —  YAO-FENG CHANG, The University of Texas at Austin, BURT FOWLER, PrivaTran, LLC, FEI ZHOU, KWANG-SUN KIM, JINA KANG, The University of Texas at Austin, THE UNIVERSITY OF TEXAS AT AUSTIN COLLABORATION, PRIVATRAN, LLC COLLABORATION — Electroforming and resistive switching in SiO\(_2\) materials are investigated by anneal temperature, etch time and operating ambient. Thermal anneal in reducing ambient lowers electroforming voltage to small than 10 V. Conductive filaments form within 4 nm of sidewall surfaces in devices with an etched SiO\(_2\) layer, whereas most filaments are larger than 10 nm from the electrode edge. Switching unpassivated devices fails at 1 atm air and pure O\(_2\)/N\(_2\), with recovery of vacuum switching at about 4.6 V after switching attempts in O\(_2\)/N\(_2\) and at about 9.5 V after switching attempts in air. Incorporating a hermetic passivation layer enables switching in 1 atm air. Discussions of defect energetics and electrochemical reactions lead to a localized switching model describing device switching dynamics. Low-frequency noise data are consistent with charge transport through electron-trapping defects. Low-resistance-state current is passivated by a thin oxide layer, which may lead to conductivity enhancement and band-gap reduction. In this work, the electronic and optical properties of \(\alpha-(\text{Fe}_{1-x}\text{V}_{x})\text{O}_3\) films are the electronic excitations from these levels to the unoccupied Fe 3d\(^{1}\) orbitals, reducing the onset of \(\alpha-(\text{Fe}_{1-x}\text{V}_{x})\text{O}_3\) photoconductivity by nearly 1.2 eV. Our calculated optical absorption spectra are in good agreement with the experiment. This insight into the electronic, atomic and spin ordering provides guiding principles for the design of new oxide semiconducting materials for efficient visible light harvesting, thus enabling the technological growth of alternate energy sources for solving the renewable solar energy and photo-chemical organic waste remediation problems.

9:00AM S9.00006 ABSTRACT WITHDRAWN
9:36AM S9.00009 Bio-Inspired Learning Demonstration with Synaptic Resistive Memory Devices, SEYOUNG KIM, TAYFUN GOKMEN, MARK RITTER, IBM T J Watson Res Ctr — Simple two-terminal semiconductor memory devices which can mimic the functions of biological synapses has recently opened up exciting opportunities for enabling native implementation of brain-inspired computing. Here, we demonstrate in hardware that a biologically-inspired architecture employing a novel resistive memory technology used to implement a simple learning algorithm that imitates some features of the sensorimotor stage of cognitive development of a newborn baby. Actuation and sensing were indicated by spiking neurons, and the associations between neurons were learned in a HfOx-based resistive memory array using a local rule. The system essentially realize a biased random walk algorithm using a fully connected spiking sensorimotor network and can be generalized to solve other optimization problems by redefining the input and output functions of the neurons. This demonstrates a new approach to solve classical problems with resilient, adaptive, and fault-tolerant non-Von Neumann architecture.

9:48AM S9.00010 Ab initio study of the epitaxial ZrO2/Si interface, MEHMET DOGAN, DIVINE KUMAH, CHARLES AHN, FREDERICK WALKER, SOHRAB ISMAIL-BEIGI, Yale University — Growing thin films of crystalline metal oxides on semiconductors has been of much scientific interest because of the potential applications of such systems in electronic devices. One particular research goal is to achieve ferroelectricity in a crystalline and thin oxide film that is epitaxial on a semiconductor. This would enable one to realize non-volatile field-effect transistors where the state of the system is encoded in the polarization direction of the oxide. In this work, we study oxides that are not ferroelectric in the bulk but become ferroelectric as an ultrathin film on a semiconductor such as silicon. Recent developments in epitaxial growth methods also permit fabrication of such systems. Here, we use density functional theory to study the interface between ZrO2 and Si. When the oxide is only 1 monolayer thick, we find a set of stable structures with a variety of positive and negative out-of-plane ferroelectric polarizations. We present an analysis of these structures as a function of oxide thickness and the size of interface unit cell. Furthermore, the ZrO2 can be used as a buffer layer to induce ferroelectricity in ultrathin perovskite oxides such as SrTiO3 on Si which can couple the oxide polarization to the silicon carrier density.

1This work is supported by the National Science Foundation through grant MRSEC NSF DMR-1110826.

10:00AM S9.00011 Band alignment in metal-oxide interface Al/SiO2 and Cu/SiO2 in presence of defect, JIANQIU HUANG, CELINE HIN, Virginia Tech, VIRGINIA TECH TEAM — Semiconductors have wide use especially in electronic devices. Technological development tends to decrease the size of the electronic devices into the nanoscale. Dielectric Breakdown was an old problem which has not been fully resolved, which exponentially related to the size of electronic devices. It causes a severe and irreversible degradation on integrated circuits. Therefore, the motivation and main purpose of this research is to explore the dominant factors that will cause dielectric breakdown to occur in order to develop techniques to effectively prevent this occurrence. Density functional theory has been used to study the interface of Al/SiO2 and Cu/SiO2. Results on the investigation of atomic and charge vacancies at the interface will be presented and compared with the defect free models. The band alignment has been constructed in order to describe the behavior of the conduction band in the depletion layer. From the comparison and band alignment, a row conclusion that causes the breakdown occurrence was made.

1Advisor

10:12AM S9.00012 Carbon impurities in oxide dielectrics, HRAL D. TAILOR, University of California, Santa Barbara, JOHN L. LYONS, Brookhaven National Laboratory, MINSEOK CHOI, Korea Institute of Materials Science, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — The high-k oxides ZrO2 and LaAlO3 can be used as dielectrics in metal-oxide-semiconductor (MOS) devices. Dielectrics and semiconductors have very strong atomic layer deposition (ALD) often leading to unintentional incorporation of impurities such as carbon from the metal-organic precursors. Experiments indicated carbon can be a significant cause of leakage current. We investigate this problem using density functional theory with a hybrid functional. Our results show that carbon substituting on the cation site undergoes an off-site displacement and forms close bonds with oxygen in ZrO2 and LaAlO3. We calculate the corresponding defect levels, and in order to determine the impact on MOS devices we align the band structures of the dielectrics with those of the semiconductor channel materials (including GaN, Si, and GaAs). We find that carbon incorporation leads to defect levels near the conduction-band minimum of the channel materials, proving potentially detrimental for n-type devices. Intriguingly, we find that the defect levels of these carbon centers in a variety of oxides and semiconductors are aligned at roughly -3.5 eV below the vacuum level.

1Work supported by NSF, ONR, and ARO.

10:24AM S9.00013 Understanding the Oxygen Vacancy in Tungsten Trioxide, WENNIE WANG, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Dept., Univ of California, Santa Barbara — Tungsten trioxide (WO3) has a variety of applications in gas sensors, photocatalysis, and smart windows. As an electrochromic BO3 can be used as dielectrics in metal-oxide-semiconductor (MOS) devices. Dielectrics and semiconductors have very strong atomic layer deposition (ALD) often leading to unintentional incorporation of impurities such as carbon from the metal-organic precursors. Experiments indicated carbon can be a significant cause of leakage current. We investigate this problem using density functional theory with a hybrid functional. Our results show that carbon substituting on the cation site undergoes an off-site displacement and forms close bonds with oxygen in ZrO2 and LaAlO3. We calculate the corresponding defect levels, and in order to determine the impact on MOS devices we align the band structures of the dielectrics with those of the semiconductor channel materials (including GaN, Si, and GaAs). We find that carbon incorporation leads to defect levels near the conduction-band minimum of the channel materials, proving potentially detrimental for n-type devices. Intriguingly, we find that the defect levels of these carbon centers in a variety of oxides and semiconductors are aligned at roughly -3.5 eV below the vacuum level.

The high-k oxides ZrO2 and LaAlO3 can be used as dielectrics in metal-oxide-semiconductor (MOS) devices. Dielectrics and semiconductors have very strong atomic layer deposition (ALD) often leading to unintentional incorporation of impurities such as carbon from the metal-organic precursors. Experiments indicated carbon can be a significant cause of leakage current. We investigate this problem using density functional theory with a hybrid functional. Our results show that carbon substituting on the cation site undergoes an off-site displacement and forms close bonds with oxygen in ZrO2 and LaAlO3. We calculate the corresponding defect levels, and in order to determine the impact on MOS devices we align the band structures of the dielectrics with those of the semiconductor channel materials (including GaN, Si, and GaAs). We find that carbon incorporation leads to defect levels near the conduction-band minimum of the channel materials, proving potentially detrimental for n-type devices. Intriguingly, we find that the defect levels of these carbon centers in a variety of oxides and semiconductors are aligned at roughly -3.5 eV below the vacuum level.

1Work supported by DOE and NSF.

10:36AM S9.00014 Muonium Diffusion in In2O3, BRITTANY BAKER, ROGER LICHTI, Texas Tech University, Y. GURKAN CELEBI, Istanbul University, PATRICK MENGYAN, Texas Tech University, Y. GURKAN CELEBI, Istanbul University, PATRICK MENGYAN, Texas Tech University — Indium oxide (In2O3) is a transparent conducting oxide (TCO) commonly found in mixtures used as windows and transparent electrodes in optical semiconductor devices (i.e. LEDs and solar cells). Hydrogen diffusion in the TCO layer and across the interface between the TCO and the semiconductor device plays an important role in the degradation of the transparency of TCO windows or electrodes. Theoretical calculations show positive H as the only stable, interstitial H charge state above the neutral H ionization temperature. Muon Spin Relaxation measurements were performed to investigate positive muon (Mu+) diffusion which are an experimentally accessible analog to H+. Three distinct Mu+ states are identified between 2 K and 1000 K; a static low temperature state, a dynamic state above room temperature, and a trapping state from 400 K to 800 K. The trap component creates complex dynamics and has been modeled assuming the Mu+ transfers between the dynamic state and the trapping state. Fits of the model to the data provide information about capture and release rates and energy barriers into and out of the trap state. Here we present and discuss results from these fits, possible site locations for each state and likely diffusion paths.

10:48AM S9.00015 Group-IV Impurity Defect Levels in beta-Gallium Oxide, STEFAN BADESCU, Wyle Aerospace/US AFRL — Beta-Gallium Oxide (β-Ga2O3) is a wide-bandgap semiconductor with a significant potential as a native substrate for electronic devices. One avenue for tuning its carrier concentration and electronic properties is doping with group-IV impurity atoms. This work presents a first-principles understanding of the effects of C, Si, Ge and Sn dopants at Ga sites. C is found to act like a bistable center whereas the other dopants preserve the symmetry of the Ga site. Hybrid functionals are used to describe accurately the effects that occur mainly in the conduction band. A Brillouin zone unfolding is used that enables a direct comparison to possible spectroscopy experiments. We delineate the effects on bandgap modulation induced by charge density on the one hand, and by conduction band resonances and effective masses on the other hand.
8:00AM S10.00001 Distorted signal transport in topological insulators and its applications\textsuperscript{1}. XIAO ZHANG, Sun Yat-Sen University, CHINGHUA LEE, Stanford University — We develop a theoretical approach for studying the distorted signal transport in topological insulators. It works for arbitrarily applied electric fields and relaxation time. Exact analytic results are obtained for generic driving fields, with a particularly elegant expression for the trigonometric function case. We analytically and numerically study the effects of temperature, relaxation time etc for topological insulators in real conditions and its applications.

\textsuperscript{1}This work is supported by the National Natural Science Foundation of China through the grant No. 11404413.

8:12AM S10.00002 Current distribution in a two-dimensional topological insulator, XIAOQIAN DANG, JOHN BURTON, EVGENY TSYMBAL, Univ of Nebraska - Lincoln — Topological insulator (TI) is a bulk insulator with spin-dependent surface (edge) states that are protected by time-reversal symmetry. This property makes TIs very interesting for potential application in electronic devices. Here we report on theoretical investigations of transport properties of a model two-dimensional (2D) TI where the conductance is controlled by the topologically protected edge states. We utilize the tight-binding form of the Bernevig-Hughes-Zhang model\textsuperscript{1} and employ the Landauer-Büttiker formalism to explore the transport properties in the presence of impurities. Using the Green’s function technique we calculate the current distribution for states within the bulk band gap of the 2D TI. Interestingly, in absence of impurities we find that the current density decays into the bulk in an oscillatory fashion reflecting an oscillatory decay pattern of the local density of states as predicted from the complex band structure.\textsuperscript{2} Non-magnetic impurities disturb this picture and lead to a complex spatial distribution of current; however, the net transmission along the edge is conserved and remains a spin conductance quantum as expected from general considerations.

\textsuperscript{1}B. A. Bernevig et al., \textit{Science}, 314, 1757 (2006).

8:24AM S10.00003 Quantum geometry and stability of the fractional quantum Hall effect in the Hofstadter model. DAVID BAUER, THOMAS JACKSON, RAHUL ROY, University of California, Los Angeles — We study the correlation between the band geometry of the Hofstadter model to the limit of small flux and the stability of fractional quantum Hall states in this system. We develop a perturbative calculation of the quantum metric that agrees well with numerical calculations. In contrast to most models studied so far where the fluctuations of the Berry curvature seem to dictate the stability of any fractionalized topological phases, we find that in the Hofstadter model, the trace of the quantum metric seems to be the predominant factor.

8:36AM S10.00004 High-field charge transport on the surface of Bi$_2$Se$_3$, M.Q. WENG, M.W. WU, University of Science and Technology of China — We present a theoretical study on the high-field charge transport on the surface of Bi$_2$Se$_3$ and reproduce all the main features of the recent experimental results, i.e., the incomplete current saturation and the finite residual conductance in the high applied field regime [Costache et al., Phys. Rev. Lett. 112, 086601 (2014)]. Due to the hot-electron effect, the conductance decreases and the current shows a tendency of saturation with the increase of the applied electric field. Moreover, the electric field can excite carriers within the surface bands through interband precession and leads to a higher conductance. As a joint effect of the hot-electron transport and the carrier excitation, the conductance approaches a finite residual value in the high-field regime and the current saturation becomes incomplete. We thus demonstrate that, contrary to the conjecture in the literature, the observed transport phenomena can be understood qualitatively in the framework of surface transport alone. Furthermore, if a constant bulk conductance which is insensitive to the field is introduced, one can obtain a good quantitative agreement between the theoretical results and the experimental data [M. Q. Weng and M. W. Wu, Phys. B 90, 125306, (2014)].

8:48AM S10.00005 Dimensional crossover of transport characteristics in topological insulator nanofilms. KEN-ICHIRO IMURA, YUKINORI YOSHIMURA, Hiroshima University, KOJI KOBAYASHI, TOMI OHTSUKI, Sophia University — Recently, much effort has been made to grow thin films of a topological insulator. Naturally, its primary purpose was to reduce the contribution of the bulk to transport quantities. Here, we propose that searching for quantized transport in thin Ti films is an efficient way for probing non-trivial topological features encoded in the 3D bulk band structure. In a recent work (Kobayashi, KI, Yoshimura & Ohtsuki, arXiv:1409.1707), we have highlighted the following issues: 1) Transport characteristics of Ti thin films is well understood by studying the conductance both in the edge and slab geometries. 2) We introduce “conductance maps” for revealing the dimensional crossover in such Ti thin films. Quantization of the conductance occurs both in the edge and in the slab geometries, but not at the same time. 3) We focus on the even-odd feature in transport with respect to the number of stacked layers. We found parameter regimes in which the even-odd feature is broken by inversion of the finite-size gap associated with hybridization of the top and bottom surface wave functions. We propose that tuning the hybridization gap of a Ti thin film and make it inverted is an effective way of realizing a 2D quantum spin Hall state.

9:00AM S10.00006 Extrinsic spin-orbit coupling and density dependent weak antilocalization in three-dimensional topological insulators, WEIZHE LIU, School of Physics, The University of New South Wales, Sydney 2052, Australia, PIERRE ADROGUER, Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany, XINTAO BI, ICQD, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui 230026, China, EWELINA HANKIEWICZ, Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany, DIMITRIE CULCER, School of Physics, The University of New South Wales, Sydney 2052, Australia — Topological insulators (TIs) have revolutionized our understanding of insulating behaviour. Three-dimensional TIs are insulators in the bulk but conducting along their surfaces. Much of recent researches on 3D TIs focus on overcoming the transport bottleneck, namely the fact that surface transport is overwhelmed by bulk transport stemming from unintentional doping. The key to overcoming this bottleneck is identifying unambiguous signatures of surface state transport. We will discuss on such signature: weak antilocalization, meaning that coherent backscattering increases the electrical conductivity. The features of this effect, however, are rather subtle, because in TIs the impurities have also strong spin-orbit coupling. I will show that spin-orbit coupled impurities introduce an additional time scale, which is expected to be shorter than the dephasing time, and the resulting conductivity has a distinguished part with linear dependent on the carrier number density. The result we predict is directly observable experimentally.

9:12AM S10.00007 Topological suppression of quantum tunneling, JIA-HUA GU, KAI SUN, University of Michigan, Ann Arbor — In this talk, we prove that if we bring together two band insulators with different topology, described by arbitrary topological indices, there must exist specific momentum points in the Brillouin zone where the wavefunctions of the two insulators are orthogonal and cannot hybridize. For 2D insulators, this conclusion implies that topology will prohibit tunneling of electrons between the two insulators at this momentum. This conclusion can also be generalized to some strongly-correlated topological systems. Explicit demonstration and proof will be provided for topological band insulators and fractional quantum Hall states.
9:24AM S10.00008 Charge Transport in 3D topological insulators in the presence of surface potential fluctuations, XINGYUE PENG, YIMING YANG, RAJIV SINGH, SERGEY SAVRASOV, DONG YU, Univ of California - Davis — Field effect measurements on the surface of a 3D topological insulator (TI) show a high minimum conductivity which is strongly dependent on sample details but the gate dependent conductivity also exhibits anomalous non-monotonic behavior which is not yet understood. Understanding the nature of this minimum conductivity is crucial for the design and fabrication of novel spintronic devices based on 3D TIs. We propose a theoretic model to explain this anomalous behavior, considering the existence of surface potential fluctuations as indicated by scanning tunneling spectroscopy (STS) and scanning photocurrent microscopy (SPCM) measurements on the surface of a 3D TI. Our model agrees well with preexisting experiments and our own transport measurements in field effect transistors (FETs) incorporating 5b-doped single Bi2Se3 nanoribbons.

9:36AM S10.00009 Effects of the boundary geometry on the edge current in the two dimensional topological insulator1, HYEONJIN DOH, HYOUNG JOON CHOI, Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University — We study the effects of the boundary shape on the edge transport of the two dimensional topological insulator described by Kane-Mele model. The edge state is robust against all time-reversal invariant defects. However, when we consider an arbitrary sample, the edge is not straight and consists of various types of boundaries. Actually, the transport property of the edge-state in the Kane-Mele model depends on the boundary type of the edge such as zigzag and armchair edges. Therefore, the edge-transport can be affected by a corner connecting two different types of edges. Here, we investigate the energy spectrum of the various shapes of finite-size honeycomb lattice with corners along the edge. We also calculate the transport properties on the edges by applying an artificial gauge field which drives a persistent current along the edges. Although the corner of the edge seems a geometrical defects and is expected to have a little effect on the transport, our results show that the geometrical defects strongly affect the edge current depending on the corner types.

1This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2013-C3-062).

9:48AM S10.00010 Distinctive features of transport in topological insulators, VINCENT SACKsteder, Nanyang Tech Univ, QUANSHENG WU, Institute of Applied Physics and Computational Mathematics, Beijing, KRISTIN ARNARDOTTIR, IVAN SHELYHKY, Nanyang Tech Univ, STEFAN KETTEMANN, Jacobs University Bremen — The surface states of a topological insulator in a fine-tuned magnetic field are ideal candidates for realizing a topological metal which is protected against disorder. Its signatures are (1) a conductance plateau in long wires and (2) a conductivity which always increases with sample size. We numerically show that the bulk substantially accelerates the conductance plateau’s decay in a magnetic field. It also reduces the effects of surface disorder and causes the magnitude of the surface conductivity and the magnetoconductivity to depend systematically on sample details such as doping and disorder strength. In addition, we predict a new signature of the topological state: at low temperatures the magnetoresistance will deviate strongly from the Hikami-Larkin-Nagaoka (HLN) formula. In this regime the magnetoresistance is dominated by scattering processes which wrap around the TI sample. The HLN formula’s shoulder is replaced by a feature with a larger critical field magnetic strength that is caused by wrapping. Inside the wrapping regime the magnetoconductance will lose its dependence on temperature. This new topological signature should be visible in the same samples and temperatures where the Altshuler-Aronov-Spivak (AAS) effect has already been observed.

10:00AM S10.00011 Berry-phase description of Topological Crystalline Insulators, ARIS ALEXANDRINATA, B. ANDREI BERNEVIG, Princeton University, XI DAI, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences — We study a class of translationally-invariant insulators protected by crystalline symmetries. Some of these insulators have no spin-orbit coupling, and may be realized in intrinsically spinless systems such as photonic crystals and ultra-cold atoms. Some of these insulators have no time-reversal symmetry as well, i.e., the relevant symmetries are purely crystalline. Nevertheless, topological phases exist which are distinguished by their robust surface modes. Their band topology is unveiled by the crystalline analog of Berry phases, i.e., parallel transport across certain non-contractible loops in the Brillouin zone. We also identify certain topological phases without any robust surface modes - they are uniquely distinguished by parallel transport along bent loops, whose shapes are determined by the symmetry group. Finally, we highlight recent interferometry experiments which demonstrate that these Berry phases are measurable.

10:12AM S10.00012 Majorana zero modes choose Euler numbers - revealed by full counting statistics, DONG E. LIU, Microsoft Research Station Q, ALEX LEVCHENKO, Michigan State University, ROMAN M. LUTCHYN, Microsoft Research Station Q — We consider a quantum dot (QD) coupled to a Majorana zero mode and two normal leads and study transport properties of the system. We investigate the full counting statistics of charge tunneling events which allows one to extract information about current fluctuations in the system. Using Keldysh path-integral approach, we compute the cumulant generating function for the quantum dot with Majorana and normal lead couplings. We first consider a non-interacting spinless QD, and find that for the symmetric dot-lead couplings, the zero-frequency cumulants exhibit a universal pattern (Euler polynomial), independent of the microscopic parameters. For a spinful QD, the Coulomb interaction effects are discussed for both strong interaction (single-electron occupancy regime) and weak interactions (perturbative regime). In the latter case, the interactions do not change the universal pattern at small voltage bias. Compared to the case without Majorana coupling, we show that, while the tunneling conductance might exhibit zero-bias anomaly due to Majorana or Kondo physics, the full counting statistics are qualitatively different in the presence of the Majorana coupling.

10:24AM S10.00013 Simple examples of Symmetry-Protected Topological phases and Symmetry-Enriched Topological phases of quantum lines, OLEKSI MOTORUNICH, SCOTT GERAEDTS, California Institute of Technology — We construct models realizing distinct confining phases of lattice gauge theories envisioned in a formal classification of gapped phases of gauge theories by Kapustin and Thorngren, arXiv:1309.4721. This generalizes ideas of Symmetry-Protected Topological (SPT) phases in Condensed Matter to systems where fundamental microscopic objects are quantum lines, which is of interest in High Energy Theory. Specifically, in (3+1)-D, we consider discrete ZN lattice gauge theory models, with two copies of ZN, and construct N distinct confining phases by engineering condensation of bound states of magnetic fluxes (which are quantum lines in 3d) and ZN electric field lines. In (4+1)D, we consider compact quantum electrodynamics (CQED) models, with two copies of CQED, and engineer condensation of bound states of monopoles (which are quantum lines in 4d) and U(1) electric field lines. When the bound states contain a single monopole, we find SPT-like phases of the lattice gauge theory, while when the bound states contain multiple monopoles, we find analogs of Symmetry-Enriched Topological phases, where in the present case we also have fractionalization of Faraday lines. The distinct character of these topological phases of quantum lines is revealed by unusual physics at a boundary.

10:36AM S10.00014 Interacting surface states of three-dimensional topological insulators, TITUS NEUPERT, Princeton University, STEPHAN RACHEL, Technische Universitaet Dresden, RONNY THOMALE, MARTIN GREITER, University of Wurzburg — We numerically investigate the surface states of a strong topological insulator in the presence of strong electron-electron interactions. We choose a spherical topological insulator geometry to make the surface amenable to a finite size analysis. The single-particle problem maps to that of Landau orbitals on the sphere with a magnetic monopole at the center that has unit strength and opposite sign for electrons with opposite spin. Assuming density-density and electron-electron interactions, we find superconducting and anomalous (quantum) Hall phases for attractive and repulsive interactions, respectively, as well as chiral fermion and chiral Majorana fermion boundary modes between different phases. Our setup is preeminently adapted to the search for topologically ordered surface termination that could be microscopically stabilized by tailored surface interaction profiles.
8:00AM S11.00001 A comparison of the superconducting states of Ta4Pd3Te16 and Nb3PdxSe7. QIU RUN ZHANG, BIN ZENG, DANIEL RHODES, LUIS BALICAS, NHMFL — We have measured the superconducting upper critical fields of a Ta4Pd3Te16 sample and a Nb3Pd3Se7 sample with very close values of $T_c$. The Maki parameter of Ta4Pd3Te16 ($H_{c2}(T \to 0K) \sim 5.57$) is small and hence it is an orbital limited system. However, $H_{c2}$ shows an unconventional linear $T$ dependence in the whole temperature range. Even though they have similar crystalline structures, the upper critical fields of Nb3Pd3Se7 are extremely high ($H_{c2}(T \to 0K) \sim 25T$) and much more anisotropic.

8:12AM S11.00002 High-field studies of the Pd-based Superconductor Ta4Pd3Te16. TONY HELM1, Lawrence Berkeley National Laboratory, PHILIP J.W. MOLL, ROBERT KEALHOFER, JAMES G. ANALYTIS, University of California — The layered Pd-based ternary chalcogenide Ta4Pd3Te16 (TPT) has not gotten much of attention since its first synthesis in 1997. Recently, TPT was found to turn superconducting (SC) below a critical temperature of $T_c = 4.5$K and up to 6.5K under pressure. The layered material has an orthorhombic crystal structure and the main conduction channel is suspected to run along one dimensional (1D) PdTe-chains. Band structure calculations find multiple bands at the Fermi level including 1D sheets. One of the striking features in the family of M3Pd3Q3 (M=Nb and Ta, Q=S and Se) is a very enhanced upper critical field. To understand the mechanism behind this enhancement TPT is of special interest since it has a similarly complex structure but much lower $H_{c2}$. Anomalous transport properties and a significant anisotropy in $H_{c2}$ have been interpreted in terms of an unconventional SC ground state present in TPT. Here we report studies of normal-state magnetotransport and magnetic torque in high fields that disclose details of TPTs electronic structure enabling us to speculate about the origin of SC in this compound.

3 Materials Science Division, Lawrence Berkeley National Laboratory; Department of Physics, University of California, Berkeley, California 94720, USA

8:24AM S11.00003 Anisotropic Superconducting Gap and Elongated Vortices with Caroli-De Gennes-Matricon States in the New Superconductor Ta4Pd3Te16. HUAN YANG, ZENGYU DU, DELONG FANG, ZHENYU WANG, YUFENG LI, GUAN DU, XIYU ZHU, HAI-HU WEN, Department of Physics, Nanjing University — The superconducting state is formed by the condensation of a large number of Cooper pairs. The normal state electronic properties can give significant influence on the superconducting state. For usual normal-state magnetotransport and magnetic torque in high fields that disclose details of TPTs electronic structure enabling us to speculate about the origin of SC in this compound.

This work was supported by the Ministry of Science and Technology of China (973 projects: 2011CBA00102, 2012CB821403), NSF of China, and PAPD.

8:36AM S11.00004 Tuning superconductivity in Nb2Pd0.81S5 using applied pressure and uniaxial strain. KUAN-WEN CHEN, QIU RUN ZHANG, NHMFL, Florida State Univ., DANIEL JACKSON, Univ. Florida, ANDREW GALLAGHER, NAOKI KIKUGAWA, SCOTT RIGGS, DAVID GRAF, NHMFL, Florida State Univ., JAMES HAMLIN, Univ. Florida, LUIS BALICAS, RYAN BAUMBACH, NHMFL, Florida State Univ. — Nb2Pd0.81S5 is a recently reported transition metal-chalcogenide superconductor ($T_c \sim 6.6$K) with unusually large upper critical fields ($H_c > 37 T$ for $H = b$) [1]. We present electrical resistivity measurements under applied pressure for this compound, where a piston cylinder cell was used with Daphne 7474 oil as the pressure transmitting medium. These measurements reveal that the superconducting transition temperature abruptly increases to 8.5 K for $P < 2$ kbar, but additional pressure (up to 16 kbar) has little effect on $T_c$. This result may indicate that while the electronic state of this compound is sensitive to strain, it is only weakly affected by hydrostatic pressure. This viewpoint is supported by subsequent experiments where application of Daphne oil or N-grease to the crystal surface results in an increase of $T_c$ to 8 K. In order to systematically disentangle the influence of pressure and strain, we will present results from resistivity measurements where the sample is uniaxially strained using a piezo-stack ("elastoresistance") along the b direction.


8:48AM S11.00005 MgB2 Coated Ellipsoids as an Approach to Investigate the Possible Enhancement of the Vortex Penetrating Field of SRF Cavities. TENG TAN, MATTHAEUS WOLAK, Department of Physics, Temple University, TSUYOSHI TAJIMA, Los Alamos National Lab, XIAOXING XI, Department of Physics, Temple University, LEONARDO CIVALE, Los Alamos National Lab — Superconducting rf (SRF) cavities fabricated from bulk niobium (Nb) are a key component for modern particle accelerators. The magnetic field distribution on the inner wall of an SRF cavity is inversely similar to the field distribution on top of a superconducting ellipsoid when we put it in a magnetic field parallel to its axis. By measuring the vortex penetration into the magnetized superconducting ellipsoids, we can deduce the behavior of SRF cavities. Magnesium diboride (MgB2) has potential to replace Nb as it has a higher $T_c$ of 39 K, a lower residual resistivity of ~0.1 $\mu$Omega cm (at 42 K), and a higher thermodynamic critical field $H_c$ value compared to Nb. In this work, we successfully coated uniform MgB2 layers on top of molybdenum and niobium ellipsoids. SQUID magnetometer measurements showed that the coated MgB2 layer has a $T_c$ above 38.5 K, and can provide a perfect magnetic shielding up to ~ 500 Oe at 1.8K. By coating MgB2 on Nb ellipsoids, we increased the vortex penetration field (the maximum field at which a cavity can be operated) by ~ 500 Oe at 2 K.

9:00AM S11.00006 ABSTRACT WITHDRAWN —
9:12AM S11.00007 Multiple Andreev Reflections in MgB$_2$/I/Pb Heterojunctions Cooled below 1 Kelvin$^1$, ROBERTO RAMOS, Indiana Wesleyan Univ, STEVEN CARABELLO, Drexel University, PENN STATE HARRIERSBURG, JOSEPH LAMBERT, Drexel University, WENQING DAI, QI LI, Penn State University, KE-CHEN, DANIEL CUNNANE, Temple University, C.G. ZHUANG, None, X.X. XU, Temple University — We have measured the I-V and dI/dV characteristics of two MgB$_2$/I/Pb heterojunctions below 1 Kelvin. In both junctions which were grown on c-axis substrates, we observed the characteristic pi peak corresponding to c-axis tunneling, consistent with theoretical predictions. Furthermore, we have observed sub-harmonic peaks in dI/dV that are consistent with Multiple Andreev Reflections (MAR) usually associated with high-transparency junctions. We also describe the temperature dependence of other sub-gap peaks observed. By systematically reducing noise in our setup and using sub-Kelvin temperatures, we were able to observe relatively sharp MAR peaks which are unusual for junctions with a large $R_{subgap}/R_n$ ratio.

9:24AM S11.00008 The Effect of Argon Ambient Pressure and Annealing Time on Bulk MgB$_2$ Superconductor$^1$, MURAT ERDEM, Abant Izzet Bayals University, OZGUR OZTURK, ELIF ASIKUZUN, SEYDANUR KAYA, Kastamonu University, SERAP SAFRAN, AHMET KILIC, Ankara University, CABIR TERZIOGLU, Abant Izzet Bayals University — The effects of Ar ambient pressure (vacuum, 0B, 105B and 20B) and annealing times (0.5 h and 1h) on microstructural, superconducting and mechanical properties of bulk superconducting MgB$_2$ are investigated. The samples are produced using the solid state reaction method. X-ray diffraction (XRD) and scanning electron microscopy (SEM) measurements were performed for determination of the crystal structure, and surface morphology of MgB$_2$ samples, respectively. The superconducting properties were studied by AC magnetic susceptibility and DC resistivity measurements. Increasing the Ar pressure decreased the lattice parameters and hence the average grain size. Increasing the annealing time results in larger lattice parameters and larger grain formation. The susceptibility measurements revealed two step transition which is reminiscent of granular superconductors. The intra-grain transition temperature is determined to be 38.4 K for all samples. The inter-grain transition temperatures of 37.2 K is obtained for samples produced under Ar ambient. These samples produced under Ar ambient have better superconducting properties than the ones produced in vacuum. Increasing the annealing time under vacuum further decreases the superconducting properties probably due to Mg loss.

9:36AM S11.00009 Isotropic superconducting gap and electron-boson coupling in MgB$_2$ multiband superconductor$^1$, DAIXIANG MOU, RUI JIANG, VALENETIN TAUFOUR, REBECCA FLINT, SERGUEI BUD’KO, PAUL CANFIELD, ADAM KAMINSKI, Division of Materials Science and Engineering, Ames Laboratory, U.S. DOE — MgB$_2$ is a prototype multiband BCS/Eliashberg superconductor with high transition temperature $T_c \sim 39$K. In this talk, we will present electronic properties of this compounds measured by tunable laser ARPES. Momentum dependent gap structure on two Fermi surface around $\Gamma$ is nearly isotropic with $\Delta \sim 0.5$meV, directly proving its s-wave pairing symmetry. Our data reveals a strong renormalization of the dispersion (kink) at $\sim 65$meV, which is caused by coupling of electrons to $\varepsilon_{2g}$ phonon mode. In contrast to cuprates, the 65 meV kink in MgB$_2$ does not change significantly across $T_c$. More interestingly, we observe strong coupling to a second, low energy collective mode at 10 meV. This excitation vanishes above $T_c$ and is likely a signature of the elusive Leggett mode.

9:48AM S11.00010 Measurement of the Penetration Depth and Coherence Length of MgB$_2$ in All Directions Using Transmission Electron Microscopy, JAMES LOUDON, University of Cambridge, S. YAZDI, T. KAMAS, Technical University of Denmark, N.D. ZHIGADLO, J. KARPINSKI, ETH Zurich — We demonstrate that images of flux vortices in a superconductor taken with a transmission electron microscope can be used to measure simultaneously the penetration depth and coherence length in all directions at the same temperature and magnetic field. This is particularly useful for MgB$_2$ where these quantities vary with the applied magnetic field and values are difficult to obtain at low field or in the c direction. We obtained images of flux vortices from a sample cut in the ab plane by focussed ion beam milling and compared these with simulations which accounted for flux vortices with a non-zero core in a thin, anisotropic superconductor. This gave penetration depths $\lambda_{ab} = 100 \pm 35$ nm, $\lambda_c = 120 \pm 15$ nm and coherence lengths $\xi_{ab} = 41 \pm 13$ nm and $\xi_c = 34 \pm 10$ nm at 10.8 K in a field of 4.8 mT. The implications of these values for type-1.5 superconductivity will be discussed.

10:00AM S11.00011 Superconductivity beyond the dimer model in 2D organic charge transfer salts$^1$, MICHAELA ALTMAYER, DANIEL GUTERDING, HARALD O. JESCHKE, ROSER VALENTI, Goethe-Universitaet Frankfurt. — We present a theoretical investigation of BEDT-TTF charge transfer salts containing $\kappa$-type layers. Using ab-initio density functional theory we construct realistic models with unprecedented accuracy for a broad variety of materials. We analyze the pairing symmetry and strength within random phase approximation spin fluctuation theory and interpret our findings microscopically in a tight-binding analysis. In particular we show that the minimal model for this class of materials needs to describe all BEDT-TTF molecules independently and give an example where the customary dimer model breaks down.

$^1$Research funded within DFG TR 49

10:12AM S11.00012 Inhomogeneous superconducting state in $\beta''$-(BEDT-TTF)$_2$S$_2$CH$_2$CF$_2$SO$_3$, GEORGIOS KOUTROULAKIS, Univ of California - Los Angeles, H. KUHNE, Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, R. KATO, Condensed Molecular Materials Laboratory, RIKEN Advanced Science Institute, J.A. SCHLUTER, Materials Science Division, Argonne National Laboratory, J. WOSNITZA, Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, S.E. BROWN, Univ of California - Los Angeles — We present nuclear magnetic resonance (NMR) measurements on the quasi-2D organic superconductor $\beta''$-(BEDT-TTF)$_2$S$_2$CH$_2$CF$_2$SO$_3$ at ultra-low temperature ($T \sim 100$K). For a magnetic field applied precisely within the conducting layers, the field evolution of the NMR spectrum reveals a phase transition within the superconducting state ($H_F > 12$T) near to the Pauli limit $H_F \sim 9.5$T. The transition is identified by the significant line-broadening of the spectrum, associated with the electronic spin polarization distribution due to the emergence of spatially inhomogeneous superconductivity, the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state. The character of this novel SC state is studied via static and dynamic (i.e. spin-lattice relaxation) NMR measurements. Moreover, the stability of the putative FFLO phase upon rotation of the field away from the in-plane condition is investigated.

10:24AM S11.00013 Electronic structure of a dual-layered organic charge transfer salt$^1$, HARALD JESCHKE, MICHAELA ALTMAYER, ROSER VALENTI, Goethe-Universitaet Frankfurt. — We examine the electronic properties of polyorphs of (BEDT-TTF)$_{2}$Ag(CH$_3$TCE) (1:1.2-chlorotrichloroethane) within density functional theory (DFT). While a phase with low superconducting transition temperature $T_c \sim 2.6$ K exhibits a $\kappa$ packing motif, two high $T_c$ phases are layered structures consisting of $\alpha'$ and $\kappa$ packed layers. We determine the electronic structures and discuss the influence of the insulating $\alpha'$ layer on the conducting $\kappa$ layer. We find that the stripes of high and low charge in the $\alpha'$ layer correspond to a stripe pattern of hopping parameters in the $\kappa$ layer. This finding is the basis for studying the effect of the different underlying Hamiltonians on the superconducting properties.

$^1$Research funded within DFG Transregio 49.
8:00AM S12.00001 Prediction of vibration modes and thermal conductivity for amorphous ZnO-based materials, YU-TING CHENG, ANINDYA ROY, MICHAEL L. FALK, Johns Hopkins University — Amorphous materials, due to their distinct physical and chemical properties, have been widely used in photovoltaics, thermoelectrics and integrated circuits. Because the thermal conductivity is critical to the performance of such devices, the thermal transport in amorphous materials has received considerable attention in the last decade. So far, a number of experimental studies and theoretical models have reported the vibration modes and thermal conductivities for amorphous Si and SiO2. However, the applicability of these vibration mode analyses and thermal conductivity models for other amorphous materials has not been studied. In this work, we employ the molecular dynamics (MD) simulations and Allen-Feldman (AF) theory [1] to investigate the vibration modes and thermal conductivity of amorphous ZnO-based materials. ZnO is basis of a promising class of n-type semiconductors for thermoelectric application. Additionally, from this work, the contribution of individual vibrational modes to the thermal conductivity can be characterized. These results are expected to guide the interpretation of thermal transport in amorphous ZnO-based materials and the optimization for their performance with different applications. [1] P. B. Allen and J. L. Feldman, Phys. Rev. B 48, 12581 (1993).

8:12AM S12.00002 Optimization of thermoelectric properties in cross-plane superlattices - A 1D NEGF Study, MISCHA THEISBERG, MAHDI POURFARTH, Vienna Univ of Technology, NEOPHYTOS NEOPHYTOU, University of Warwick, HANS KOSINA, Vienna Univ of Technology — Thermoelectric materials utilize carrier energy filtering through potential barriers to achieve improvements in the Seebeck coefficient. Barriers, however, tend to drastically reduce the electrical conductivity, and power factor improvements are difficult to be realized. In this work we present a fully quantum mechanical simulation study of thermoelectric transport in the presence of barriers for energy filtering. For this, we use the non-equilibrium Green’s function (NEGF) method, including both acoustic and optical phonons. We show that power factor improvements can be achieved by properly adjusting a series of interrelated parameters: i) the position of the Fermi level, ii) the width, size and shape of the barriers as well as the separation between them, iii) the optical phonon energies. Our results provide insight on how to optimize superlattices and nanocomposite materials for enhanced thermoelectric properties.

8:24AM S12.00003 Sub-Band engineering through superlattice based barrier heterostructures for higher thermoelectric efficiency, MAHYAR POURHASEMI, JIVTESH GARG, Univ of Oklahoma — There is a huge desire to increase operation speeds in modern integrated circuits as they get more compact. Heat generation in such a submicron devices is a key factor limiting their performances. As a solution, thermoelectric cooling in heterostructures can address heat dissipation issue in submicron devices. Performance of single barrier heterostructures depends strongly on several parameters including barrier height, barrier width and thermal conductivity of barrier. Superlattice structures have been known to have the lowest thermal conductivities reported for crystalline materials. Low thermal conductivity is beneficial for thermoelectric cooling as it reduces the heat flow from hot end to cold junction. Moreover the band offset between the barrier and base material can be easily tuned by changing the superlattice period. By optimizing the conduction band offset (barrier height), it is possible to control the Joule heating and also optimize the amount of heat absorbed due to Peltier cooling. We investigate the feasibility of using PbSe/PbSnTe superlattices in heterostructures using Monte Carlo simulation. The effect of different parameters such as barrier height, barrier width and superlattice thermal conductivity on thermoelectric cooling of such structures will be presented.
Development of thermal rectifier using unusual electron thermal conductivity of icosahedral quasicrystals. TSUNEHIRO TAKEUCHI, Toyota Technological Inst — The bulk thermal rectifiers usable at high temperature were developed using the unusual increase of electron thermal conductivity of icosahedral quasicrystals (ICQ) at high temperature. Our previously performed analyses in terms of linear response theory suggested that the unusual increase of electron thermal conductivity of ICQ was brought about by the synergy effect of quasiperiodicity and narrow pseudogap at the Fermi level. Since the linear response theory suggests that the unusual increase of electron thermal conductivity is coupled with the small magnitude of Seebeck coefficient, the composition of Al-Cu-Fe ICQ, where the thermal conductivity shows the most significant increase with increasing temperature, was determined with a great help of Seebeck coefficient measurements. Consequently obtained $A_{11,5}Cu_{26},Fe_{12},0 ICQ, which was characterized by the small magnitude of Seebeck coefficient, possessed 9 times larger value of thermal conductivity at 1000 K than that observed at 300 K. The increasing tendency of electron thermal conductivity with increasing temperature was further enhanced by means of small amount of Re substitution for Fe. This substitution definitely reduced the lattice thermal conductivity while the electron thermal conductivity was kept unchanged. The lattice thermal conductivity was reduced by 35 % under the presence of 0.5 at. % Re, and the thermal conductivity at 1000 K consequently became about 11 times larger than that at 300 K. The thermal rectifiers were constructed using our newly developed ICQ ($A_{11,5}Cu_{26},Fe_{12},0$ or $A_{12},5Si_{10},Cu_{26},Fe_{11},0$) together with one of the selected materials (Si, Al$_2$O$_3$, Cu$_2$Te$_2$ or Ag$_2$Te) that possess thermal conductivity decreasing with increasing temperature. The heat current flowing in the rectifiers was confirmed to show significant direction dependence. The consequently obtained $TRR = |J_{\text{large}}/ |J_{\text{small}}|$ for the composite consisting of $A_{11,5}Si_{10},Cu_{26},Fe_{12},0$ or $A_{12},5Si_{10},Cu_{26},Fe_{11},0$ reached 2.24, and that is the largest value ever reported for the bulk thermal rectifiers.

9:12AM S12.00005 Thermopower measurements of atomic and molecular junctions using microheater-embedded mechanically-controllable break junctions, MAKUSU TSUTSUI, TAKANORI MORIKAWA, AKIHIDE ARIMA, MASATERU TANIGUCHI, ISIR, Osaka University — There has been growing interest in developing high-performance thermoelectric materials for realizing thermoelectric power generation. Quantum effects in low-dimensional structures are expected to provide high electronic density of states for enhanced thermopower, and thus considered as a promising approach for achieving a high figure of merit (M. S. Dresselhaus et al., Adv. Mat. 19 (2007) 1043-1053). From this respect, it is interesting to study thermoelectric properties of atomic and molecular junctions and evaluate their potential as a thermoelectric material. Recently, we have developed a heater-embedded micro-fabricated mechanically-controllable break junction (MCBJ) for investigating the thermoelectric transport in single-atom and –molecule junctions. Using the MCBJ devices, we could repeatedly form stable junctions at room temperatures via a self-breaking mechanism with one side being heated by the adjacent microheater. In my presentation, I will show the results of simultaneous measurements of the thermoelectric voltage and the electrical conductance of atom-sized Au junctions and Au-benzenedithiol-Au junctions and discuss on the geometrical dependence of thermoelectric transport.

9:24AM S12.00006 Phonon thermal conductivity of a nanowire attached to leads, SELMAN HERSHFIELD, KHANDKER MUTTALIB, Department of Physics, University of Florida — There is experimental evidence as well as theoretical proposals that nanowires can be made to have high thermoelectric efficiency by tuning the electronic properties; however, there is always a phonon contribution to the heat transport which reduces the thermoelectric efficiency. In the harmonic approximation we compute the transmission of phonons through a nanowire coupled to large leads. There is a finite thermal conductance because of the restriction provided by the nanowire. The nanowire reduces the thermal transport because of the mismatch between the leads and wire modes. We examine the effect of disorder in three places: in the wire, in the leads near the wire, and in the leads far way from the wire. In some cases disorder can increase the thermal conduction because of enhanced mode coupling. We will discuss the implications of our results for thermoelectric nanowire devices.

9:36AM S12.00007 Measurement of thermal boundary conductance at sintered Si-Si interface, MASANORI SAKATA, TAKUMA HORI, TAKAFUMI OYAKE, Department of Mechanical Engineering, The University of Tokyo, JEREMIE MAIRE, MASAHIRO NOMURA, Institute of Industrial Science, The University of Tokyo, JUNICHIRO SHIOMI, Department of Mechanical Engineering, The University of Tokyo — Performance of thermoelectric materials is enhanced by reducing thermal conductivity (TC) without appreciably decreasing electrical properties. Recently, nanocrystalline formed by compaction of nanopowder by sintering has been shown to be a promising solution for low TC and high scalability However, little is known about the thermal boundary conductance (TBC) of the grain boundaries, which dominantly affect the TC, because of the difficulty to directly measure the TBC of the local boundaries. We have therefore developed a process to fabricate a highly planar and uniform bonded-interface between Si thin film and Si substrate, which is suitable for measuring the TBC of the interfaces with time-domain thermoreflectance method. We have found that sintering temperature and HF removal of native oxide on the wafers can change the interface structures from uniform to local SiO$_x$ structures, which alter the TBC from 0.1 to 1 G$\text{W}^{-1}\text{K}^{-1}$ order. Moreover, crystal orientation mismatch can change the TBC by several times. Together with theoretical calculation that relates the TBC and TC of nanocrystalline Si, the measurement results identify the route to reduce the TC less than the state-of-art value.

9:48AM S12.00008 Tuning nanoscale thermoelectricity with electron-electron interactions, ARUNIMA COOMAR, CHARLES STAFFORD, University of Arizona — The Nonequilibrium Green’s Function (NEGF) formalism is a powerful tool that provides a microscopic theory for interacting quantum systems out of equilibrium. In this talk, I will be presenting a few results obtained using the NEGF approach combined with pi-electron effective field theory to study the thermoelectric properties such as the thermopower (S) and the dimensionless figure of merit (ZT) across single-molecule junctions with pi-conjugated molecular systems, which exhibit destructive quantum interference of the electron waves. Some interesting results showcasing the tuning of the thermoelectric properties by embedding the junctions in a dielectric medium will be presented, along with our ongoing investigations of the transmission node spectrum in these molecular junctions, and the enhanced thermoelectricity resulting from it.

1 This research is partially supported by KAKENHI 2679009.

10:00AM S12.00009 Thermal Transport Properties of Low Dimensional SI, GE, and SI-GE Superlattice Structures, ALI KANDEMIR, Department of Materials Science and Engineering, Faculty of Engineering, Anadolu University, CEM SEVK, Department of Mechanical Engineering, Faculty of Engineering, Anadolu University — Potential low dimensional thermoelectric materials have captured considerable attention of researchers due to their possible adaptation in power generation, energy conversion, and solid-state cooling applications. Due to enhanced electrical conductivity of these systems, researchers mainly focused on to find a way of reducing thermal conductivity of these systems to enhance their thermoelectric performance. With this intention a number of theoretical and experimental studies have been carried out. Due to their extraordinary transport properties carbon based nano materials have been studied intensively and several different researchers have pointed out their highly efficient thermoelectric properties. Furthermore, as another nanostructure material family Si, Ge, and Si-Ge based nano systems have attracted attention and ZT values larger than 2.0 have been reported for some Si nanostructures. Considering the potential of these materials, we systematically investigate the thermal transport properties of bulk and nano superlattice structures of Si, Ge and SiGe by equilibrium molecular dynamics simulations. We predicted quite low lattice thermal conductivity for some specific structures of these materials. Our results show that the thermal conductivity of these structures can be suppressed up to 75 percent of bulk superlattice or pure nanowire structures.
10:12AM S12.00010 Thermoelectric Properties of Carbon nanohybrids Incorporated Polymer Nanocomposites1, KUN ZHANG, SHIREN WANG, Texas Tech University — In this work, non-covalently functionalized graphene with fluorinated fullerene (F-C60) by π-π stacking was integrated into poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS). F-C60 as a p-type semiconducting material was used. Polylithium intercalation during growth (P(O2)) after deposition of F-C60 on SiO2. The conduction behavior which changes from strongly localized transport that fits a Variable Range Hopping (VRH) model (low P(O2)) to thermally activated transport (high P(O2)) during growth determines the conduction behavior which changes from strongly localized transport that fits a Variable Range Hopping (VRH) model (low P(O2)) to thermally activated transport (high P(O2)). The transition is observed when P(O2) increases from 0.02% to 0.2%. The single-phase STO/Si films were of high crystalline quality as verified by x-ray diffraction, transmission electron microscopy, and atomically flat. Transport measurements were performed on the STO/Si structures in a Van der Pauw configuration. The P(O2) during growth determines the conduction behavior which changes from strongly localized transport that fits a Variable Range Hopping (VRH) model (low P(O2)) to thermally activated transport (high P(O2)). The resistivity of the strongly disordered STO/Si films decreased from 1 Ohm-cm to 3x10^-2 Ohm-cm as the film thickness increased (3nm-60nm). The perpendicular magnetoresistance (MR) is positive at 300K and becomes negative at T<20K. We consider competing effects on the STO/Si heterostructure such as 1.7% compressive strain resulting in SrTiO3 nanoparticle growth, changes in the piezoelectric field, changes in the lattice constant, changes in the band gap, and changes in the occupation of the conduction and valence bands.

1 NSF

10:24AM S12.00011 Non-linear thermoelectricity in disordered nanowires, KHANDKER MUTTALIB, SELMAN HERSHEYFIELD, University of Florida — We consider non-linear thermoelectric transport in an effectively one-dimensional disordered semiconductor nanowire connected to a pair of three-dimensional perfectly conducting semi-infinite leads, where the impurity band of the disordered wire can be shifted relative to the conduction band of the leads by applying a gate voltage. We show how the gate voltage can be tuned to optimize a unique interplay between the microscopic parameters characterizing the transmission of electrons through the nanowire and the thermodynamic parameters that characterize the Fermi functions in the leads. Assuming a Lorentzian distribution of disorder in the wire, we calculate the full non-linear thermodynamic efficiency η as well as the power output P. We show that for a fixed set of microscopic and thermodynamic parameters η can be increased from zero to η > 0.5ηC, where ηC is the Carnot efficiency, by simply changing the gate voltage. The power output P can then be scaled by connecting many wires in parallel.

10:36AM S12.00012 Tuning the Thermoelectric Properties of a Single-Molecule Junction by Mechanical Stretching1, RENATO PONTE, Federal University of Goias, ALBERTO TORRES, Federal University of Santa Catarina, ANTONIO J.R. DA SILVA, Brazilian Synchrotron Light Laboratory (LNLS), ADALBERTO FAZZIO, Sao Paulo University — We theoretically investigate, as a function of the stretching, the behaviour of the thermoelectric properties - Seebeck coefficient (S), the electronic heat conductance (γe) - and the figure of merit (ZT) - of a molecule-based junction composed by benzene-1,4-dithiol molecule (BDT) coupled to Au(111) surfaces at room temperature. We show that the thermoelectric properties of a single molecule can be tuned by mechanical stretching. The Seebeck coefficient can be positive, indicating that it is dominated by HOMO. Furthermore, it increases as the HOMO level, which is associated to the sulphur atom, goes to energies close to the Fermi level. By modelling the transmission coefficient of the system as a single Lorentzian peak, we propose a scheme to obtain the maximum ZT of any molecular junction.

1 The authors thank the Brazilian funding agencies CNPq, CAPES and FAPESP. We also thank CENAPAD-SP for the computational facilities.

10:48AM S12.00013 First-Principles Study on Thermoelectric Properties of Carbon Nanotubes, JOUNGHEE LEE, EUI-SUP LEE, YONG-HYUN KIM, KAIST — Carbon nanotubes (CNTs) have attracted much attention because of their extraordinary material properties such as strong mechanical strength, chirality- and diameter-dependent electronic structure, and high thermal conductivity. As an electronic material, CNTs can be used as high-performance thermoelectric materials. In this work, we studied the thermoelectric properties of CNTs using first-principles calculations. We found that the thermoelectric properties of CNTs can be tuned by changing the chirality and diameter of the CNTs. The Seebeck coefficient of (9,9) metallic CNTs is 1.3 mV/K with appropriate doping level, while it is 0.8 mV/K for (10,8) semiconducting CNTs with similar diameter. When the diameter is smaller, the Seebeck coefficient of one-dimensional CNT systems based on coherent electron transport within first-principle calculations and Landauer formulation. We will also estimate a contribution from diffusive transport, comparing to experimental results. The calculated maximum Seebeck coefficient is 0.13 mV/K for (9,9) metallic CNTs, while it is 0.8 mV/K for (10,8) semiconducting CNTs with similar diameter. When the diameter is smaller, the Seebeck coefficient of semiconducting CNTs can be as big as 1.3 mV/K with appropriate doping level.

10:50AM S13.00001 Electrical characterization of n-SrTiO3δ−/p-Si(100)epitaxial diode structures1, RYAN COTTIER, DANIEL CURR, NIKOLETA THEODOROPOULOU, Texas State University — Semiconducting, single crystalline n-p (n-STO/p-Si) junctions were grown by MBE (Molecular Beam Epitaxy) using a technique that suppresses the formation of a SiOx interfacial layer. The STO layer thickness varied from 3.6 to 30 nm, and oxygen vacancies were induced during growth by controlling the background O2 pressure (P(O2)) during growth. Incorporating of STO/F-C60 nanohybrids into highly conductivity metallic PEDOT:PSS formed Schottky barrier to selectively scatter low-energy carriers. Enhanced thermoelectric power factor of rGO/F-C60/PEDOT:PSS nanocomposites were observed with the optimized power factor of 83.2 µV/m.K2, which is 19 times of that of the highly conductive PEDOT:PSS. Additionally, the F-C60 nanoparticles on rGO surfaces hinder thermal transport by phonon scattering, resulting in the synergistic effect on enhancing thermoelectric properties. As a result, a figure of merit (ZT) of 0.10 was achieved.

1 NSF

10:52AM S13.00002 Transport properties of SrTiO3δ−/p-Si thin films grown by Molecular Beam Epitaxy on p-Si(001) substrates1, NIKOLETA THEODOROPOULOU, DANIEL CURR, RYAN COTTIER, Physics Dpt., Texas State University, ARTURO PONCE-PEDRAZA, JESUS CANTU, OSCAR VILLARREAL, Physics, Dpt., University of Texas-San Antonio — SrTiO3 (STO) films were grown on p-Si(001) and STO(001) bulk substrates using molecular beam epitaxy (MBE). Oxygen vacancies were introduced by controlling the Oxygen pressure during growth (P(O2)): 4 × 10^-6 - 8 × 10^-7 resulting in SrTiO3δ− with δ ∼ 0.02% for the lowest P(O2). The single-phase STO/Si films were of high crystalline quality as verified by x-ray diffraction, transmission electron microscopy, and atomically flat. Transport measurements were performed on the STO/Si structures in a Van der Pauw configuration. The P(O2) during growth determines the conduction behavior which changes from strongly localized transport that fits a Variable Range Hopping (VRH) model (low P(O2)-high disorder) to thermally activated transport (high P(O2)-low disorder). The resistivity of the strongly disordered STO/Si films decreased from 1 Ohm-cm to 3x10^-2 Ohm-cm as the film thickness increased (3nm-60nm). The perpendicular magnetoresistance (MR) is positive at 300K and becomes negative at T<20K. We consider competing effects on the STO/Si heterostructure such as 1.7% compressive strain induced by lattice mismatch to Si, defects due to oxygen vacancies, the bulk STO antiferrodistortive phase transition at 105K, and structural dislocations.

1 Funded by NSF Career Award DMR-1255629.
9:12AM S13.00005 Continuous strain modulation of strontium titanate (SrTiO$_3$) on semiconductor interface by thermal strains LEI ZHANG, YAKUN YUAN, SHIMING LEI, BERND KABIUS, VENKATRAMAN GOPALAN, ROMAN ENGEL-HERBERT, Pennsylvania State Univ. — Strain engineering is a general strategy for tuning the desired material properties, such as enhancing carrier mobility and increasing the spontaneous polarization and Curie temperature in ferroelectric films. Control over the strain state in thin film is provided by the substrate with lattice mismatch. Although growth of strained perovskite oxides was demonstrated, the limited number of suitable substrates of high quality imposed difficulty towards utilizing the strain. We’ll discuss a novel route towards wafer-scale strain engineering of ferroelectric oxide based on large thermal mismatch between film and substrate, enabling to continuously modulate the strain state. SrTiO$_3$ films were grown on Si (001) between 400 $^\circ$C and 900 $^\circ$C above the critical film thickness. The films relaxed at growth temperature and accumulated a tensile strain ranging from 0.2% to 0.7% during cool-down, which was proportional to the temperature difference. X-ray reciprocal space maps and geometric phase analysis obtained from cross section transmission electron microscopy have been used to relate the film’s strain state to the ferroelectric properties, probed by second harmonic generation and piezo force microscopy.

9:24AM S13.00006 Switchable two-dimensional electron gas at the interface of a ferroelectric and nonpolar insulator: BaTiO$_3$/SrTiO$_3$ KURT FREDRICKSON, ALEX DEMKOV, Univ of Texas, Austin — We theoretically investigate the interface between a ferroelectric BaTiO$_3$ film and a nonpolar insulating SrTiO$_3$ substrate. We find that thin BaTiO$_3$, under 5 nm, can stabilize two polarization states. While the nonpolarized state is insulating, for the polarized heterostructure, we discovered the existence of two-dimensional gases. In this case, the heterostructure undergoes an electronic reconstruction in order to prevent the polar catastrophe. The two-dimensional gases, formed as a result, screen the polarization, leading to a substantially reduced potential drop across the ferroelectric film. We emphasize that the two-dimensional electron and hole gases are created by the polarization of the sample, and is not due to the polar nature of either material or doping.

9:36AM S13.00007 Electronic carrier transport at epitaxial oxide-semiconductor interfaces LIOR KORNBLUM, ERIC JIN, CHARLES AHN, FRED WALKER, Dept. of Applied Physics and Center for Research on Interface Structures and Phenomena, Yale University, New Haven, CT 06511, USA — The epitaxial growth of transition metal perovskite oxides on conventional semiconductors is a promising approach for integrating the wealth of electronic phenomena found in these oxides with existing devices and technologies. Some oxide functionalities require charge transport to and from the semiconductor, making the semiconductor-oxide interface an important focal point in the utilization of epitaxial oxides in electronic devices. We present our findings on electronic carrier transport in the conduction band of titanate perovskites (TiO$_x$) epitaxially grown on silicon and on germanium. Metal-semiconductor contacts were fabricated by epitaxial deposition of metallic contacts on top of epitaxially-grown oxides on semiconductors. Transport measurements show diode-like transport across the interface of some of the structures, whereas whereas leakage currents are observed in others. These results are discussed in light of the physical and electronic structure at the oxide-semiconductor interface.

8:48AM S13.00008 Growth of Dielectric SrTiO$_3$(111) Film with Atomiically Well Defined Surface1 JIANDONG GUO, YAN LIANG, WENTAO LI, SHUYUAN ZHANG, Institute of Physics, Chinese Academy of Sciences — Oxide heterointerfaces exhibit novel properties that can be controlled by external fields. The (111) surfaces of perovskite oxides are particularly interesting since the six-fold symmetry is compatible with other quantum materials, e.g., topological insulators. We grow high quality SrTiO$_3$(111) film on Nb-doped substrate by oxide molecular beam epitaxy. By adjusting the flux rates of Sr and Ti, we keep the reconstruction of film surface unchanged as that on substrate all through the growth. Thus the cation stoichiometry is achieved since the surface reconstruction is determined by Sr:Ti concentration ratio and can be monitored in real-time. Moreover reconstruction allows the stable layer-by-layer growth of the polar film. In situ scanning tunneling microscope shows the atomically well defined film surface with broadened terraces. And the C-V measurements indicate that the tunable range of the carrier density is 2E13 per cm2 for a 50 nm film. This insulator/metal homoeptaxial system provides a template for the growth of novel low-dimensional structures with flexible tunability by gate voltage.

1This work is supported by Chinese NSF (11225422) and 973 project (2012CB921700).
10:00AM S13.00009 Growth of epitaxial poly-crystalline transition metal oxide thin films. SUNGMIN WOO, HOIDONG JEONG, SANG A LEE, HOSUNG SEO, Sungkyunkwan University, MORGANE LACOTTE, ADRIAN DAVID, CNRS UMR 6508, HYUN YOON KIM, Chungnam National University, WILFRID PRELLIER, CNRS UMR 6508, YUNSEOK KIM, WOO SEOK CHOI, Sungkyunkwan University — By comparing single- and poly-crystalline transition metal oxides (TMOs), one can study intriguing physical phenomena such as electronic and ionic conduction at the grain boundaries, phonon propagation, and various domain properties. In this work, we propose an approach to simultaneously fabricate single- and poly-crystalline epitaxial TMO thin films using substrate epitaxy of poly-crystalline SrTiO$_3$ (STO). In order to grow TMO thin films epitaxially with atomic precision, and to achieve a flat surface of the substrate is required. We fabricated SrTiO$_3$ (001), (110), and (111) oriented single-crystalline STO surfaces, which required different annealing conditions to achieve an atomically flat surface. A poly-crystalline STO surface was then prepared at the optimum condition for which all the domains with different crystallographic orientations could be successfully flattened. Studying the surface properties (surface potential, topography, and orientation) of poly-crystalline STO helped us to understand the formation of the atomically flat surface. Based on our research, we envision expansion of the studies regarding the epitaxial poly-crystalline TMO thin films and heterostructures.

10:12AM S13.00010 The surface of SrTiO$_3$ (111): effect of annealing in vacuum and in oxygen. MOHAMMAD SAGHAYEZHIAN, LINA CHEN, GAOMIN WANG, HANGWEN GUO, JIANDI ZHANG, EARL W. PLUMMER, Louisiana State Univ. — Baton Rouge — The surface of SrTiO$_3$ (111) have created a new playground for new physics, exhibiting novel properties such as 2DEG and topological phases such as quantum spin Hall effect. Due to the polar nature of the surface, it is very susceptible to different kinds of reconstructions which results in various terminations. There has been a fair amount of investigations on SrTiO$_3$ (111) as a function of sputtering and annealing, while less attention has been paid to its reconstruction when the surface comes in contact with oxygen or the mere effect of annealing in vacuum. We have focused on the surface reconstruction and chemical composition of SrTiO$_3$ (111) as a function of annealing temperature and oxygen pressure using LEED and ARXPS. We observed that annealing in oxygen brings more Ti to the surface in comparison with annealing in vacuum. Our data show that the SrTiO$_3$ (111) surface is highly reactive and easily absorbs carbon. Furthermore, we show that in contrast to SrTiO$_3$ (001), where carbon tends to be physisorbed and can easily be removed by low temperature annealing, on SrTiO$_3$ (111), carbon only leaves the surface after annealing to very high temperature. Also, our data show that the presence of oxygen can facilitate de-contamination of the surface and makes the surface more ordered.

1Supported by U.S. DOE under Grant No. DOE DE-SC0002136.

10:24AM S13.00011 Influence of Strain on the Thermoelectric Properties of electron-doped SrTiO$_3$ Thin Films. ALEXANDROS SARANTOPoulos, ELIAS FERREIRO-VILA, CIQUIS, Universidad de Santiago de Compostela, Santiago de Compostela, España, CESAR MAGEN, LMA, INA, Universidad de Zaragoza, 50018 Zaragoza, Spain & Fundación ARAID, 50018 Zaragoza, Spain, MYRIAM H. AGUIRRE, LMA, INA, Universidad de Zaragoza, 50018 Zaragoza, Spain, VICTOR PARDO, Instituto de Investigaciones Tecnológicas, Universidad de Santiago de Compostela, Spain, FRANCISCO RIVADULLA, CIQUIS, Universidad de Santiago de Compostela, 50018 Santiago de Compostela, España — The discovery of a two dimensional electron gas with high mobility at the interface between insulating LaAlO$_3$/SrTiO$_3$ (LAO/STO) opened the possibility of fabricating functional devices based on this interfacial effect. Therefore, it is important to study the influence of the growth parameters on the properties of the constituent materials. Here, we demonstrate that the thermoelectric properties of epitaxial thin films of Nb:STO can be finely tuned by adjusting the growth conditions in a PLD system. By growing the sample on different substrates, we demonstrate that the amount of vacancies depends on the degree of epitaxial compressive stress. The vacancies produced lead to impurity scattering at low temperatures. We show that the magnetoresistance response, and non-linear behavior of the Hall effect, characteristic of LaO/STO interfaces, can be reproduced in thin films of Nb:STO with a controlled number of vacancies. Moreover, we show that the Seebeck coefficient is a valid tool to obtain information about the degeneracy of the electronic band structure.

1We acknowledge support from the ERC 2D Therms project.

10:36AM S13.00012 Spectroscopic ellipsometry study on doped SrTiO$_3$ superlattice films. YUNSANG LEE, Y.K. SEO, Soongsil University, CHOI, J.W. SEO, J. LEE, Sungkyunkwan University — We report on the spectroscopic ellipsometry study on the low-dimensional confinement of chemical doping in SrTiO$_3$. We fabricated superlattice films composed of the stacking of insulating SrTiO$_3$ (STO) and metallic La-doped SrTiO$_3$ (SLTO) layers. As the dimensionality is varied from three to two dimensions by changing the thickness of the SrTiO$_3$ layers, phase transition from metal to insulator occurred through interplay of charge, spin, orbital, and lattice degrees of freedom. The optical conductivity spectra obtained from the spectroscopic ellipsometry show a significant change below the charge transfer gap near 3 eV through the insulator-metal transition. We detail our research expansion of the studies regarding the epitaxial poly-crystalline TMO thin films and heterostructures.

10:48AM S13.00013 Two-dimensional electron gas at surfaces of (001), (110), and (111) oriented SrTiO$_3$ induced by Ar$^+$-irradiation. LUDI MIAO, RENZHONG DU, YUEWEI YIN, QI LI, Penn State University — Two-dimensional electron gases (2DEGs) at transition metal oxide surfaces and interfaces have attracted much attention due to their fascinating exotic properties such as superconductivity, large magnetoresistance (MR), and ferromagnetism. We have created 2DEGs at the surfaces of (001), (110), and (111) oriented SrTiO$_3$ (STO) by Ar$^+$-irradiation and measured their transport properties. The 2DEGs exhibit a fully metallic behavior with the 2D charge carrier density around $2 \times 10^{14}$ cm$^{-2}$ and the mobility as large as 5500 cm$^2$V$^{-1}$s$^{-1}$ at low temperatures, which is tunable by electric fields applied through STO back gates. We have measured MR anisotropy of the 2DEGs at surfaces of STO with all orientations. We observed combinations of two types of components in their anisotropic MR at low temperatures. While the first type is an STO-orientation-independent two-fold component results from the Lorentz force effect, the second type shows stark differences between these 2DEGs as a consequence of distinct Fermi surface symmetries with different STO orientations. Indeed, it is four-fold for STO (001), two-fold for STO (110) and six-fold for STO (111), respectively.

Thursday, March 5, 2015 8:00AM - 11:00AM — Session S14 DMP FIAP: Focus Session: Dopants and Defects in III-V and II-VI Semiconductors

008A - Kirstin Alberi, National Renewable Energy Laboratory
8:00AM S14.00001 Carrier Decay and Diffusion Dynamics in Single-Crystalline CdTe as seen via Microphotoluminescence1. ANGELO MASCARENHAS, BRIAN FLUEGEL, KIRSTIN ALBERI, NREL, YONG-HANG ZHANG, Arizona State Univ. — The ability to spatially resolve the degree to which extended defects impact carrier diffusion lengths and lifetimes is important for determining upper limits for defect densities in semiconductor devices. We show that a new spatially and temporally resolved photoluminescence (PL) imaging technique can be used to accurately extract carrier lifetimes in the immediate vicinity of dark-line defects in CdTe/MgCdTe double heterostructures. A series of PL images captured during the decay process show that extended defects with a density of 1.4x10^{-5} cm^{-2} deplete photogenerated charge carriers from the surrounding semiconductor material on a nanosecond time scale. The technique makes it possible to elucidate the interplay between nonradiative carrier recombination and carrier diffusion and reveals that they both combine to degrade the PL intensity over a fractional area that is much larger than the physical size of the defects. Carrier lifetimes are correctly determined from numerical simulations of the decay behavior by taking these two effects into account. Our study demonstrates that it is crucial to measure and account for the influence of local defects in the measurement of carrier lifetime and diffusion, which are key transport parameters for the design and modeling of advanced solar-cell and light-emitting devices.

1We acknowledge the financial support of the Department of Energy Office of Science under Grant No. DE-AC52-06CH11357.

8:12AM S14.00002 Carrier scattering mechanisms in p-type transparent copper-alloyed ZnS: Crystalline vs. amorphous, RACHEL WOODS-ROBINSON, Materials Sciences Division, Lawrence Berkeley National Laboratory, ALIREZA FAGHANINIA, Department of Energy, Environmental and Chemical Engineering, Washington University in St. Louis, JASON K. COOPER, HIEU H. PHAM, Materials Sciences Division, Lawrence Berkeley National Laboratory, CYNTHIA LO, Department of Energy, Environmental and Chemical Engineering, Washington University in St. Louis, LIN-WANG WANG, JOEL W. AGER, Materials Sciences Division, Lawrence Berkeley National Laboratory — Crystalline (wurtzite and sphalerite) and amorphous forms of copper-alloyed ZnS (Cu_{x}Zn_{1−x}S) are p-type conducting transparent thin film materials with near-record figures of merit for applications in photovoltaics and optoelectronics. Remarkably, the conductivity of amorphous Cu_{x}Zn_{1−x}S, 42 S/cm at x = 0.30, is nearly as high as crystalline Cu_{x}Zn_{1−x}S (54 S/cm at x = 0.21). This contrasts with typical observations of poorer carrier transport in amorphous materials. By combining experiment and computation, we investigate the defect physics underlying hole transport in amorphous and crystalline Cu_{x}Zn_{1−x}S. Structural probes (EXAFS, TEM and wide-angle XRD) are used to determine bonding characteristics and lattice order, and serve as inputs to ab initio hybrid functional HSE calculations of the electronic structure. Hall effect, temperature dependent conductivity (15K to 580K), and XPS valence band measurements and ab initio calculations show that hole conduction occurs in a hybridized S-3p and Cu-3d valence band for amorphous and crystalline films. The hole scattering mechanisms which limit the conductivity will be discussed in the context of theoretical carrier transport model based on Boltzmann transport equation, ab initio calculated band structure, and phonon dispersion.

8:24AM S14.00003 Diffusion of Interstitial Defects in CdTe, SU-HUI AI, JI-HUI YANG, JIE MA, JOONGOO KANG, National Renewable Energy Laboratory — CdTe is one of the most promising candidates for thin-film photovoltaic applications and it is well known that Cu and Cl diffusions play critical roles in improving the CdTe solar cell efficiency. However, the diffusion behavior of these impurities as well as the host elements in CdTe has not been clearly understood. Using first-principles calculations, we determine the diffusion behaviors of the cation atoms (Cd and Cu) and the anion atoms (Te and Cl) at different charged states is investigated. We find that, due to different electronic level occupations and level splittings, the diffusion of the cation atoms and anion atoms are very different. We explain why Cu can diffuse much faster than other elements and show that the diffusion speeds of the impurities can be controlled by tuning the Fermi level of CdTe. We have also developed a general diffusion coefficient theory for multi-barrier diffusion. Our calculated diffusivity of the interstitial impurities agrees well with available experimental measurements.

2This work is supported by US/DOE/EEERE PREDICTS program.

8:36AM S14.00004 ABSTRACT WITHDRAWN —

8:48AM S14.00005 First-principles study of low Σ grain boundaries in CdTe, JI-SANG PARK, Natl Renewable Energy Lab, JOONGOO KANG, DGIST, JI-HUI YANG, WYATT METZGER, SU-HUI AI, Natl Renewable Energy Lab — Grain boundaries (GBs) play critical roles in determining physical properties of polycrystalline materials. In this study, we investigate stability and electronic structure of GBs in CdTe through first-principles density functional calculations. We consider low-Σ symmetric tilt GBs including Σ=111, Σ=112, Σ=120, and Σ=130 GBs. We find that the Σ=111 GB is more stable than the other GBs considered in this study because it contains no dangling bonds and wrong bonds. The stability of the Σ=112 GBs is independent on the chemical potential of Cd and Te whereas that of the Σ=130 GBs depends on the chemical potentials. Unexpectedly, we find that the Σ=120 GBs are more stable than the Σ=112 GBs, despite that the Σ=120 GBs have often been used as a model system to study GBs in polycrystalline thin-film photovoltaic materials. The Σ=120 GBs found in this study are not electrically harmful even though the GBs contain wrong bonds.

9:00AM S14.00006 Role of phonon-assisted processes in Auger recombination in InAs, JIMMY-XUAN SHEN, DANIEL STEIAUF, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Univ of California - Santa Barbara — Auger recombination has been identified as an important loss mechanism in InAs and InAs-based alloyed thin emitters, yet the mechanisms are not fully understood. In particular, it is unclear whether direct or indirect processes dominate. The direct process involves only Coulomb interaction, while the indirect process is mediated by the absorption or emission of a phonon. We present results of first-principles calculations of the direct and indirect phonon-assisted Auger coefficients in InAs and related alloys. The direct process is usually assumed to occur in small-band-gap semiconductors. However, we find that indirect phonon-assisted processes also contribute significantly to the Auger rate. We untangle the contributions of the electron-electron-hole and hole-hole-electron processes, and pinpoint the phonon modes that are most relevant to the indirect process.

9:12AM S14.00007 Electrical characterization of GaAsN and GaAsBi single-quantum-well diodes1, JO. OCCENA, R.L. FIELD III, A.S. TERAN, T. JEN, C. KURDACK, J.D. PHILLIPS, R.S. GOLDMAN, Univ of Michigan - Ann Arbor — The highly mismatched alloys GaAsN and GaAsBi have been identified as promising candidates for the active layer of optoelectronic devices because their bandgaps can be tuned with minimal change in lattice parameter. Since the conduction band minimum (CBM) of GaAsBi and the valence band maximum (VBM) of GaAsN are approximately aligned with the CBM and VBM of GaAs, with corresponding significant valence and conduction band offsets, GaAsN/GaAsBi is expected to exhibit a staggered Type II band-offset. The resulting spatial separation of charge and optical absorption at wavelengths larger than the fundamental bandgap, on either side of the junction, is promising for both infrared detectors and solar cells. To date, few groups have grown GaAsBi alloys and the GaAsN/GaAsBi heterostructure has yet to be realized. To explore the N- and Bi-related states near the CB and VB in GaAsN(Bi) alloys, Schottky diodes containing GaAsN(Bi) quantum wells (QWs) are grown by molecular-beam epitaxy at low temperature, using Si as either an n- or p-type dopant. For both GaAsN and GaAsBi QWs, rectifying current-voltage characteristics are observed, with reasonable diode ideality factors. We will discuss the influence of increasing N and Bi fraction on the formation of N- and Bi-related states. We will also discuss progress towards measurements of the VB and CB offsets using admittance spectroscopy.

1This material is based upon work supported by NSF grants DMR-1006835 and DMR-1410282.
GaAsBi and related bismuthide alloys. In addition, a comparison of the photoluminescence spectra of films grown with both As using As
4
and As
5
. The preference for Bi incorporation with As
4
over As
5
emerges as the ratio was increased from 15 to 40. As the growth temperature was decreased from 595 to 550 °C, the layers became more defective. Moreover, the layers became more defective. The strong radiative emission is concentrated in two narrow bands (~ 90 μeV width) at either 828.65 or 830.40 nm depending on the stacking fault orientation. Stacking fault defects can be imaged using far-field confocal microscopy by the narrow band photoluminescence. Polarization-resolved photoluminescence and magnetic field measurements are consistent with a theory of light-hole excitons bound to the stacking fault plane with a quantization axis normal to the plane. More recently, excitons bound to stacking faults were aligned with the temperature gradient-induced voltage, which is then converted to the local Seebeck coefficient, S. The S profile is then converted to a conduction band-
4
or Fe2
3
+ state to the stacking fault plane. The strong perturbation of the strain potential due to this fundamental growth defect. The narrow linewidth and high homogeneity across many defects suggests excitons are bound to a single atomically-thin stacking fault plane. This work opens the door to a novel, highly homogeneous, 2D light-hole excitonic system in the well-characterized material GaAs.


10:00AM S14.00011 Excitons bound to stacking fault planes in GaAs: a novel 2D excitonic system 1

1
 research was supported by the AFOSR FA9550-14-1-0179.

10:12AM S14.00012 Raman scattering and time-resolved photoluminescence characterization of defects in GaAs/AlGaAs double heterostructures 1

1
 research was supported by the U.S. DoE under Award Number DE-P0000012, the NSF GRFP under Grant No. DGE-1256082, the U.S. DoE under contract DE-FG02-06OR23100, and CSTEC, an EFRC funded by the U.S. DoE under Award No. DE-SC0000957.

10:24AM S14.00013 Profiling the local carrier concentration across a semiconductor quantum dot 3

3
 This material is based upon work supported by the U.S. DoE under Award Number DE-P0000012, the NSF GRFP under Grant No. DGE-1256082, the U.S. DoE under contract DE-FG02-06ER46339, and CSTEC, an EFRC funded by the U.S. DoE under Award No. DE-SC0000957.

10:36AM S14.00009 Isoelectronic Traps in Gallium Phosphide , THERESA CHRISTIAN, University of Colorado, Boulder and National Renewable Energy Laboratory.

10:24AM S14.00008 First-Principle Tight Binding-Like Parametrizations of GaAs
1−x
Bi
x
and InAs
1−x
Bi
x
, Electronic Structures , S.C. BADESCU, Wyle Aerospace/US AFRL, M.E. GRUPEN, US AFRL, J. HADER, J.V. MOONEY, NLCSTR, US, S.W. KOCH, Marburg Univ., Germany — The anion substitution with Bi atoms in large concentration (1-5%) has been proven to be an effective means for tuning the energy bandgap and the spin-orbit in materials like GaAs and InAs. In order to describe these materials in opto-electronic device simulations it is necessary to use simple and accurate parametrizations of their bandstructures. We describe here tight binding-like parametrizations of first-principle bandstructures to compare the better-known GaAs
1−x
Bi
x
with the newer InAs
1−x
Bi
x
. Accurate bandgaps are included via hybrid density functionals, and spin-orbit split-offs of the valence bands as well as the d-orbitals for In are found to be crucial. Essential features such as the strong perturbation of the Luttinger Hamiltonian and the strong anticovalence between valence bands and impurity d-orbitals are captured in a zone-unfolding picture.

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 NSF Grant No. 1150647, DGE-1256082.
We find the acceptor bound-exciton lifetimes to be lifetimes for the 12-state three-carrier complex. We confirm this prediction through polarization dependent and time-resolved photoluminescence experiments. We present a convenient formalism for predicting the optical properties of k=0 excitons with an arbitrary number of charge carriers in different symmetry environments. Using this formalism, we investigate the radiative lifetime of the neutral acceptor-bound exciton (A0) and the major parameter to control cell function is of great therapeutic interest. We developed a theoretical-experimental approach to investigate the biophysical mechanisms of EF interaction with cells in electrode-free physiologically-relevant configuration. Our numerical results demonstrated that EF frequency is the fundamental tool to control cell function. In contrast, high-frequency EF penetrates the cell membrane and reaches cell cytoplasm, where it may directly activate intracellular responses. Our theoretical predictions were confirmed in our experimental studies of the effects of applied EF on vascular cell function. Results show that non-oscillating EF increases vascular endothelial growth factor (VEGF) expression while field polarity controls cell adhesion rate. High-frequency, but not low frequency, EF provides differential regulation of cytoplasmic focal adhesion kinase and VEGF expression depending on the substrate, with increased expression in cells cultured on RGD-rich synthetic hydrogels, and decreased expression for matrigel culture. A theoretical-experimental approach to investigate the biophysical mechanisms of EF interaction with cells in electrode-free physiologically-relevant configuration. Our numerical results demonstrated that EF frequency is the non-invasive tool to control cell function and highlight the importance of a unified treatment of all recombination pathways when deriving the radiative properties of multi-carrier excitons.

1This material is based upon work supported by the National Science Foundation under Grant No. 1150647, DGE-0718124 and DGE-1256082.

Thursday, March 5, 2015 8:00AM - 11:00AM

Session S15 FIAP: Bio/Nano Applications Including Sensors
008B - Ernesto E. Marinero, Purdue University

8:00AM S15.00001 Regulation of cellular function via electromagnetic field frequency and extracellular environment: A theoretical- experimental approach1, TOLOO TAGHIAN, Univ of Cincinnati, ABDUL SHEIKH, Yale University, DARIA NAROMEVA, ANDREI KOGAN, Univ of Cincinnati — Application of external electric field (EF) as a non-pharmacological, non-invasive tool to control cell function is of great therapeutic interest. We developed a theoretical-experimental approach to investigate the biophysical mechanisms of EF interaction with cells in electrode-free physiologically-relevant configuration. Our numerical results demonstrated that EF frequency is the major parameter to control cell response to EF. Non-oscillating or low-frequency EF leads to charge accumulation on the cell surface membrane that may mediate membrane initiated cell responses. In contrast, high-frequency EF penetrates the cell membrane and reaches cell cytoplasm, where it may directly activate intracellular responses. The theoretical predictions were confirmed in our experimental studies of the effects of applied EF on vascular cell function. Results show that non-oscillating EF increases vascular endothelial growth factor (VEGF) expression while field polarity controls cell adhesion rate. High-frequency, but not low frequency, EF provides differential regulation of cytoplasmic focal adhesion kinase and VEGF expression depending on the substrate, with increased expression in cells cultured on RGD-rich synthetic hydrogels, and decreased expression for matrigel culture.

1The authors acknowledge the financial support from the NSF (DMR-1206784 & DMR-0804199 to AK); the NIH (1R21 DK078814-01A1 to DN) and the University of Cincinnati (Interdisciplinary Faculty Research Support Grant to DN and AK).

8:12AM S15.00002 Tunnel-Current based Single-Molecule Detection Method of Biopolymer Identification, TAKAHITO OHSHIRO, MAKUSU TSUTSUI, KAZUMICHI YOKOTA, MASATERU TANIGUCHI, Osaka Univ, BIONANOTECHNOLOGY TEAM — We have been proposed a tunneling-current based identification as a single-molecule biopolymer sequencing. This methodology is based on sequentially reading the tunneling-current across the single-synthetic polymer in the sequence, resulting in a high-speed electrical discrimination of the individual nucleotides. In this study, we report on a read of nucleotide sequence by the transverse electron transport through nanogap-electrode. We measured the extent of the electron-tunneling by using nanofabricated, mechanically controllable break junction, and determined the conductance values for deoxyribo/ribo-nucleoside monophosphates. When the molecules passed between the nanoelectrodes separated by a sub-nanometer gap, the tunneling-current through the molecules was increased, relative to that in the absence of molecules. The current intensity is found to be closely related to the individual molecular energy level. We also applied this method to base-pairing in oligonucleotides. Based on the electrical conductivity for single-nucleotides, we read the fragment of sample nucleotide passing through the sensing electrode. On the basis of a reconstruction of the read fragment sequences, we successfully determined a sample nucleotide sequence.

8:24AM S15.00003 Multiplexed microfluidic quantification of proteins in serum, NITIN RAJAN, SUKUMAR RAJARIA, ANDREW CLELAND, Univ of California - Santa Barbara — Rapid and low cost immunoassays targeting proteins in blood or other bodily fluids are highly sought after for point-of-care devices and early screening of patients. Immunoturbidimetric assays utilize latex particles functionalized with antibodies, with particle aggregation in the presence of the analyte detected by a change in absorbance. Using a high throughput micro-fluidic particle analyzer based solely on electrical signals (resistive pulse sensing), we are able to accurately quantify the degree of aggregation by analyzing the changes in the particle size distribution. Thus we study the aggregation of streptavidin (SAv) coated beads in the presence of biotinylated bovine serum albumin as a proof-of-principle assay and extract the binding capacity of the SAv beads from the dose-response curve. We also use our aggregation measurement platform to characterize a commercial C-reactive protein (CRP) immunoturbidimetric assay (hsCRP, Diazyme Inc.). We obtain a linear calibration curve as well as a better limit of detection of CRP than that obtained by absorbance measurements. By using different bead sizes functionalized with different antibodies, multiplexed analyte detection is also possible. We demonstrate this by combining the commercial anti-CRP functionalized beads (0.4 microns) with biotin coated beads (1.0 microns), and carry out the simultaneous detection of SAv and CRP in a single sample.

8:36AM S15.00004 ABSTRACT WITHDRAWN –

8:48AM S15.00005 Self-Assembled DNA Structures for Molecular Force Measurement: A Magnetically Actuated Approach, M. ARMSTRONG, S. LAUBACK, C. MILLER, C. PEACE, C. CASTRO, R. SOORYAKUMAR, Ohio State Univ - Columbus — Understanding molecular forces is important to comprehend many of the underlying properties of molecular machines and biological processes. The relevant forces in these cases often lie in the piconewton range, and thus experiments on individual biomolecules must integrate techniques capable of measuring such forces. A mechanical system to measure molecular forces associated with interacting DNA strands is being developed by using self-assembled DNA nanostructures and super-paramagnetic beads. The DNA nanostructure consists of single-stranded DNA molecules which can be folded into a precise compact geometry using hundreds of short oligonucleotides, i.e., staples, via programmed molecular self-assembly. These nanostructures can be polymerized into micron-scale filaments. By functionalizing the filament ends with bispesific conjugate staples, the structure can be attached to a surface as well as labeled with magnetic beads in order to apply a force on the system. Externally magnetic fields provide the means to maneuver and manipulate the magnetically labeled DNA structures. Preliminary findings associated with the DNA constructs and their manipulation lay the groundwork to establish real-time control of DNA nanodevices with micromanipulation.
9:00AM S15.00006 Sensitization of sub 10 nm Yb\(^{3+}\)-doped NaYF\(_4\) nanoparticles with visible light through 1,2,3,4,5,6,7-heptaoctfluoro-8-hydroxyanthracene-9,10-dione chromophore. HAIZHOU LU, School of Physics and Astronomy, Queen Mary University of London, Mile End Road, London, E1 4NS, UK, YU PENG, School of Biological and Chemical Sciences, Queen Mary University of London, Mile End Road, London, E1 4NS, UK, IGNACIO HERNANDEZ, Dpto. CITIMAC, Universidad de Cantabria, Facultad de Ciencias, Avda. Los Castros, 39005, Santander, Spain, WILLIAM GILLIN, School of Physics and Astronomy, Queen Mary University of London, Mile End Road, London, E1 4NS, UK — Uniform sub 10 nm Yb\(^{3+}\)-doped NaYF\(_4\) nanoparticles were prepared using a conventional hydrothermal method. Yb\(^{3+}\) ions doped inside the NaYF\(_4\) nanoparticles can be sensitized with 1,2,3,4,5,6,7-heptaoctfluoro-8-hydroxyanthracene-9,10-dione (HL), which is bounded onto the surface of the nanoparticle, through the so-called "antenna effect." Strong sensitization is achieved with the broad visible light excitations. The overall near infrared (NIR) emission from Yb\(^{3+}\) ions is increased by a factor of 5 as a result of the broad and strong absorption of HL chromophore compared with the ytterbium's intrinsic absorption during the 980 nm regime. Interestingly, an energy migration process from Yb\(^{3+}\) ions on the surface to inner-side Yb\(^{3+}\) ions of doped nanoparticle is demonstrated by the time-resolved spectroscopy method. It gives a direct evidence that the local environment between the surface and center of the nanoparticle is different. We believe our material will contribute to the NIR emitters with a strong visible absorption for the bio-materials.

9:12AM S15.00007 Low cost sensing technology for type 2 diabetes monitoring. PRASHANT SARSWAT, MICHAEL FREE, University of Utah — Alpha-hydroxybutyrate (2-hydroxybutyrate or α-HB) is becoming more widely recognized as an important metabolic biomarker that has been shown to be highly correlated with prediabetes and other metabolic diseases. In 2012 there were 86 million Americans with prediabetes, many of whom are not aware they have prediabetes, but could be diagnosed and treated to prevent type 2 diabetes if a simple, low-cost, convenient test were available. We have developed new, low-cost, accurate α-HB detection methods that can be used for the detection and monitoring of diseases such as prediabetes, type 2 diabetes, β-cell dysfunction, and early hyperglycemia. The new sensing method utilizes a diode-connection microchip, additives, and a phototransistor to detect α-HB at levels near 1 micro g/l in the presence of serum compounds such as lactic acid, sodium pyruvate, and glucose. The objective of this research is to improve the understanding of the interactions that enhance α-HB detection to enable additional improvements in α-HB detection as well as improvements in other biosensor applications.

9:24AM S15.00008 A pH-gradient induced method for wetting metal-layer embedded nanopores. VENKAT BALAGURUSAMY, GUSTAVO STOLOVITZKY, IBM T.J. Watson Research Center, Yorktown Heights, NY — Solid-state nanopores made on a single layer of Silicon nitride are wet by a number of methods by different workers. Typically, they involve using some low-surface tension liquid like isopropanol for pre-wetting before filling with the electrolyte solution of interest e.g., a buffered KCl solution both sides of the chamber that partitions the nanopore. These methods can also be preceded by a cleaning step which may involve either oxygen plasma or piranha treatment. However we found that these methods were not successful in wetting certain batches of nanopores drilled in a stack of SiO\(_2\)/TiN/SiO\(_2\)/Si layers. We found that applying buffer solutions at different pH on the two sides of the nanopore greatly accelerated the wetting process from days to few hours and resulted in nanopores with near linear I-V behavior for high salt concentration buffer solutions. We will describe this method and the results for a number of nanopores. [1] Nanopores wet with this pH gradient method translocate DNA molecules like nanopores wet by other methods mentioned here. We believe that the actual mechanism of this wetting process is influenced strongly by the pH effect on SiO\(_2\) surface. Efforts are underway to understand the working of this wetting method by quantum computer simulation methods [2]. [1] V.S.K.Balagurusamy, US Patent 8702944 (April 2014), “A novel nanopore device wetting method ” [2] R.Zhou, Soft matter theory/simulations group, IBM Watson Research Center, personal communication

9:36AM S15.00009 Nanoribbon field-effect transistors as direct and label-free sensors of enzyme-substrate interactions. LUYE MU, Electrical Engineering, Yale University, ILIA DROUJININE, Genetics, Harvard Medical School, NITIN RAJAN, SONYA SAWTELLE, Applied Physics, Yale University, MARK REED, Electrical Engineering and Applied Physics, Yale University — The ability to measure enzyme-substrate interactions is essential in areas such as diagnostics, treatment, and biochemical screens. Many enzymatic reactions alter the pH of its environment, suggesting a simple and direct method for detection. We show the ability of Al\(_2\)O\(_3\)-coated Si nanoribbon field-effect biosensors to sensitively measure various aspects of enzyme-substrate interactions through measuring the pH. [Urea in phosphate buffered saline (PBS) and penicillinase in PBS and urine were measured to limits of -200 μM and 0.02 units/mL, respectively. We also show the ability to extract accurate kinetics from the interaction of acetylcholine and its esterase. Prior work on FET sensors has been limited by the use of surface functionalization, which not only alters enzyme-substrate affinity, but also makes enzyme activity quantification difficult. Our method involves direct detection of reactions in solution without requiring alteration to the reactants, allowing us to obtain repeatable results and sensitive limits of detection. This method is a simple, inexpensive, and effective platform for detection of enzymatic reactions, and can be readily generalized to many unrelated classes of reactants.

[1] This work was supported in part by U.S. Army Research Office and Air Force Research Laboratory


9:48AM S15.00010 ToF-SIMS Characterization of Biocompatible Silk/Poly(pyrrole) Electromechanical Actuators. NATHAN BRADSHAW, SEAN SEVERT, Western Washington Univ, ZHAOYING WANG, Pacific Northwest National Laboratory, CARLY KLEMEK, JESSE LARSON, Western Washington Univ, ZHIJIA ZHU, Pacific Northwest National Laboratory, AMANDA MURPHY, JANELLE LEGER, Western Washington University — Materials capable of controlled movements that can also interface with biological environments are highly sought after for biomedical devices such as valves, blood vessel sutures, cochlear implants and controlled drug release devices. Recently we have reported the synthesis of films composed of a conductive interpenetrating network of the biopolymer silk fibroin and poly(pyrrole). These silk-Ppy composites function as bilayer electromechanical actuators in a biologically-relevant environment, can be actuated repeatedly, and are able to generate forces comparable with natural muscle (>0.1 MPa), making them an ideal candidate for interfacing with biological tissues. Here, time of flight secondary ion mass spectrometry was used to investigate the migration of ions in the devices during actuation. These findings will be discussed in the context of the actuation mechanism and opportunities for further improvements in device stability and performance.

10:00AM S15.00011 Biocompatible Silk-Poly(Pyrrole) Composite Trilayer Electromechanical Actuators. CARLY KLEMEK, NATHAN BRADSHAW, JESSE LARSON, SEAN SEVERT, NICHOLAS OSTROVSKY-SNIDER, AMANDA MURPHY, JANELLE LEGER, Western Washington University — Biocompatible materials capable of controlled actuation are in high demand for use in biomedical applications such as dynamic tissue scaffolding, valves, and steerable surgical tools. Conducting polymers (CPs) have some desirable traits for use as an actuator, such as the ability to operate in biologically relevant fluids and responsiveness to low voltages. However CPs alone are limited due to their brittle nature and poor solubility. Recently we have shown that a composite material of silk and the CP poly(pyrrole) (Ppy) shows promising characteristics as an actuator; it is mechanically robust as well as fully biocompatible. Initial proof-of-concept experiments demonstrated that these composites bend under an applied voltage (or current) using a simple bilayer device. Here we present the development of a trilayer device, composed of two conductive layers separated by an insulating silk layer. This configuration has twice the active surface area as a bilayer, potentially increasing the amount of mechanical motion per volt applied. We will discuss the fabrication and characterization of these devices, as well as their performance and future applications of this technology.
10:12AM S15.00012 Developing a nanoscale pressure sensor utilizing the Plasmon Ruler, ALEX TAYLOR, DAVID CARROLL, Wake Forest Univ — We demonstrate a novel method for detecting pressure by utilizing the Plasmon Ruler; the effect by which the frequency of light scattered by a nanoparticle (NP) is red shifted when brought into close proximity with another NP. This distance dependent phenomenon is leveraged by a film/NP architecture, wherein silver NPs are suspended above a silver film by a polymer spacing layer. As the fluid pressure above the rigid substrate is increased, the polymer layer is compressed and the NP height is decreased, leading to a measurable redshift in the plasmon resonance frequency. Thus, by factoring in the strength of the polymer layer’s restoring force we can determine the pressure being applied. These devices were constructed onto optic wires, which allow us to probe the device using the evanescent field from light inside the glass core. This naturally leads to in vivo medical applications, such as inter-compartment or inter-cranial pressure sensing via the inserted fiber optic probe.

10:24AM S15.00013 Highly Selective and Sensitive Detection of Acetylcholine Using Receptor-Modified Single-Walled Carbon Nanotube Sensors, SHIHONG XU, BYEONGJU KIM, HYUN SEOK SONG, HYE JUN JIN, EUN JIN PARK, SANG HUN LEE, Seoul National University, BYUNG YANG LEE, Korea University, TAI HYUN PARK, SEOUNGUN HONG, Seoul National University — Acetylcholine (ACh) is a neurotransmitter in a human central nervous system and is related to various neural functions such as memory, learning and muscle contractions. Dysfunctional ACh regulations in a brain can induce several neuropsychiatric diseases such as Alzheimer’s disease, Parkinson’s disease and myasthenia gravis. In researching such diseases, it is important to measure the concentration of ACh in the extracellular fluid of the brain. Herein, we developed a highly sensitive and selective ACh sensor based on single-walled carbon nanotube-field effect transistors (swCNT-FETs). In our work, M1 muscarinic receptor protein, an ACh receptor, was expressed in E.coli and coated on swCNT-FETs with lipid membranes. Here, the binding of ACh onto the receptors could be detected by monitoring the change of electrical currents in the underlying swCNT-FETs, allowing the real-time detection of ACh at a 10 pM concentration. Furthermore, our sensor could selectively detect ACh from other neurotransmitters. This is the first report of the real-time sensing of ACh utilizing specific binding between the ACh and M1 mAChR, and it may lead to breakthroughs in various biomedical applications such as drug screening and disease diagnosis.

10:36AM S15.00014 Nanovesicle-Carbon Nanotube Hybrid Structures Mimicking Mammalian Pain Sensory System, YOUNG TAK CHO, HYE JUN JIN, Department of Physics and Astronomy, Seoul National University, JEONG MI AN, Department of Oral Biology, College of Dentistry Yonsei University, JUHUN PARK, Department of Physics and Astronomy, Seoul National University, SEOK JUN MOON, Department of Oral Biology, College of Dentistry Yonsei University, SEOUNGUN HONG, Department of Physics and Astronomy, Seoul National University — We developed a “chemical-pain sensor” based on a single-walled carbon nanotube-based field effect transistor (SWNT-FET) functionalized with rat pain sensory receptor, rat transient receptor potential vanilloid 1 (rTRPV1) mimicking a mammalian pain sensory system. The sensor can selectively detect chemical pain stimuli such as capsaicin and resiniferatoxin with a sensitivity of 1 pM detection limit. Since this sensor allows one to quantitatively measure the concentration of chemical pain stimuli just like animal sensory systems, it can be used for various practical applications such as food screening. In addition, TRP families including rTRPV1 protein used for the sensor are now suggested as potential drug targets related to nerve and circulation disorders. Thus, the capability of measuring TRP responses using our sensor platform should open up other applications such as drug screening and basic research related with nerve and circulation systems.

10:48AM S15.00015 Floating Electrode Sensor based on CNT-FET for the Detection of DNAs, MINJU LEE, BYEONGJU KIM, JOOHYUNG LEE, SEON NAMGUNG, JOEONGSU KIM, Seoul Natl Univ, JAE YEOL PARK, Doowon Technical University College, MOON-SOOK LEE, Samsung Advanced Institute of Technology, SEOUNGUN HONG, Seoul Natl Univ — DNA sensors based on carbon nanotube (CNT) networks have been drawing much attention due to their high sensitivities. In the CNT network-based DNA sensors, the modulation of the Schottky barrier by the DNA hybridization has been known to play an important role in detecting target DNAs. In such applications, many researchers have tried to enhance the sensitivity of the Schottky barrier-based sensors through various methods such as the formation of a nonsymmetrical Schottky contact or the increase of the Schottky contact area. However, these methods suffered from some limitations such as the difficulty of controlling the sensor response for applications. Here in, we developed a floating electrode-based DNA sensor with controllable responses. In this strategy, metallic floating electrodes were fabricated to form Schottky barriers between CNTs and floating electrodes. We showed that the increased number of floating electrodes could enhance the sensitivity of our sensor. We also analyzed our results based on the Langmuir isotherm theory. This efficient approach could be an important strategy to improve the sensitivity and to control the response of CNT network-based sensors. Our work should provide an important insight regarding Schottky barrier-based sensors.

Thursday, May 3, 2015 8:00AM - 11:00AM
Session S16 DMP: Focus Session: Graphene Devices: Function, Fabrication, and Characterization: van der Waals Heterostructures 101AB - Akm Nawaz, San Francisco State University

8:00AM S16.00001 Bilayer Graphene-Hexagonal Boron Nitride Heterostructure Negative Differential Resistance Interlayer Tunnel FETs, SANGWOO KANG, BABAK FALLAHZAD, KAYOUNG LEE, HEMA MOVVA, KYOUNGHWAN KIM, CHRIS CORBET, Univ of Texas, Austin, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan, LUIGI COLOMBO, Texas Instruments Incorporated, LEONARD REGISTER, EMANUEL TUTUC, SANJAY BANERJEE, Univ of Texas, Austin — We present the operation of a vertical tunneling field effect transistor using a stacked double bilayer graphene (BLG) and hexagonal boron nitride (hBN) heterostructure. The device is fabricated with the so-called Van der Waals transfer method with the edges of the top and bottom BLG flakes being rotationally aligned to roughly 60°. The device shows multiple negative differential resistance (NDR) peaks which can be adjusted through the gate bias. Temperature dependent measurements show that the peak width of the differential conductance broadens and the height lowered when the temperature is increased, which is indicative of resonant tunneling. Three electron states at the Fermi level are seen, it is shown that the multiple peaks occur when the two conduction bands at the K-point of the top and bottom bilayer graphene become aligned at certain bias conditions. It is also shown that by adjusting the rotational alignment of the bands of the top and bottom BLG through an in-plane magnetic field, the conductance peaks can be broadened. In addition, utilizing the NDR characteristic of the device, one-transistor latch or SRAM operation is demonstrated.

8:12AM S16.00002 Resonant Tunneling in Double Bilayer Graphene Heterostructures, BABAK FALLAHZAD, KAYOUNG LEE, SANGWOO KANG, JIAMIN XUE, STEFANO LAURENTIS, CHRISTOPHER CORBET, KYOUNGHWAN KIM, HEMA MOVVA, Univ of Texas Austin, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan, LEONARD REGISTER, SANJAY BANERJEE, EMANUEL TUTUC, Univ of Texas, Austin — We present the realization and characterization of independently contacted and rotationally aligned double bilayer graphene heterostructures, that show gate-tunable tunneling resonances and negative differential resistance in their interlayer current-voltage characteristics. Our devices are fabricated by successively stacking mechanically exfoliated bilayer graphene and hexagonal boron nitride dielectric using a layer-by-layer transfer technique. The bilayers are rotationally aligned during the device fabrication by selecting flakes with straight edges, and using them as a reference for alignment. We determine the heterostructure energy band alignment at the tunneling resonance using the individual layer carrier densities, and including the chemical potential dependence on the carrier density. Our analysis show that the tunneling resonances occur when the charge neutrality points of the two bilayer graphene flakes are energetically aligned, which suggests the resonances stem from the momentum conserving tunneling.
8:24AM S16.00003 Graphene superlattices in van der Waals heterostructures, VLADIMIR FALKO, Lancaster University — The technological development of graphene has generated new high-quality systems offer access to the earlier inaccessible extremes of quantum physics. When graphene is placed on an atomically flat substrate with hexagonal lattice with a close lattice constant, such as boron nitride (hBN), and their crystalline axes are aligned, a long-wavelength perfectly periodic moiré pattern forms for electrons in graphene. Various regimes of possible moiré minibands at zero magnetic field [Phys. Rev. B 87, 245408 (2013); Phys. Rev. B 88, 205418; Phys. Rev. B 88, 155415 (2013); New J. Phys. 15, 123009 (2013)] and strong magnetic field [Nature 497, 594 (2013), Nature Physics 10, 525 (2014); Phys Rev B 89, 075401 (2014)] will be discussed. Experimentally available graphene samples are enough to provide flux \( \psi \) through the moiré superlattice cell comparable to the magnetic flux quantum \( \phi_0 \) and reach the regime of fractal Hofstadter spectra. As a result, a single device can offer a multiplicity of two-dimensional electron systems, realised at rational flux values \( \psi = \phi_0, \phi_0/2, 2\phi_0/3, \) etc., each with its own intrinsic topological properties, including quantum Hall effect physics related to the effective Landau levels emerging from these magnetic minibands at the nearby range of magnetic fields.

9:00AM S16.00004 A boron nitride - graphene - C\textsubscript{60} heterostructure, CLAUDIA OJEDA-ARISTIZABAL, UC Berkeley, ELTON J.G. SANTOS, University of California, Berkeley, JAIRO VELASCO JR., SALMAN KAHN, UC Berkeley, AIMING YAN, UC Berkeley, JOSEF YOUNG, Lawrence Berkeley National Laboratory, KAVIENERGY, Lawrence Berkeley National Laboratory — We have fabricated a new van-der-Waals heterostructure composed by BN/graphene/C\textsubscript{60}. We performed transport measurements on the preliminary BN/graphene device finding a sharp Dirac point at the neutrality point. After the deposition of a C\textsubscript{60} thin film by thermal evaporation, we have observed a significant n-doping of the heterostructure. This suggests an unusual electron transfer from C\textsubscript{60} into the BN/graphene structure. This BN/graphene/C\textsubscript{60} heterostructure can be of interest in photovoltaic applications. It can be used to build devices like p-n junctions, where C\textsubscript{60} can be easily deposited in defined regions of a graphene junction by the use of a shadow mask. Our results are contrasted with theoretical calculations.

9:12AM S16.00005 Tunneling measurements in graphene-hexagonal boron nitride-based heterostructures\(^1\), U. CHANDNI, Institute for Quantum Information and Matter and Department of Physics, California Institute of Technology, Pasadena, California 91125, USA, K. WATANABE, T. TANIGUCHI, National Institute for Materials Science, 1-1 Namiki, Tsukuba Ibaraki 305-0044, Japan, J.P. EISENSTEIN, Institute for Quantum Information and Matter and Department of Physics, California Institute of Technology, Pasadena, California 91125, USA — Van der Waals heterostructures is an emerging field involving the study of layered materials consisting of various crystalline atomic planes exfoliated from bulk crystals and then stacked, often by hand, in custom-made patterns. Vertical tunneling structures made out of such quasi-2D crystals are potentially very interesting and may provide a new playground to observe electron-electron interaction effects in graphene and related materials. In the present work, we report the fabrication and study of several such tunnel junctions, including metal-hexagonal boron nitride (hBN)-metal, metal-hBN/graphite and metal-hBN-graphene tunneling devices. Tunneling measurements done at low temperatures and high magnetic fields reveal interesting and distinct features in each of these designs.

\(^1\)We acknowledge funding provided by the National Institute of Information and Matter, an NSF Physics Frontiers Center with support of the Gordon and Betty Moore Foundation through Grant GBMF1250.

9:24AM S16.00006 Ultra-sensitive Hall sensors based on graphene boron nitride heterostructures, JAN DAUBER, JARA-FIT and II. Institute of Physics, RWTH Aachen University, Aachen, Germany, ABHAY A. SAGADE, Advanced Microelectronics Center Aachen (AMICA), AMO GmbH, Aachen, Germany, MARTIN OELLERS, JARA-FIT and II. Institute of Physics, RWTH Aachen University, Aachen, Germany, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan, DANIEL NEUMAIER, Advanced Microelectronics Center Aachen (AMICA), AMO GmbH, Germany, CHRISTOPH STAMPFPER, JARA-FIT and II. Institute of Physics, RWTH Aachen University, Aachen, Germany — Recent developments of encapsulating graphene in hexagonal boron nitride lead to well protected graphene with very high material quality. This opens interesting possibilities for applications, such as graphene-based Hall sensors. Magnetic field sensors using Hall effect are widely used in different fields of applications, e.g. automotive and consumer electronics. Their performance benefits greatly from high room temperature mobility and low charge carrier density, which is achievable with the integrated material for the sensor and the sensor elements based on graphene boron nitride heterostructures. We show a detailed characterization including Hall effect measurements under ambient and vacuum conditions. We achieve current- and voltage-related sensitivity up to 5700 V/AT and 3V/VT, respectively, outpacing state-of-the-art silicon and III/V Hall sensor devices. Finally, we determine a magnetic resolution limited by low frequency electric noise less than 0.5 mG/Hz.

9:36AM S16.00007 Colossal Coulomb Drag in Double Bilayer Graphene Heterostructures\(^1\), KAYOUNG LEE, JAIMIN XUE, The University of Texas at Austin, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, EMANUEL TUTUC, The University of Texas at Austin — Double-layer electron systems, where charge carriers are apart into two parallel layers, have been of interest thanks to their various interlayer interaction phenomena. One of the peculiar interaction features is Coulomb drag, in which current flowing in one layer (driving layer) induces voltage drop in the opposite layer (drag layer) via interlayer momentum transfer. Recent progress in the fabrication of heterostructures consisting of atomic layer materials such as graphene and hexagonal boron nitride (hBN) has led to high mobility double layer systems. Here we probe Coulomb drag in double bilayer graphene heterostructures separated by 2 – 5 nm thick hBN dielectrics. At temperatures \( T \) lower than 30 K, we observe an anomalous Coulomb drag in the vicinity of the drag layer charge neutrality points, which increases as \( T \) is reduced. At \( T = 1.4 \) K, the lowest temperature studied here, the drag resistivity becomes comparable to the layer resistivity at a finite drag layer density \( n_{\text{drag}} \). The ratio of the drag to layer resistivity increases as the hBN thickness reduces, and also as the drag layer mobility increases. At \( T > 50K \), we observe diffusive drag, which increases with \( T \).

\(^1\)We thank ONR, NRI and Intel for support.

9:48AM S16.00008 Encapsulated Superconducting Graphene Nanodevices for Transport and Spectroscopic Studies, JOEL I-JAN WANG, Massachusetts Institute of Technology/Harvard School of Engineering and Applied Sciences, PATRICK BACK, Swiss Federal Institute of Technology in Zurich (ETHZ), YU-AN CHEN, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science (NIMS), Japan, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — Through proximity effect, graphene provides an ideal platform to study mesoscopic superconductivity and other quantum phenomena as it is in contact with superconductors. The advancement in the fabrication techniques of 2-D Van der Waals heterostructures has brought the superconducting graphene nanodevice into ballistic regime and made it suitable for a variety of studies. We show superconducting graphene nanodevices encapsulated in hexagonal boron nitride (hBN) thin films. The pristine graphene can be proximitized by superconducting leads, manipulated by local gating and probed by tunneling leads in order to explore various kinds of physics.
Topological materials may exhibit Hall-like currents flowing transversely to the applied electric field even in the absence of a magnetic field. In graphene superlattices, which have broken inversion symmetry, topological currents originating from graphene’s two valleys are predicted to flow in opposite directions. This work was supported in part by the Center for Low Energy Systems Technology (LEAST), one of the six SRC STARnet Centers, sponsored by MARCO and DARPA.

1We gratefully acknowledge support for this work from ONR (N00014-13-1-0806) and AFOSR (FA9550-12-1-0268).

10:24AM S16.00011 Electric field effects in graphene-complex-oxide heterostructures1. GIRRIRAJ JNAWALI, MENGCHEN HUANG, JEN-FENG HSU, FENG BI, LU CHEN, RONGPU ZHOU, Department of Physics and Astronomy, University of Pittsburgh, HYUNGWOO LEE, SANGWOO PYU, CHANG-BEOM EOM, Materials Science and Engineering, University of Wisconsin-Madison, PATRICK IRVIN, BRIAN D’URSO, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — Graphene has excellent electrical, chemical, and mechanical properties, which make it a promising material for developing nanoscale electronic devices, while complex-oxide heterostructure provide sharply confined multifunctional interfaces that can be tailored at nanodimension scales. The combination–graphene-complex-oxide heterostructures–merge the multifunctional properties of oxide interfaces such as high dielectric constant, metal-insulator-transition, magnetism, and superconductivity, with the unique electronic properties of graphene. Here we demonstrate some simple three-terminal field-effect devices that can realize the electronic properties of these two systems. Nanoscale devices are fabricated from graphene/LaAlO$_3$/SrTiO$_3$ heterostructures using c-AFM lithography. We demonstrate field effects in both the graphene and LaAlO$_3$/SrTiO$_3$ interfaces. These novel heterostructures open new avenues for creating devices that combine the most interesting and unique properties of the coupled two-dimensional electronic system.

1This work was supported in part by the Center for Low Energy Systems Technology (LEAST), one of the six SRC STARnet Centers, sponsored by MARCO and DARPA.

10:36AM S16.00012 Inelastic vertical tunneling in graphene-based heterostructures1. SERGIO DE LA BARRERA, RANDALL FEENSTRA, Carnegie Mellon University, Department of Physics — Lateral momentum conservation of tunneling states in graphene / hexagonal boron nitride / graphene heterostructures causes intriguing resonant behavior and negative differential resistance. We explain this phenomenon in terms of a simple model which includes electrostatic gating, rotational alignment between graphene layers, elastic scattering, and inelastic tunneling effects for both monolayer and bilayer graphene. We highlight recent experimental efforts to observe these effects in fabricated devices and compare with theory to validate our theoretical model. In order to improve future fabrication, we discuss disorder mechanisms, the differences between monolayer and bilayer graphene configurations, and the critical parameters which govern the characteristics of these devices.

1We gratefully acknowledge support for this work from ONR (N00014-13-1-0806) and AFOSR (FA9550-12-1-0268).

10:48AM S16.00013 Sensitive room-temperature graphene-BN atomic stack terahertz detector. JIAYUE TONG, MARTIN MUTHUE, SHAO-YU CHEN, SIGFIRD K YNGVESSON, JUN YAN, University of Massachusetts Amherst — Due to its high mobility, weak electron-phonon interaction and tunable broadband optical response, graphene is a promising material for high-speed optoelectronics such as terahertz (THz) detectors. In this presentation, we will discuss our studies of THz detection with graphene-BN heterostructure devices. Using a double-patch antenna that operates at around 1.9THz and an on-chip silicon lens, we demonstrate that asymmetrically-contacted graphene-BN heterostructure samples can efficiently detect THz laser radiation. Strong polarization dependence of our device indicates significant sensitivity improvement by antenna coupling and silicon lens coupling. We also find that responsivity can be tuned by changing the charge carrier density. Our work expands the methodology for making graphene-based THz detectors.

Thursday, March 5, 2015 8:00AM - 11:00AM – Session S17 DCMP: Graphene: Transport Properties 102AB - Inti Sodermann, Massachusetts Institute of Technology

8:00AM S17.00001 Detecting topological currents in graphene superlattices, GELIANG YU, ANDREY KRETININ, School of Physics and Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, UK, JUSTIN SONG, Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA, ROMAN GORBACHEV, Centre for Mesoscience and Nanotechnology, University of Manchester, Manchester M13 9PL, UK, LEONID LEVITOV, Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA, KONSTANTIN NOVOSELOV, ANDRE GEIM, School of Physics and Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, UK — Topological materials may exhibit Hall-like currents flowing transversely to the applied electric field even in the absence of a magnetic field. In graphene superlattices, which have broken inversion symmetry, topological currents originating from graphene’s two valleys are predicted to flow in opposite directions and combine to produce long-range charge neutral flow. We observed this effect as a nonlocal voltage at zero magnetic field in a narrow energy range near Dirac points at distances as large as several micrometers away from the nominal current path. Locally, topological currents are comparable in strength with the applied current, indicating large valley-Hall angles. The long-range character of topological currents and their transistor-like control by means of gate voltage can be exploited for information processing based on valley degrees of freedom.
8:12AM S17.00002 Quantum Spin Hall phase in multilayer graphene\textsuperscript{1}, NOEL GARCIA, JOSE LUIS LADO, JOAQUIN FERNANDEZ-ROSSIO, International Iberian Nanotechnology Laboratory (INL), THEORY OF NANOSTRUCTURES TEAM — We address the question of whether multilayer graphene systems are Quantum Spin Hall (QSH) insulators. Since interlayer coupling copes $p_z$ orbitals with $s$ orbitals of different layers and Spin-Orbit (SO) couples $p_z$ orbitals with $p_x$ and $p_y$ of opposite spins, new spins mixing channels appear in the multilayer scenario that were not present in the monolayer. These new spin-mixing channels cast a doubt on the validity of the spin-conserving Kane-Mele model for multilayers and motivates our choice of a four orbital tight-binding model in the Slater-Koster approximation with intrinsic Spin-Orbit interaction. To completely determine if the QSH phase is present we calculate for different number of layers both the $Z_2$ invariant for different stackings (only for inversion symmetric systems), and the density of states at the edge of semi-infinite graphene ribbon with armchair termination. We find that QSH systems with even number of layers are normal insulators while systems with odd number of layers are QSH insulators, regardless of the stacking.

\textsuperscript{1}We acknowledge financial support by Marie-Curie-ITN 607904-SPINOGRAPH

8:24AM S17.00003 Probing layer localization in twisted graphene bilayers via cyclotron resonance\textsuperscript{1}, CHI-KEN LU, National Taiwan Normal University, H.A. FERTIG, Indiana University Bloomington — Electron wave functions in twisted bilayer graphene may have a strong single-layer character or be intrinsically delocalized between layers, with their nature often determined by how energetically close they are to the Dirac point. We demonstrate that in magnetic fields, cyclotron resonance spectra contain signatures that may be used to distinguish the nature of these wave functions at low energies, as well as to locate low-energy critical points in the zero-field energy spectrum. Optical absorption for two different configurations–electric field parallel and perpendicular to the bilayer–is calculated, and the configurations are shown to have different selection rules with respect to which states are connected by the perturbation. Interlayer bias further distinguishes transitions involving states of a single-layer nature from those with support in both layers. For doped systems, a sharp increase in intra-Landau-level absorption occurs with increasing field as the level passes through the zero-field saddle-point energy, where the states change character from single layer to bilayer. The effects of impurity scattering will be discussed too.

\textsuperscript{1}This work was supported by the NSF through Grant No. DMR-1005035, the U.S.-Israel Binational Science Foundation, and Ministry of Science and Technology Taiwan Grant No. 103-2112-M-003-012-MY3

8:36AM S17.00004 Spin and valley polarized quantum Hall edge states in monolayer graphene, DI WEI, School of Engineering and Applied Sciences, Harvard University, JAVIER SANCHEZ-YAMAGISHI, Physics Department, Massachusetts Institute of Technology, TOENO VAN DER SAR, Physics Department, Harvard University, PABLO JARILLO-HERRERO, Physics Department, Massachusetts Institute of Technology, AMIR YACOBY, Physics Department, Harvard University — Studying edge transport in the quantum Hall regime provides insight into the nature of partially filled Landau levels. Previous reports on graphene have shown that when the four-fold degeneracy of each Landau level is lifted, spin and valley polarizations influence scattering between edges. We report progress on the fabrication of monolayer graphene devices encapsulated in hexagonal boron nitride (hBN), a technique which allows us to produce pristine graphene samples showing robust broken symmetry quantum Hall states. Additionally, graphene encapsulation allows us to create both globally and locally gated regions with sharp carrier density boundaries due to our thin hBN gate dielectrics. Here we study the transport of spin and valley polarized edge currents at these junctions.

8:48AM S17.00005 Twisting the physics in bilayer graphene, JASON LUO, JAVIER SANCHEZ-YAMAGISHI, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute of Materials Science, Japan, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — Twisted bilayer graphene is the ultimate limit of a bilayer 2DEG, where two graphene layers are stacked with an interlayer distance of only 0.34nm. The interlayer tunnel coupling can be continuously tuned by twisting the two layers, leading to different physics in the small and large twist angle limits. At small twist angles, the two layers form a large superlattice unit cell and the hybridization of the layers leads to low-energy van Hove singularities in the electronic spectrum, resulting in a strong departure from the typical monolayer graphene transport properties. At large twist angles, the system behaves as two decoupled monolayer graphene sheets, and the occupation of quantum Hall edge modes on each layer can be independently controlled. This allows for the realization of a quantum spin Hall state in twisted bilayer graphene by doping to form an electron-hole bilayer at moderate magnetic fields. I will discuss our magnetotransport measurements of high-quality twisted bilayer graphene, and how, by independently controlling the total charge density and applied electric field, we can realize different novel electronic states in this system.

9:00AM S17.00006 Ballistic transport and density of states of modulated bilayer graphene, LIUBOV ZHEMCHUZHNA, Hunter College, CUNY, DANHONG HUANG, Air Force Research Laboratory, Space Vehicles Directorate, GODFREY GUMBS, Hunter College, CUNY and Donostia International Physics Center (DIPC), ANDRII IUROV, University of New Mexico and Hunter College, CUNY — The magnetic band structure for electrostatically modulated bilayer graphene is calculated. We include the $K$ and $K'$ valleys. A and B sublattices as well as the bilayer crystalline structure. The energy eigenvalues are obtained as functions of wave vector as well as magnetic field. Our results are then employed in calculating density-of-states and ballistic conductance. Comparison with recent experimental results is presented.

9:05AM S17.00007 SU(4) symmetry breaking revealed by magneto-optical spectroscopy in epitaxial graphene\textsuperscript{1}, LIANG Z TAN, Univ of California - Berkeley, MILAN ORLITA, MAREK POTEMSKI, LNCMI, CNRS, MIKE SPRINKLE, CLAIRE BERGER, WALTER DE HEER, Georgia Institute of Technology, STEVEN LOUIE, University of California - Berkeley, GERARD MARTINEZ, LNCMI, CNRS — Electron-electron and electron-phonon interactions break the spin and valley degeneracies of the lowest Landau level (LL) in graphene. Multiple theoretical models have been proposed for the broken symmetry ground state. Previous tilted magnetic field transport experiments have obtained partial information on the ground state by probing the spin degree of freedom. In this work, we show that, via the valley-dependent electron-phonon interaction, symmetry breaking of the valley degree of freedom can be detected in infra-red transmission signatures close to magneto-phonon resonances. We have performed infra-red magneto-transmission experiments on multi-layer epitaxial graphene samples in magnetic fields up to 35 T. Following the main optical transition involving the lowest LL, we observe a new absorption transition increasing in intensity with magnetic fields greater than 26 T. Our theoretical calculations quantitatively explain these features, and unambiguously identify the charge density wave as the ground state in our samples.


9:12AM S17.00008 SU(4) symmetry breaking revealed by magneto-optical spectroscopy in epitaxial graphene\textsuperscript{1}, LIANG Z TAN, Univ of California - Berkeley, MILAN ORLITA, MAREK POTEMSKI, LNCMI, CNRS, MIKE SPRINKLE, CLAIRE BERGER, WALTER DE HEER, Georgia Institute of Technology, STEVEN LOUIE, University of California - Berkeley, GERARD MARTINEZ, LNCMI, CNRS — Electron-electron and electron-phonon interactions break the spin and valley degeneracies of the lowest Landau level (LL) in graphene. Multiple theoretical models have been proposed for the broken symmetry ground state. Previous tilted magnetic field transport experiments have obtained partial information on the ground state by probing the spin degree of freedom. In this work, we show that, via the valley-dependent electron-phonon interaction, symmetry breaking of the valley degree of freedom can be detected in infra-red transmission signatures close to magneto-phonon resonances. We have performed infra-red magneto-transmission experiments on multi-layer epitaxial graphene samples in magnetic fields up to 35 T. Following the main optical transition involving the lowest LL, we observe a new absorption transition increasing in intensity with magnetic fields greater than 26 T. Our theoretical calculations quantitatively explain these features, and unambiguously identify the charge density wave as the ground state in our samples.

\textsuperscript{1}This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by the NSF through XSEDE resources at NICS.
9:24AM S17.00008 Combination of conductance oscillation in the quantum Hall regime and charge trap flash memory phenomena in graphene field effect transistor, YOOJOO YUN, HAEYONG KANG, JOONG-GYU KIM, JEONCMIN PARK, THUY KIEU TRUONG, NAHEE PARK, JEONG-GYUN KIM, YOURACK LEE, CINAP, IBS, DOES, SunghyunKwanUniv., HOYEOL YUN, SANG WOOK LEE, School of Physics, Konkuk Univ., YOUNG HEE LEE, DONGSEOK SUH, CINAP, IBS, DOES, SunghyunKwanUniv., CINAP, IBS, DOES, SUNGYUNKWAN UNIV, TEAM, SCHOOL OF PHYSICS, KONKUK UNIV, COLLABORATION — We present the feature of conductance oscillation in the quantum Hall regime graphene FET on top of large gate-voltage hysteresis (up to 100 V). A mono-layer graphene was put on the hBN flake on the wet silicon oxide/silicon substrate. At 300 K, the normal conductance versus gate-voltage curve was observed showing the charge neutrality point without hysteresis. At 2 K, however, there was a huge conductance hysteresis during the sweep of gate-voltage, which could be attributed to the characteristics of charge-trap memory behavior because of defects located inside the dielectric playing a role of charge-trap sites. Even though the hysteresis during gate-voltage sweeping was enormous, in our device having hBN for graphene device preventing the deteriorating impacts from the defective SiO₂, the conductance oscillation during the gate-voltage sweep was observed from the magnetic field 4 T. In summary, the results proved that the combination of quantum Hall related transport phenomena and the charge-trap memory operation was achieved successfully without affecting each other in our graphene-on-hBN FET device.

9:36AM S17.00009 Transport in graphene on boron nitride, ASHLEY DASILVA, University of Texas at Austin, JEIL JUNG, National University of Singapore, SHAFFIQUE ADAM, Yale NUS College and National University of Singapore, ALLAN MACDONALD, University of Texas at Austin — The lattice mismatch and twist angle of graphene on boron nitride contributes to a long wavelength moire pattern in the atomic positions. This superlattice structure and the sublattice symmetry breaking in the hexagonal boron nitride layer lead to observable transport features in the graphene layer. We show a decreased conductivity at the Dirac point due to an opening of the band gap. There is also a decreased conductivity when the Fermi level is tuned to four carriers per moire unit cell, which is the position of the secondary Dirac points in perfectly matched and sublattice symmetric hexagonal bilayers. We show both intraband and interband contributions to the conductivity, the latter is peaked when the Fermi level is tuned inside the gaps, either at the Dirac point or the secondary Dirac points.

9:48AM S17.00010 Graphene-based quantum Hall resistance standards grown by chemical vapor deposition on silicon carbide, REBECA RIBEIRO-PALAU, FABIEN LAFONT, Laboratoire National de Metrologie et d’Essais, DIMITRIS KAZAZIS, Laboratoire de Photonique et de Nanostructures, ADRIEN MICHON, Centre de Recherche sur l’Hétéroépitaxie et ses Applications, OLIVIER COUTURAUD, CHRISTOPHE CONSEJO, BENOIT JOUAILT, Laboratoire Charles Coulomb, WILFRID POIRRIER, FELICIEN SCHOPFER, Laboratoire National de Metrologie et d’Essais — Replace GaAs-based quantum Hall resistance standards (GaAs-QHRS) by a more convenient one, based on graphene (Gr-QHRS), is an ongoing goal in metrology. The new Gr-QHRS are expected to work in less demanding experimental conditions than GaAs ones. It will open the way to a broad dissemination of quantum standards, potentially towards industrial end-users, and it will support the implementation of a new International System of Units based on fixed fundamental constants. Here, we present accurate quantum Hall resistance measurements in large graphene Hall bars, grown by the hybrid scalable technique of propane/hydrogen chemical vapor deposition (CVD) on silicon carbide (SiC). This new Gr-QHRS shows a relative accuracy of 1 × 10⁻¹¹ of the Hall resistance under the lowest magnetic field ever achieved in graphene. These experimental conditions surpass those of the most widely used GaAs-QHRS. These results confirm the promises of graphene for resistance metrology applications and emphasize the quality of the graphene produced by the CVD on SiC for applications as demanding as the resistance metrology.

10:00AM S17.00011 Observation of conducting edge states in graphene at zero magnetic field, MONICA ALLEN, Harvard University, ION FULGA, Weizmann Institute of Science, OLES SHTANKO, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, Massachusetts Institute of Technology, ANTON AKHMEROV, Delft University of Technology, LEONID LEVITOV, Massachusetts Institute of Technology, AMIR YACOBY, Harvard University — The electronic nature of edge states confined to the boundaries of a graphene crystal remains an outstanding question. Primarily, range from Anderson localization to chiral zero-energy edge modes, but a full microscopic picture of edge transport remains elusive. We directly image current transmission in real space by coupling superconducting electrodes to a graphene crystal and measuring quantum interference as a function of applied magnetic flux. To obtain a more quantitative picture, we employ Fourier techniques to extract the real space current distribution with nanoscale precision. We observe robust confinement of current to the edges of the crystal approaching the Dirac point and show that relative edge and bulk contributions are tunable via electrostatic gating. A strong candidate consistent with our data is the proposal of chiral edge modes that arise from sublattice symmetry breaking at the edge, sustained in all crystallographic edge orientations except atomically perfect armchair. Our techniques also open the door to fast spatial imaging of current distributions along more complicated networks of domains in larger crystals.

10:12AM S17.00012 ABSTRACT WITHDRAWN

10:24AM S17.00013 Experimental evidence of one-dimensional edge states at the line junction of two oppositely biased bilayer graphene, J. LI, Department of Physics, Penn State University, University Park, USA, K. WATANABE, T. TANIGUCHI, National Institute for Material Science, 1-1 Namiki, Tsukuba, Japan, ZHU, Department of Physics, Penn State University, University Park, USA — A one-dimensional edge (kink) state is predicted to exist at the line junction of two gapped bilayer graphene with opposite electric field bias or the stacking fault of AB-BA stacked bilayer regions. The conductance of the kink state is expected to be quantized at 4e²/h in the absence of K'-K' valley mixing, counting spin and layer degeneracy. This novel 1D system has not been realized experimentally due to fabrication challenges. Here we report evidence of the kink state in split dual-gated bilayer graphene, where the top and bottom splits are approximately 70 nm and precisely aligned. h-BN encapsulation ensures the high quality of the device, which allows us to make the bulk bilayer graphene very insulating at moderate E-fields of less than 0.3V/nm. The junction resistance RＪ exhibits drastic contrast between low resistances of several tens of KΩ when the two bilayers are oppositely biased, versus high resistances of several MΩ when the two E-fields have the same polarity. The low-resistance states are weakly insulating in temperature dependence and their resistances drop substantially in a perpendicular magnetic field. We discuss the nature of the kink state and possible reasons that RＪ deviates from the single-particle prediction of 4ℏ/π².

10:36AM S17.00014 Semiconducting transport characteristics of monolayer graphene through substrate-induced functionalization, PO-HSIANG WANG, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan, LO-YUEH CHANG, National Synchrotron Radiation Research Center, Taiwan, FU-YU SHIH, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan, PO-HSUN HO, Department of Materials Science and Engineering, National Taiwan University, Taiwan, CHIA-HAO CHEN, National Synchrotron Radiation Research Center, Taiwan, CHUN-WEI CHEN, Department of Materials Science and Engineering, National Taiwan University, Taiwan, WEI-HUA WANG, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan — We report semiconducting transport behaviors of monolayer graphene functionalized through chemically reactive substrates. In contrast to pristine graphene, graphene on activated SiO₂/Si substrates exhibits a transport gap at cryogenic temperature, nonlinear transfer characteristics, and insulating transport behaviors. Raman spectroscopy was performed to provide evidence of sp³ hybridization of graphene and confirms the presence of chemical bonding in the graphene samples. Moreover, we observe hopping transport characteristics at cryogenic temperature. Our study points toward an alternative method to control the functionalization of graphene and its transport behaviors.
10:48AM S17.00015 Tunable Optoelectronic Properties of Semiconducting Graphene1. MARC DVORAK, ZHIGANG WU, Department of Physics, Colorado School of Mines — If patterned properly, structural modifications on graphene can induce intervalley scattering between Dirac points and open a sizeable band gap. Such two-dimensional semiconductors could offer great tunability in electronic and optical properties. We performed calculations based on many-body perturbation theory using Green’s functions to obtain quasiparticle energies and optical absorption spectra for these semiconducting graphene structures, focusing on the role of defect size, type, and geometric configuration. Our results show a strong renormalization of the band gap over Kohn-Sham energy levels and exciton binding energies greater than 0.4 eV. By stacking monolayer defected graphene with various defect sizes and configurations, one could create an excellent photovoltaic absorber layer that efficiently absorbs photons with energy larger than 1.0 eV. 

1This work was supported by a U.S. DOE Early Career Award (Grant No. DE-SC0006433).

Thursday, March 5, 2015 8:00AM - 10:24AM –
Session S18 GSNP: Invited Session: Statistical Physics for Electric Grids Mission Room 103A - Guido Caldarelli, IMT Alti Studi Lucca

8:00AM S18.00001 Realistic modeling and analysis of synchronization dynamics in power-grid networks1. TAKASHI NISHIKAWA, Northwestern University — An imperative condition for the functioning of a power-grid network is that its power generators remain synchronized. Disturbances can prompt desynchronization, which is a process that has been involved in large power outages. In this talk I will first give a comparative review of three leading models of synchronization in power-grid networks. Each of these models can be derived from first principles under a common framework and represents a power grid as a complex network of coupled second-order phase oscillators with both forcing and damping terms. Since these models require dynamical parameters that are unavailable in typical power-grid datasets, I will discuss an approach to estimate these parameters. The models will be used to show that if the network structure is not homogeneous, generators with identical parameters need to be treated as non-identical oscillators in general. For one of the models, which describes the dynamics of coupled generators through a network of effective interactions, I will derive a condition under which the desired synchronous state is stable. This condition gives rise to a methodology to specify parameter assignments that can enhance synchronization of any given network, which I will demonstrate for a selection of both test systems and real power grids. These parameter assignments can be realized through very fast control loops, and this may help devise new control schemes that offer an additional layer of protection, thus contributing to the development of smart grids that can recover from failures in real time.

1Funded by ISEN, NSF, and LANL LDRD.

8:36AM S18.00002 Complex Dynamics of the Power Transmission Grid (and other Critical Infrastructures). DAVID NEWMAN, Univ. of Alaska Fairbanks — Our modern societies depend crucially on a web of complex critical infrastructures such as power transmission networks, communication systems, transportation networks and many others. These infrastructure systems display a great number of the characteristic properties of complex systems. Important among these characteristics, they exhibit frequent large cascading failures that often obey a power law distribution in their probability versus size. This power law behavior suggests that conventional risk analysis does not apply to these systems. It is thought that much of this behavior comes from the dynamical evolution of the system as it ages, is repaired, upgraded, and as the operational rules evolve with human decision making playing an important role in the dynamics. In this talk, infrastructure systems as complex dynamical systems will be introduced and some of their properties explored. The majority of the talk will then be focused on the electric power transmission grid though many of the results can be easily applied to other infrastructures. General properties of the grid will be discussed and results from a dynamical complex systems power transmission model will be compared with real world data. Then we will look at a variety of uses of this type of model. As examples, we will discuss the impact of size and network homogeneity on the grid robustness, the change in risk of failure as generation mix (more distributed vs centralized for example) changes, as well as the effect of operational changes such as the changing the operational risk aversion or grid upgrade strategies. One of the important outcomes from this work is the realization that “improvements” in the system components and operational efficiency do not always improve the system robustness, and can in fact greatly increase the risk, when measured as a risk of large failure.

9:12AM S18.00003 Self Healing Percolation1. ANTONIO SCALA, CNR — We introduce the concept of self-healing in the field of complex networks modelling; in particular, self-healing capabilities are implemented through distributed communication protocols that exploit redundant links to recover the connectivity of the system. Self-healing is a crucial in implementing the next generation of smart grids allowing to ensure a high quality of service to the users. We then map our self-healing procedure in a percolation problem and analyse the interplay between redundancies and topology in improving the resilience of networked infrastructures to multiple failures. We find exact results both for planar lattices and for random lattices, hinting the role of duality in the design of resilient networks. Finally, we introduce a cavity method approach to study the recovery of connectivity after damage in self-healing networks.

1CNR-PNR National Project “Crisis-Lab,” EU HOME/2013/CIPS/AG/4000005013 project CI2C and EU FET project MULTIPLEX nr.317532

9:48AM S18.00004 Easily repairable networks1. THOMAS FINK, London Institute for Mathematical Sciences / CNRS — We introduce a simple class of distribution networks which withstand damage by being repairable instead of redundant. Instead of asking how hard it is to disconnect nodes through damage, we ask how easy it is to reconnect nodes after damage. We prove that optimal networks on regular lattices have an expected cost of reconnection proportional to the lattice length, and that such networks have exactly three levels of structural hierarchy. We extend our results to networks subject to repeated attacks, in which the repairs themselves must be repairable. We find that, in exchange for a modest increase in repair cost, such networks are able to withstand any number of attacks.

1We acknowledge support from the Defense Threat Reduction Agency, BCG and EU FP7 (Growthcom).

Thursday, March 5, 2015 8:00AM - 11:00AM –

8:00AM S19.00001 Historical Overview of 3-D Printing: Do inventors know what they are doing? . MICHAEL CIMIA, Massachusetts Institute of Technology — No abstract available.
8:36AM S19.00002 Functional Structures for System Integrity and Security . DAVID M. KEICHER, Sandia National Laboratories — The 3D printing revolution is redefining manufacturing and has given rise to a new industry segment called Additive Manufacturing (AM). Assemblies of mechanical components can now be integrated into a single printed structure. A logical next phase in this revolution is to assimilate multiple technologies to functionalize these 3D printed structures. Some applications include embedding of simple sensors for structural health monitoring and tamper protection to fully integrating electronics onto nontraditional surfaces such as the inside shell of a housing. Electronic printing technologies provide an enabling tool to this end. This talk will describe work in printing large area sensors for temperature, strain and proximity detection applications. A critical aspect will also cover improvements made to aerosol based printing technologies to provide a more robust printing solution that both demonstrates improved printing performance over existing technologies and lowers the barrier to entry for high precision conformal printing of electronics.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.


9:48AM S19.00004 Additive Manufacturing and High-Performance Computing: A Disruptive Latent Technology BRUCE GOODWIN, Lawrence Livermore National Laboratory — This presentation will discuss the relationship between recent advances in Additive Manufacturing (AM) technology, High-Performance Computing (HPC) simulation and design capabilities, and related advances in Uncertainty Quantification (UQ), and then examines their impacts upon national and international security. The presentation surveys how AM accelerates the fabrication process, while HPC combined with UQ provides a fast track for the engineering design cycle. The combination of AM and HPC/UQ almost eliminates the engineering design and prototype iterative cycle, thereby dramatically reducing cost of production and time-to-market. These methods thereby present significant benefits for US national interests, both civilian and military, in an age of austerity. Finally, considering cyber security issues and the advent of the “cloud,” these disruptive, currently latent technologies may well enable proliferation and so challenge both nuclear and non-nuclear aspects of international security.

10:24AM S19.00005 Additive Manufacturing and Medical Devices: Case studies, Technical Concerns and Research KATHERINE VORVOLAKOS, Food and Drug Administration — The past decade has seen a steady increase in the marketing of medical devices produced via additive manufacturing (AM). This presentation discusses the technical concerns surrounding AM in the context of medical devices. While unprecedented complexity is possible, maintaining safety and effectiveness requires a more nuanced understanding of the interdependent chemical, physical, software and process traits of creating an AM medical device. This presentation will feature historical perspective, cite specific technical concerns and describe a few medical device case studies. Additionally, it will highlight FDA research and an upcoming FDA guidance document, both of which aim to identify and help address these technical concerns.

Thursday, March 5, 2015 8:00AM - 11:00AM –
Session S20 DPOLY: Invited Session: Ion-Containing Polymers Ballroom B - Kevin Cavicchi, University of Akron

8:00AM S20.00001 Thermal and pH Transitions in Polyelectrolyte Complexes and Multilayers JODIE LUTKENHAUS, Texas A&M University — When oppositely charged polymers are mixed in water, they form a polyelectrolyte complex. Analogously at a surface, oppositely charged polymers can be assembled to form a polyelectrolyte multilayer. Complexation is entropically driven, as it results in the release of small counter ions and water molecules into the surrounding media. First, the effect of time and temperature on the formation of polyelectrolyte complexes containing model polyelectrolytes poly(diallyldimethyl ammonium chloride) and poly(styrene sulfonate) is presented. We show that complexation is a time-dependent phenomenon, which is consistent with complexes existing in a kinetically trapped state, rather than a thermodynamic equilibrium. Upon heating, a glassy-viscous transition that shows features of an LCST is demonstrated. Second, the effect of pH on polyelectrolyte multilayer microtubes is presented. The microtubes are made of poly(allylamine) and poly(acrylic acid), both of which are weak polyelectrolytes. Modulating the pH induces a nanoporous transition that results in nanoporous microtubes. These results, in summary, show that noncovalent interactions are very sensitive to external stimuli such as temperature and pH.

8:36AM S20.00002 Multicomponent transport in membranes for redox flow batteries . CHARLES MONROE, University of Michigan — Redox flow batteries (RFBs) incorporate separator membranes, which ideally prevent mixing of electrochemically active species while permitting crossover of inactive supporting ions. Understanding crossover and membrane selectivity may require multicomponent transport models that account for solute/solute interactions within the membrane, as well as solute/membrane interactions. Application of the Onsager–Stefan–Maxwell formalism allows one to account for all the dissipative phenomena that may accompany component fluxes through RFB membranes. The magnitudes of dissipative interactions (diffusional drag forces) are quantified by matching experimentally established concentration transients with theory. Such transients can be measured non-invasively using DC conductometry, but the accuracy of this method requires precise characterization of the bulk RFB electrolytes. Aqueous dissipative interactions (diffusional drag forces) are quantified by matching experimentally established concentration transients with theory. Such transients can be measured non-invasively using DC conductometry, but the accuracy of this method requires precise characterization of the bulk RFB electrolytes. Aqueous solutions containing both vanadyl sulfate (VOSO$_4$) and sulfuric acid (H$_2$SO$_4$) are relevant to RFB technology. One of the first precise characterizations of aqueous vanadyl sulfate has been implemented and will be reported. To assess the viability of a separator for vanadium RFB applications with cell-level simulations, it is critical to understand the tendencies of various classes of membranes to absorb (uptake) active species, and to know the relative rates of active-species and supporting-electrolyte diffusion. It is also of practical interest to investigate the simultaneous diffusion of active species and supports, because interactions between solutes may ultimately affect the charge efficiency and power efficiency of the RFB system as a whole. A novel implementation of Barnes’s classical model of dialysis-cell diffusion [Physics 5:1 (1934) 4-8] is developed to measure the binary diffusion coefficients and sorption equilibria for single solutes (VOSO$_4$ or H$_2$SO$_4$) in porous membranes and cation-exchange membranes. With the binary diffusion and uptake measurement in hand, a computer simulation that extends the approach of Heintz, Wiedemann and Ziegler [J. Membrane Science 137:1-2 (1997) 121-132] is used to establish Onsager resistances that describe the drag forces VOSO$_4$ and H$_2$SO$_4$ exert on each other as they interdiffuse. The ramifications of these interactions for different classes of membranes – and for RFB applications – will be discussed.

1 NSF CBET-1253544
9:12AM S20.00003 Morphology control in solid polymer electrolytes, CHRISTOPHER LI, Drexel University — Solid polymer electrolytes (SPEs) with high ionic conductivity are important for energy-related applications, such as solid state batteries and fuel cells. In this talk, I will discuss how morphology affects the properties of SPEs. In the first part of the talk, I will show quantitatively that the effect of polymer crystallization on ion transport is twofold: structural (tortuosity) and dynamic (tethered chain confinement). We decouple these two effects by designing and fabricating a model polymer single crystal electrolyte system with controlled crystal structure, size, crystallinity, and orientation. Ion conduction is confined within the chain fold region and guided by the crystalline lamellae. We show that, at low ion content, due to the tortuosity effect, the in-plane conductivity is 2000 times greater than through-plane.1. Contrary to the general view, the dynamic effect is negligible at moderate ion contents. Our results suggest that semicrystalline polymer is a valid system for practical polymer electrolytes design. In the second part of the talk, I will discuss how to use holographic photopolymerization (HP) to fabricate long-range, defect-free, ordered SPEs with tunable ion conducting pathways. By incorporating polymer electrolytes into the carefully selected HP system, electrolyte layers/ion channels with length scales of a few tens of nanometers to micrometers can be formed. Confinement effects on ion transport will be reported.

9:48AM S20.00004 Morphology and Ionic Conductivity of Block Copolymer Electrolytes Containing Ionic Liquids, MOON JEONG PARK, Pohang University of Science and Technology (POSTECH) — The global energy crisis and an increase in environmental pollution in the recent years have drawn the attention of the scientific community towards the development of efficient electrochemical devices. Polymers containing charged species have the potential to serve as electrolytes in next-generation devices and achieving high ion transport properties in these electrolytes is the key to improving their efficiency. Although the synthesis and characterization of a wide variety of ion-containing polymers have been extensively reported over the last decade, quantitative understanding of the factors governing the ion transport properties of these materials is in its infancy. In this talk, I will present the current understanding of the diverse factors affecting the thermodynamics, morphologies and ion transport of ion-containing polymers by focusing on the use of ionic liquids (ILs). Various strategies for accessing improved transport properties of IL-containing polymers are elucidated by focusing on the role of IL-polymer interactions. The major accomplishment of obtaining well-defined morphologies for these IL-containing polymers by the use of block copolymer is particularly emphasized as a novel means of controlling the transport properties. The application of IL-incorporated polymer electrolytes in high temperature fuel cells and electro-active actuators is also enclosed.

10:24AM S20.00005 Ionomer Dynamics: Insights from Broadband Dielectric Spectroscopy*1, JAMES RUNT, Pennsylvania State University — Ionomers (polymers containing ionic functionality) have been traditionally used as packaging materials and in molding applications, and are now of increasing interest as candidate single ion conductors for energy storage devices, in energy conversion, and for other electroactive materials applications. The focus of this presentation is on the insight that broadband dielectric (impedance) spectroscopy brings to our understanding of ion and polymer dynamics of this family of materials. As an example of our recent work on relatively conductive ionomers, the first portion of the presentation will focus on anion conducting polyphosphazene ionomers, in which polymer bound cations are quaternized with either short alkyl or short ether oxygen chains. The low Tg, amorphous nature, and cation-solvating backbone distinguish polyphosphazenes as promising materials for ion conduction, the iodide variants being of particular interest in solar cells. In the second part of this overview, the first findings on the molecular dynamics of linear precise polyethylene-based ionomers containing 1-methylimidazolium bromide pendants on exactly every 9th, 15th, or 21st carbon atom will be summarized. In order to develop a robust interpretation of the dynamics of these materials, it is imperative to develop a thorough understanding of microphase separation (e.g. ion aggregation), and each of the above studies is complemented by multiange X-ray scattering experiments.

1Supported by the NSF Polymers Program and DOE Basic Energy Sciences

Thursday, March 5, 2015 8:00AM - 11:00AM — Session S21 GIMS: Spectroscopic Techniques 201 - Dennis Mills, Argonne National Laboratory

8:00AM S21.00001 Nanoscale imaging of nonequilibrium polymer films, JOHN KING, STEVE GRANICK, University of Illinois, Urbana-Champaign — In recent years there have been exciting advances in sub-diffraction limited imaging based on fluorescence microscopy. While most applications of super-resolution microscopy focus on static biological imaging, we are interested in extending these techniques to the study of polymer dynamics. To this end, we couple stimulated emission depletion (STED) with spectroscopic detection, relying on spectral features of fluorescence emission to serve as the imaging contrast agent. We aim to adapt fluorescent dyes responsive to environmental properties (polarity, mobility, current, temperature, etc.) to STED imaging. Using the fluorescent spectral response as a contrast agent allows for nanoscopic environments to be directly imaged without the need for specific labeling. Rapid acquisition of images allows for slow dynamic processes in nonequilibrium polymer films to be imaged in real time. We demonstrate the power of super-resolution spectroscopic imaging by directly imaging several topical problems in materials science.

8:12AM S21.00002 Nonlinear photothermal Mid-Infrared Microspectroscopy with Superresolution1, SHYAMSUNDER ERRAMILLI, Physics department & the Photonics Center, Boston University, ALKET MERTIRI, Department of Biology, Boston University, HUI LIU, ATCHA TOTACHAWATTANA, Electrical and Computer Engineering, Boston University, MI HONG, Physics department, Boston University, MICHELLE SANDER, Electrical and Computer Engineering, Boston University — We describe a nonlinear method for breaking the diffraction limit in mid-infrared microscopy using nonlinear photothermal microspectroscopy. A Quantum Cascade Laser (QCL) tuned to an infrared active vibrational molecular normal mode is used as the pump laser. A low-phase noise Erbium-doped fiber (EDFL) laser is used as the probe. When the incident intensity of the mid-infrared pump laser is increased past a critical threshold, a nanobubble is nucleated, strongly modulating the scatter of the probe beam, in agreement with prior work. Remarkably, we have also found that the photothermal spectral signature of the mid-infrared absorption bifurcates and is strongly narrowed, consistent with an effective “mean-field” theory of the observed forkich bifurcation. This ultrasharp narrowing can be exploited to obtain mid-infrared images with a resolution that breaks the diffraction limit, without the need of mechanical scanning near-field probes. The method provides a powerful new tool for hyperspectral label-free mid-infrared imaging and characterization of biological tissues and materials science and engineering.

1We thank our collaborators H. Altug, L. D. Ziegler, J. Mertz, for their advice and generous loan of equipment.

8:24AM S21.00003 Novel Raman instrumentation for characterizing 2D nanomaterials, ANGELA HIGHT WALKER, National Institute of Standards and Technology, Gaithersburg, MD 20899 — We have designed and constructed a unique Raman microscope system to enable diffraction limited measurements of graphene and two-dimensional transition-metal dichalcogenides (TMDs). The design enables low frequency phonon measurements down to ten wavenumbers through a triple grating Raman spectrometer, as well as resonance Raman spectroscopy through multiple laser excitation lines throughout the visible region. Through coupling to a cryogen-free magnet system, Raman spectra can be collected while the sample is in fields up to 9 Tesla and at temperatures from 4 K to 400 K. Uniquely, both Farady and Voight geometries are accessible. Furthermore, multiple electronic feedthroughs permit collecting Raman scatter from devices at varying voltages. Proof of concept measurements on TMDs will highlight the full capabilities of the instrumentation. Collaborations are sought to demonstrate the utility of the new instrumentation.
9:00AM S21.00006 High Power Terahertz Conductive Antenna with Chaotic Electrodes

Christopher Kim, Benjamin Graber, Dong HO Wu, Naval Research Laboratory — Time domain terahertz spectroscopy (TDTS) is now widely adopted and being used for various purposes, including chemical and material analysis as well as detection of hazardous materials in the laboratories. While there are several different methods available to generate a wideband terahertz pulse for the TDTS, currently a terahertz photoconductive antenna may be the most popular one, as it can produce a wideband terahertz pulse very efficiently. However, our experimental investigation indicates that the conventional photoductive antenna with a pair of parallel electrodes can produce a terahertz pulse at most about 100 micro-Watts. When attempted to produce a higher power terahertz pulse, the antenna may experience irreversible failure. In order to overcome this problem, we recently redesigned the photoconductive antenna and implemented electrodes that lead to a chaotic trajectories of charged particles. With the new electrodes we have demonstrated a high power (>2 mW) coherent terahertz beam, and we found that the lifetime of the antenna is also substantially longer than that of the conventional antenna. In this talk, I will present our experimental results and disclose some of our new antenna designs.


Fidele Twagi-Rayezu, Wilhemus J. Geerts, Yubo Cui, Texas State Univ-San Marcos — The study of optical properties of Nickel (Ni) is important, given the pivotal role it plays in the semiconductor and nano-electronics technology. Ni films were made by DC and RF magnetron sputtering in an ATC Orion sputtering system of AJA on various substrates. The optical properties were studied ex situ by variable angle spectroscopic (220-1000 nm) ellipsometry at room temperature. The data were modeled and analyzed using the Woollam CompleteEase Software fitting ellipsometric and transmission data. Films sputtered at low pressure have optical properties similar to that of Palik [1]. Films sputtered at higher pressure however have a lower refraction index and extinction coefficient. It is expected from our results that the density of the sputtered films can be determined from the ellipsometric quantities. Our experiments also revealed that Ni is susceptible to a slow oxidation changing its optical properties over the course of several weeks. The optical properties of the native oxide differ from those of reactive sputtered Ni similar as found by [2]. Furthermore the oxidation process of our samples is characterized by at least two different time constants.

1Supported by DTRA


9:24AM S21.00008 Practical Framework for an Electron Beam Induced Current Technique Based on a Numerical Optimization Approach

Hideshi Yamaguchi, Takeshi Soeda, Fujitsu Laboratories Ltd. — A practical framework for an electron beam induced current (EBIC) technique has been established for conductive materials based on a numerical optimization approach. Although the conventional EBIC technique is useful for evaluating the distributions of dopants or crystal defects in semiconductor transistors, issues related to the reproducibility and quantitative capability of measurements using this technique persist. For instance, it is difficult to acquire high-quality EBIC images throughout continuous tests due to variation in operator skill or test environment. Recently, due to the evaluation of EBIC equipment performance and the numerical optimization of equipment items, the constant acquisition of high contrast images has become possible, improving the reproducibility. As well as field yield regardless of operator skill or test environment. The technique proposed herein is even more sensitive and quantitative than scanning probe microscopy, an imaging technique that can possibly damage the sample. The new technique is expected to benefit the electrical evaluation of fragile or soft materials along with LSI materials.


Xuetao Zhu, Yanwei Cao, Shuyuan Zhang, Xun Jia, Qinlin Guo, Fang Yang, Institute of Physics, Chinese Academy of Sciences, Linfan Zhu, University of Science and Technology of China, Larry Kessmodel, Indiana University, Bloomington, Jiandi Zhang, Ward Plummer, Louisiana State University, Jiandong Guo, Institute of Physics, Chinese Academy of Sciences — High resolution electron energy loss spectroscopy (HREELS) has been demonstrated as a powerful technique to probe vibrational and electronic surface excitations of solids. The dispersion relation of the surface excitations, i.e. energy as a function of momentum, can be obtained via the angle resolved measurements by rotating the sample or the analyzer in a conventional HREELS measurement. The sampling density in the momentum space and the detecting efficiency are restricted by the mechanical rotation. Here we introduce a new design of the HREELS system, by combining the traditional Ibach-type electron source with the mainstream hemispherical electron energy analyzer, which could simultaneously measure the energy and momentum of the scattered electrons without any mechanical rotation. The new system possesses higher efficiency and sampling density of momentum-resolved measurements by at least one order of magnitude than conventional spectrometers without deteriorating the resolution of energy and momentum. Using Bi$_2$Sr$_2$CaCu$_2$O$_{8+}$$\delta^+$ as an example, we show that an energy loss spectrum can be scanned throughout the first Brillouin zone and a momentum-dependent spectral intensity distribution could be obtained in one measurement.
10:00AM S21.00011 Measurement of the low energy spectral contribution in coincidence with valence band (VB) energy levels of Ag(100) using VB-VB coincidence spectroscopy . P.V. JOGLEKAR, R. GLADEN, Z.H. LIM, K. SHASTRY, University of Texas at Arlington, S.L. HULBERT, Photon Science Directorate, Brookhaven National Laboratory, A.H. WEISS, University of Texas at Arlington — A set of coincidence measurements were obtained for the study and measurement of the electron contribution arising from the inter-valence band (VB) transitions along with the inelastically scattered VB electron contribution. These Auger-unrelated contributions arise in the Auger spectrum (Ag 4p NVV) obtained using Auger Photoelectron Coincidence Spectroscopy (APECS). The measured Auger-unrelated contribution can be eliminated from Auger spectrum to obtain the spectrum related to Auger. In our VB-VB coincidence measurement, a photon beam of energy 180eV was used to probe the Ag(100) sample. The coincidence spectrum was obtained using two Cylindrical Mirror Analyzers (CMA’s). The scan CMA measured the low energy electron contribution in the energy range 0-70eV in coincidence with VB electrons measured by the fixed CMA. In this talk, we present the data obtained for VB-VB coincidence at the valence band energy of 171eV along with the coincidence measurements in the energy range of 4p core and valence band.

10:12AM S21.00012 High repetition rate source of narrowband extreme-ultraviolet harmonics for time-resolved ARPES . H. HE WANG, YIMING XU, STEFAN ULONSKA, PREDRAG RANITOVIC, JOSEPH ROBINSON, ROBERT KAINDL, Lawrence Berkeley National Laboratory — We present a highly efficient table-top source of extreme ultraviolet (XUV) femtosecond pulses operating at 50-kHz repetition rate. A bright XUV source flux of 3x10^13 photons/s is generated at 22.3 eV by driving high-harmonic generation with the ultraviolet second-harmonic of a laser amplifier focused tightly into Kr gas. The conversion efficiency (5x10^-12) is enhanced by two orders-of-magnitude in this cascaded scheme, exceeding dipole wavelength scaling and evidencing enhanced phase matching conditions as confirmed by simulations. Importantly, the spectral structure enables the direct, high-contrast isolation of a single, narrowband harmonic with 72 meV linewidth. The high repetition rate, narrow bandwidth, and high flux (10^{11}-10^{12} ph/s at the sample) of this source is ideal for time-resolved photoemission or nanoscale imaging. First applications in time- and angle-resolved photoemission (trARPES) will be discussed.

10:24AM S21.00013 Instrumentation for Cyclotron Resonance and Electron Spin Resonance in Pulsed Magnetic Fields . CHRISTOPHER BEEDEL, Los Alamos Natl Lab, PAUL GODDARD, Warwick University, United Kingdom, NIEL HARRISON, Los Alamos Natl Lab, JAMIE MANSON, Eastern Washington University, ROSS MCDONALD, JOHN SINGLETON, Los Alamos Natl Lab — Pulsed electron spin resonance (ESR) and cyclotron resonance (CR) are widely used in structure and magnetic resonance of materials. For example, CR can yield the strength of electron-electron correlations via the dynamic mass, and determine the Fermi surface topology. However, very high magnetic fields are required to extend CR to heavy mass and/or disordered correlated-electron systems, and to cuprate superconductors, where the upper critical field must be exceeded. Similarly, magnetic fields ~ 100 T in conjunction with high-frequency ESR could access the magnetic interactions in highly anisotropic spin-gap materials and molecular quantum magnets, probe phase transitions in f-electron systems, and examine the electronic structure of organic radicals. Pulsed magnets are therefore required for such ultra-high-field CR and ESR experiments; but the resulting extreme environment presents challenges in resonant cavity and waveguide design. In this presentation, we describe probe designs tailored to CR and ESR experiments spanning fields up to 100 T and frequencies from 40 GHz to 4 THz. These new techniques will be illustrated using experimental ESR data from organic quantum magnets.

10:36AM S21.00014 High speed nonlinear optical harmonic generation rotational anisotropy measurements for sensitive detection of crystallographic and electronic symmetry breaking . LAUREN NIU, Institute for Quantum Information and Matter, California Institute of Technology, ANTONI WOSS, University of Cambridge, JOHN HARTER, DARIUS TORCHINSKY, DAVID HSIEH, Institute for Quantum Information and Matter, California Institute of Technology — The rotational anisotropy of optical nonlinear harmonic generation (NHG) on a crystalline material can be used to probe the symmetries of both its lattice structure and underlying ordered electronic phases. Presently however, low temperature experimental setups require both optics and detectors to be mechanically rotated during measurement [1], which makes the data collection slow and thus susceptible to low frequency sources of noise. We present a new method to perform rotational anisotropy measurements based on a triple beam-splitter setup and a spatially sensitive detection scheme. This method increases the data collection frequency by over three orders of magnitude by removing nearly all rotating parts from the experiment. We will report the improved sensitivity to symmetry changes in a material and discuss the potential to carry out wavelength dependent and time-resolved NHG measurements using this method.

10:48AM S21.00015 Electron Energy-Loss Spectroscopy (EELS) Calculation in Finite-Difference Time-Domain (FDTD) Package: EELS-FDTD . NICOLAS LARGE, YANG CAO, ALEJANDRO MANJAVacas, PETER NORDLANDER, Rice University — Electron energy-loss spectroscopy (EELS) is a unique tool that is extensively used to investigate the plasmonic response of metallic nanostructures since the early works in the ’50s. To be able to interpret and theoretically investigate EELS results, a myriad of different numerical techniques have been developed for EELS simulations (BEM, DDA, FEM, GDTD, Green dyadic functions). Although these techniques are able to predict and reproduce experimental results, they possess significant drawbacks and are often limited to highly symmetrical geometries, non-penetrating trajectories, small nanostructures, and free-standing nanostructures. We present here a novel approach for EELS calculations using the Finite-difference time-domain (FDTD) method: EELS-FDTD. We benchmark our approach by direct comparison with results from the well-established boundary element method (BEM) and published experimental results. In particular, we compute EELS spectra for spherical nanoparticles, nanoparticle dimers, nanodisks supported by various substrates, and gold bowtie antennas on a silicon nitride substrate. Our EELS-FDTD implementation can be easily extended to more complex geometries and configurations and can be directly implemented within other numerical methods.

1Work funded by the Welch Foundation (C-1222, L-C-004), and the NSF (CNS-0821727, OCI-0959097).
Room-Temperature Studies of Li$_{10}$Mo$_9$O$_{17}$ by Scanning Tunneling Microscopy

Michael Boyer, Ling Fu, Aaron Kraft, Clark University, Martha Greenblatt, Rutgers University — The lithium purple bronze (Li$_{10}$Mo$_9$O$_{17}$) is a quasi-1-dimensional material as evidenced by high anisotropy in resistivity and thermal conductivity measurements. The material has garnered interest due to experimental evidence for Luttinger Liquid physics from 25 K to 300 K. Here we present our room-temperature topographic and spectroscopic scanning tunneling microscopy measurements on Li$_{10}$Mo$_9$O$_{17}$. We interpret the observed topographic and spectroscopic features in the context of previous bulk and surface measurements as well as theoretical models describing the 1-dimensional physics of the lithium purple bronze.

Thermoelectric effects in the field-suppressed superconducting state of quasi-one-dimensional Li$_{10}$Mo$_9$O$_{17}$

Joshua L. Cohn, University of Miami, Carlos A. M. Dos Santos, Escola de Engenharia de Lorena - USP, Brazil, John J. Neumeier, Montana State University — We present resistivity, thermopower (S), and Nernst (ν) measurements in the range 0.4 K ≤ T ≤ 20 K on single crystals of the quasi-one-dimensional (q1D) metal, Li$_{10}$Mo$_9$O$_{17}$ (LiPB) along the q1D metallic chains. The low-T limits of S/T and ν/T, determined in the magnetic-field suppressed superconducting state (T$_{c}$ = 2 K), indicate a very small Fermi temperature (T$_{F}$ ~ 30 K), contrary to expectations from prior work including photoemission. Possible insights from these results into the nature of the mysterious density-wave order, responsible for the upturn in resistivity below ~25 K will be discussed.

Topological character and chiral solitons in double Peierls-distorted chains

Sangmo Cheon, Tae-Hwan Kim, Sung-Hoon Lee, Han Woong Yeom, Caldes, Institute for Basic Science and POSTECH, Korea — Chiral edge states have played an important role in understanding condensed matter systems such as quantum Hall systems and topological insulators. In 1D electronic systems, Peierls-distorted atomic chains such as polyacetylene have two topologically different ground states and thus have topological edge states between them. The edge states—topological solitons—show novel properties of charge-spin separation and fractional charge. Here, we present theoretical results on the topological properties of double Peierls-distorted chains with interchain coupling. The double Peierls chains support a dynamically generated topological structure with four-fold symmetric ground states and have topological solitons with a new degree of freedom, chirality, which is absent in a single chain. We also discuss experimental evidence of the chiral solitons in the 1D charge-density wave (CDW) system of indium atomic nanowires on silicon substrates.

Photoinduced Dynamics of Charge Density Waves in Mott-Peierls Systems

Yao Wang, Stanford University/Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Chen-Chien Chen, Advanced Photon Source, Argonne National Laboratory, Chunjing Jia, Stanford University/Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Michael Van Veenendaal, Advanced Photon Source, Argonne National Laboratory/Department of Physics, Northern Illinois University, Thomas Devereaux, Stanford University/Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Brian Moritz, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory — We study the time-dependent evolution of photoinduced optical excitations in a model for organic solids, using the density matrix renormalization group method. The model consists of the quarter-filled one-dimensional extended Peierls-Hubbard Hamiltonian interacting with a classical time-dependent electric field. Our main results show that the overall dynamics of the dominating $k_F\rho$ bond and charge instabilities correspond to a gigantic fluctuating behavior as a function of time, whereas the 2$k_F$ state remains largely unaffected. These results remain valid regardless of the nature of the optical excitations and whether the system is driven resonantly or not. We compare our calculations with experimental pump-and-probe ultrafast spectroscopy studies of the optical conductivity in organic compounds.

Bond patterns in 1/4-filled spin-Peierls materials

Andrew Ward, R. Torsten Clay, Mississippi State University, Niladri Comes, Sumit Mazumdar, University of Arizona — In the 1/4-filled quasi-one-dimensional molecular charge transfer solids (CTS) there exist two distinct classes of spin-Peierls (SP) transitions. The two classes are distinguished by differing bond patterns: either the pattern Strong-Medium-Weak-Medium (SMMW), or the pattern Strong-Weak-Strong-Weak’ (SWSW’). Experimentally the SP transition temperature of CTS of the first type (SMMW) is much higher than those of the second type (SWSW”). This indicates that the small change in bond patterns within the SP phase greatly affects the electronic behavior of the CTS. We show that these two bond patterns can be explained within the one dimensional Extended Hubbard Model. We use quantum Monte Carlo and finite-size scaling to create a phase diagram for the 1/4-filled 1D CTS and discuss charge order amplitude and other experimental observables.

Charge fluctuations in the metallic phase of Lithium purple bronze

Jose Alvarez, Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid, Jaime Merino, Departamento de Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid, Natalia Lera, Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid — We study the role of charge fluctuations for a model of the quasi-one-dimensional Li$_{10}$Mo$_9$O$_{17}$ and study their influence in ARPES experiments. Coulomb repulsion induces a charge ordering (CO) transition in a multiorbital extended Hubbard model. The ordering pattern is different from the one present in a conventional CDW driven by Fermi surface nesting. We assume that purple bronze lays in the metallic side of this phase diagram, but still very close to the CO transition. In these regime, strong charge fluctuations manifest themselves through low-energy collective excitations softening in the proximity the transition, which may be directly visible in HRRIX experiments. We discuss specific role of quasi-one-dimensionality in this context. We argue that the electronic scattering by these charge fluctuations can lead to the upturn in the resistivity observed at 24K and the deviations of scaling observed in ARPES.
Local correlation effects on pyrochlore iridate thin films in [111] direction

QI CHEN, HSIAO-HSUAN HUNG, XIANG HU, GREGORY A. FIETE, Univ of Texas, Austin — We study the local correlation effects on topological phases of matter in pyrochlore oxide thin films of the form $A_2B_2O_7$, oriented along the [111] direction. We examine bilayer and trilayer lattice models, including an on-site Hubbard interaction, by cellular dynamical mean field theory. The local correlation effects on the topological and magnetic phases are explored in both thin film geometries. Our focus is on the stability of the interaction induced Chern Insulator phases found in mean-field (Hartree-Fock) studies. By including dynamical fluctuations and computing the topological invariants from the single-particle Greens function, we corroborate the results of the Hartree-Fock mean field study and point out the differences. We discuss the likelihood of the Chern insulator phase being experimentally realized in transition metal oxide thin films.

Perfect Metal Phases of One-Dimensional and Anisotropic Higher-Dimensional Systems

EUGENIU PLAMADEALA, Univ of California - Santa Barbara, MICHAEL MULLIGAN, Stanford University, CHETAN NAYAK, Univ of California - Santa Barbara, Microsoft Station Q — We show that a 1D quantum wire with 23 channels of interacting fermions has a perfect metal phase in which all weak perturbations that could destabilize this phase are irrelevant. Consequently, weak disorder does not localize it, a weak periodic potential need not open a gap, and contact with a superconductor also fails to open a gap. Similar phases occur for $N \geq 24$ channels of fermions, except for $N=25$, and for $k\ell$ channels of interacting bosons, with $k \geq 3$. Arrays of perfect metallic wires form higher-dimensional fermionic or bosonic perfect metals, albeit highly-anisotropic ones.

Observation of a hierarchy of modes in an interacting one-dimensional system

CHRISTOPHER FORD, MARIA MORENO, YIQING JIN, WOOI KIAT TAN, IAN GRIFFITHS, IAN FARRER, GEB JONES, University of Cambridge, ANNE ANTHORE, Universite Paris Diderot, DAVID RITCHIE, University of Cambridge, OLEKSANDR TSYPLYATYEV, ANDREW SCHOFIELD, University of Birmingham — Studying interacting fermions in 1D at high energy, we find a hierarchy in the spectral weights of the excitations theoretically and we observe evidence for second-level excitations experimentally. Diagonalising a model of fermions (without spin), we show that levels of the hierarchy are separated by powers of $\mathcal{R}^2/L^2$, where $\mathcal{R}$ is a length-scale related to interactions and $L$ is the system length. The first-level (strongest) excitations form a mode with parabolic dispersion, like that of a renormalised single particle. The second-level excitations produce a singular power-law finite size scaling of these first-level modes and multiple power-laws at the spectral edge. We measure momentum-resolved tunneling of electrons (fermions with spin) from/to a wire formed within a GaAs heterostructure, which shows parabolic dispersion of the first-level mode and well-resolved spin-charge separation at low energy with appreciable interaction strength. We find structure resembling the second-level excitations, which dies away quite rapidly at high momentum.
8:00AM S23.00001 The importance of the finite-temperature exchange-correlation for warm dense matter studies\textsuperscript{1}. \textsc{V.V. Karasiev, S.B. Trickey}, Physics and QTP, Univ. Florida — Matter at extremely elevated temperature (thousands to millions Kelvin) under a wide range of pressures usually is treated by ab initio molecular dynamics driven by free-energy DFT. Whether in the Kohn-Sham or orbital-free forms, implementation requires a reliable exchange-correlation (XC) free energy approximation. Finite-temperature Hartree-Fock calculations\textsuperscript{1} suggest strongly that the explicit T-dependence of X is important. The recently developed first rung XC free-energy functional, the finite-T local density approximation (LDA)\textsuperscript{2}, captures that explicit T-dependence for the homogeneous electron gas. We report study of the impact of explicit T-dependence in the LDA on the properties of matter in the warm dense regime and conclude that there is a need to develop a T-dependent and density gradient-dependent XC functional. Next, we analyze the finite-T gradient expansion for X and C, extract from it the appropriate reduced density gradients for X and C with explicit T-dependence, introduce the next-run GGA XC free-energy functionals, and discuss their behavior and properties.

\textsuperscript{1} Work supported by U.S. Dept. of Energy, grant DE-SC0002139.

8:12AM S23.00002 Theoretical Investigation of Differing Ion and Electron Temperatures in Hydrogen\textsuperscript{1}. \textsc{Keith Runge, Valentin Karasiev}, Department of Physics, University of Florida, Pierre Deymier, Materials Science and Engineering, University of Arizona — Andrew Ng\textsuperscript{1} has reported experimental results for silicon and gold in warm, dense matter conditions that have been modeled by use of distinct temperatures for the ions and electrons. Here we investigate the implications of such differing ion and electron temperatures for hydrogen using path-integral molecular dynamics (PIMD) for protons which interact with electrons described by orbital-free density functional theory (OF-DFT). Temperatures ranging from room temperature to many kilokelvin are considered for the protons, while the electron temperatures are fixed in the kilokelvin range. Recent advances\textsuperscript{2} in OF-DFT not only allow for faster generation of first principles forces but also include the effects of temperature on the electron density. Comparisons are made with classical molecular dynamics to allow us to quantify the quantum nuclear effects captured by PIMD.

\textsuperscript{1} Work supported by U.S. Dept. of Energy, grant DE-SC0002139.

8:24AM S23.00003 High-throughput calculations of pressure-induced phase transitions in tungsten nitride\textsuperscript{1}. \textsc{Michael Mehl}, Naval Research Laboratory, Washington DC, Daniel Finkenstadt, United States Naval Academy, Annapolis MD, Gus Hart, Brigham Young University, Provo UT, Stefano Curtarolo, Duke University, Durham NC — We have previously used high-throughput electronic structure calculations\textsuperscript{2} to determine the ground state structures of the tungsten-nitride system as a function of composition. In doing this, we found many structures with are close to the W-N convex hull and apparently metastable. The question then arises if any of these structures can be stabilized under pressure. To test this, we have determined the ground state hull as a function of pressure up to 50 GPa. We find that the structures on the hull change with pressure. We discuss some of the more interesting structures, and show how the choice of density functional changes our predictions.

\textsuperscript{1} Partial support from US-ONR and US DoD HPC.


8:36AM S23.00004 Self-diffusion and viscosity for warm dense systems by orbital-free density functional theory. \textsc{Travis Sjostrom, Jerome Daligault}, Los Alamos National Laboratory — Evaluation of transport properties requires significantly longer molecular dynamics simulations than, for example, equation of state calculations. The standard approach at lower temperatures is to use Kohn-Sham (orbital dependent) density functional theory to find the quantum electron density at every molecular dynamics step. However, the Kohn-Sham approach becomes computationally prohibited at higher temperatures for equation of state, let alone for transport properties. Our recent orbital-free approach\textsuperscript{1} has shown excellent agreement with Kohn-Sham method at lower temperatures and extends to very high temperatures. Here we evaluate self-diffusion and viscosity from low to high temperatures and compare with Kohn-Sham methods where applicable as well as with recent approaches of kinetic theory.

8:48AM S23.00005 A New Force-Matched Reactive Force Field for Bulk Water Under Extreme Thermodynamic Conditions. \textsc{Laurence Fried, Lucas Koziol}, Lawrence Livermore National Laboratory — A many-body classical force field is presented for water under dissociative thermodynamic conditions. The force field is optimized by force-matching to ab initio molecular dynamics (AIMD) simulations calculated with Density Functional Theory (DFT). The force field contains short-ranged central terms, many-body over-coordination terms, and long-range Ewald electrostatics. It is optimized and tested on water at density 1.5 g/mL and 2000 K, which is approximately 10% dissociated according to DFT. Molecular dynamics simulations closely reproduce DFT radial distribution functions, as well as the distribution of H$_2$O and dissociation products. The calculated atomic self-diffusion constants appear about 50% lower than in DFT, although precise comparison is impossible due to the short timescale accessible to AIMD (about 20 ps). The force field is also compared to ReaxFF using the CHO parameter set of Chenowith et al. ReaxFF structural and dynamical properties are in overall fair agreement with DFT, although ReaxFF water is not dissociative at these conditions.

9:00AM S23.00006 N Dependence of the Equilibrium Free Energy from the Canonical Ensemble\textsuperscript{1}. \textsc{Debajit Chakraborty, QTP}, Department of Physics, University of Florida, James Dufty, Department of Physics, University of Florida — Free-energy density functional theory conventionally is formulated in the Grand Canonical ensemble but implemented computationally in the Canonical ensemble. To investigate the effects of this disjuncture, the equilibrium free energy per particle for a uniform non-interacting gas is calculated from the Canonical ensemble for given particle number $N$ and fixed volume. The same calculation is performed from the Grand Canonical ensemble for the corresponding average $<N>$ and same volume. In dimensionless forms the latter depends only on the reduced temperature, $t = T/T_F$. In contrast, of course, the Canonical result depends on both $t$ and $<N>$. The results are compared for $1 <N> <100$. Next, the same calculations are performed for a non-uniform gas generated by an external ion using a regularized Coulomb potential. The number dependence is explored for positions near and far from the ion. The implications for free-energy density functional theory are discussed.

\textsuperscript{1} Research supported by US DOE Grant DE-SC0002139.
9:12AM S23.00007 Pressure-stabilized lithium cesides with cesium anions beyond the -1 state
, JORGE BOTANA, Beijing Computational Science Research Centre, Beijing 10084, China., MAO-SHENG MIAO, Materials Research Laboratory, University of California, Santa Barbara, California Q3 93106-5050, USA. — Main group elements usually assume a typical oxidation state while forming compounds with other species that depends on the occupation of the outermost orbital. Group I elements are usually in the +1 state in inorganic materials. Our recent work on Cs-F compounds reveals that pressure may make the inner shell 5p electrons of Cs reactive, causing Cs to expand beyond the +1 oxidation state. In our study, we have found that pressure can cause large electron transfer from light alkali metals such as Li to Cs, causing Cs to become anionic with a formal charge much beyond -1. Li and Cs only form alloys at ambient conditions, but by studying the thermodynamic stability of the intermetallic compounds Li$_m$Cs$_n$ (n=1-5, m=1; n=1,m=1-4), we have found that some Li$_m$Cs (n=1,3,4,5) compounds become stable under pressures higher than 100 GPA. Once formed, these compounds exhibit interesting structural features, including capped cuboids and dimerized icosahedra. Finally, we have also found superconductivity in metastable LiCs and that the unusual anionic state of Cs has a strong effect on the transition temperature.

9:24AM S23.00008 Bypassing the malfunction junction in warm dense matter simulations
, ATTILIA CANGI, Max Planck Institute of Microstructure Physics, AURORA PRIBRAM-JONES, University of California, Irvine — Simulation of warm dense matter requires computational methods that capture both quantum and classical behavior efficiently under high-temperature and high-density conditions. The state-of-the-art approach to model electrons and ions under those conditions is density functional theory molecular dynamics, but this method's computational cost skyrockets as temperatures and densities increase. We propose finite-temperature potential functional theory as an in-principle-exact alternative that suffers no such drawback[1]. In analogy to the zero-temperature theory developed previously[2,3], we derive an orbital-free free energy approximation through a coupling-constant formalism. Our density approximation and its associated free energy approximation demonstrate the method's accuracy and efficiency.

9:36AM S23.00009 Interaction of Short Pulse Laser Irradiation with Metal Targets under Condition of Spatial Confinement
, MAXIM SHUGAEV, EAMAN KARIM, CHENG-YU SHIH, CHENPING WU, LEONID ZHIGILEI, Univ of Virginia — While the general mechanisms of laser interactions with metals in vacuum have been broadly investigated experimentally, theoretically and computationally, the effect of strong spatial confinement by solid or liquid overlayers on the laser induced processes remains largely unexplored. In this work, the results of large-scale atomic simulations of short pulse laser irradiation of metal targets in liquid environment and in the presence of a transparent silica glass overlay are used to reveal the effect of the spatial confinement on the material response to the fast laser energy deposition. The ability of the overlayer to suppress generation of unloading tensile wave, prevent photomechanical spallation and explosive decomposition of the surface region of the target, and facilitate the formation of a high pressure and temperature supercritical state near the interface is revealed in the simulations. The results of the simulations clarify the mechanisms responsible for structural and morphological changes in the interfacial region, formation of voids and crystal defects, and generation of nanoparticles.

9:48AM S23.00010 ABSTRACT WITHDRAWN —

Thursday, March 5, 2015 8:00AM - 11:00AM –
Session S24 DCOMP: Quantum Many-Body Systems and Methods I 203AB - Chris Marianetti, Columbia University

8:00AM S24.00001 ABSTRACT WITHDRAWN —

8:12AM S24.00002 Entanglement spectrum and covalent bonding
, DAVID YANG, NORM TUBMAN, Univ of Illinois - Urbana. — We present an approach for computing the entanglement spectrum with quantum Monte Carlo for both continuum and lattice Hamiltonians. This method provides direct access to the matrix elements of the spatially reduced density matrix, using a generalization of the SWAP operator. We apply this method to several diatomic molecules and describe how the spatial entanglement spectrum encodes a covalent bond that includes all the many-body correlations. Of particular focus is the C$_2$ molecule, which has been subject to recent controversy. Our results suggest that entanglement-based methods can lead to more realistic analysis of covalent bonds than possible before.

8:24AM S24.00003 Power law violation of the area law in quantum spin chains
, RAMIS MOVASSAGH, Northeastern Univ. / MIT, PETER SHOR, MIT, Mathematics — The sub-volume scaling of the entanglement entropy with the system's size, $n$, has been a subject of vigorous study in the last decade. The area law provably holds for gapped one dimensional systems and it was believed to be violated by at most a factor of log($n$) in physically reasonable models such as critical systems. We first describe and then generalize our earlier spin-1 model [PRL 109, 207202 (2012)] to all integer spin-s chains, whereby we introduce a class of exactly solvable models that are physical yet violate the area law by a power law [arXiv:1408.1657 quant-ph]. This rules out the possibility of these models being described by a conformal field theory. We analytically show that the Schmidt rank grows exponentially with $n$ and that the half-chain entanglement entropy to the leading order scales as $\sqrt{n}$. Lastly, we introduce an external field which allows us to remove the boundary terms yet retain the desired properties of the model.
8:36AM S24.00004 Quantum criticality in “easy-plane” SU(N) spin model. JONATHAN DEMIDIO, RIBHU K. KAUL, Univ of Kentucky — We investigate a two dimensional quantum spin model with “easy-plane” SU(N) anisotropy which describes an N = 1 component superfluid of hard-core bosons. This model exhibits a transition from a magnetically ordered state, corresponding to superfluid order of the bosons, to a non-magnetic state with broken lattice translation symmetry (a valence bond solid). It has been shown previously that the fully SU(N) symmetric version of this model exhibits a continuous phase transition consistent with the scenario of deconfined quantum criticality. Using quantum Monte Carlo techniques we study the critical properties in the “easy-plane” case.

1 NSF DMR-1056536

8:48AM S24.00005 Matrix-product Ansatz for Fermions in a 1D Continuum, S.S. CHUNG, University of Cincinnati, K. SUN, University of Texas at Dallas, C.J. BOLECH, University of Cincinnati — We present a novel implementation of a matrix-product ansatz for fermions in a 1D continuum, which correctly predicts the ground state properties of a homogeneous interacting spin-1/2 system. This includes the signatures of a partially polarized regime, in agreement with a large amount of theoretical work which has guided, and/or has been inspired by, recent cold-atom experiments.


1 DOE FG02-12ER46875.

9:12AM S24.00007 Momentum-space Entanglement Spectrum of Bosons and Fermions with Interactions, REX LUNDGREN, JONATHAN BLAIR, University of Texas at Austin, MARTIN GREITER, Institue for Theoretical Physics, University of Wuerzburg, ANDREAS LAEUCHLI, Institut fuer Theoretische Physik, Universität Innsbruck, GREGORY FIEITE, University of Texas at Austin, RONNY THOMALE, Institute for Theoretical Physics, University of Wuerzburg — We study the momentum space entanglement spectra of bosonic and fermionic formulations of the spin-1/2 XXZ chain with analytical methods and exact diagonalization. We investigate the behavior of the entanglement gaps, present in both partitions, across quantum phase transitions in the XXZ chain. In both cases, finite size scaling reveals that the entanglement gap closure does not occur at the physical transition points. For bosons, we find that the entanglement gap observed in [Thomale et al., Phys. Rev. Lett. 105, 116805 (2010)] depends on the scaling dimension of the conformal field theory as varied by the XXZ anisotropy. For fermions, the infinite entanglement gap present at the XX point persists well past the phase transition at the Heisenberg point. We elaborate on how these shifted transition points in the entanglement spectra may in fact support the numerical study of the physical transitions in the momentum space density matrix renormalization group. Accepted by Physical Review Letters (arXiv:1404.7545) This work was supported by an National Science Foundation Graduate Research Fellowship

9:24AM S24.00008 Failure of the GGE for integrable models with bound states, NATAN ANDREI, GARRY GOLDSTEIN, Rutgers University — In this work we study the applicability of the local GGE to integrable one dimensional systems with bound states. We find that the GGE, when defined using only local conserved quantities, fails to describe the long time dynamics for most initial states including eigenstates. We present our calculations by studying the attractive Lieb-Liniger gas and the XXZ magnet, though similar results may be obtained for other models.

1 This research was supported by NSF grant DMR 1006684 and Rutgers CMT fellowship.

9:36AM S24.00009 Steady-state phases of the non-equilibrium Rabi-Hubbard Model, HAKAN TURECI, Princeton University, CHAITANYA JOSHI, University of St Andrews, MYKOLA BORDYUYH, Princeton University, ROSARIO FAZIO, Scuola Normale Superiore, JONATHAN KEELING, University of St Andrews, MARCO SCHIRO, Institut de Physique Theorique, CEA, CNRS-URA — We study the realization of a tunable Rabi-Hubbard Model with a coupled cavity array containing Raman-pumped 4-level qubits. This effective model is found to display a phase diagram that features a normal phase (vanishing polarization and photon coherence) and a finite-frequency ordered phase. The ordered phase may either display a “ferro-electric” order where the photon coherence is uniform through the array, or one with an alternating phase that we refer to as “anti-ferroelectric.”

9:48AM S24.00010 Local density fluctuation approach to Fermionic lattice models, ZHENGQIAN CHENG, CHRIS MARIANETTI, Columbia University — We formulate an effective action as a function of selected Hubbard operators which reproduces the local density fluctuations of a given lattice model. The relevant Hubbard operators emerge via mapping the lattice Hamiltonian to a composite system with auxiliary holes and gauge bosons which mediate the inter-cell hopping. After a mean field approximation of the gauge bosons, we get an effective local model which reproduces the expectation value of the relevant Hubbard operators. We apply our method to the one band Hubbard model in one and infinite dimensions, demonstrating good agreement between our computed static observables and the exact solutions. While our approach does not address frequency dependent observables, it has a negligible computational cost as compared to dynamical mean field theory and could be highly applicable in the context of real materials.

10:00AM S24.00011 Density-matrix renormalization group study of triangular and square Hubbard models, TAKAMI TOHYAMA, Tokyo University of Science, SHIGETOSHI SOTA, RIKEN AICS, TOMONORI SHIRAKAWA, SEIJI YUNOKI, RIKEN — We perform large-scale density-matrix renormalization group calculations for two-dimensional Hubbard models with a triangular lattice and a square lattice. In the triangular Hubbard model, we determined a boundary between metal and insulator and a boundary between spin-liquid and antiferromagnetic phases. The presence of spin-liquid phase is confirmed by spin-spin correlation function. In the square Hubbard model, we introduce a second-neighbor hopping interaction and calculate the dynamical spin correlation function to clarify the doping dependence of magnon excitations. We find a shift of a peak position toward higher energy in the electron-doped side, being consistent with recent resonant-inelastic x-ray scattering.

10:12AM S24.00012 Many-body localization edge in the random-field Heisenberg chain, DAVID J. LUITZ, NICOLAS LAFLORENCIE, FABIEN ALET, CNRS and Université Paul Sabatier de Toulouse — We present a large scale exact diagonalization study of the one dimensional spin 1/2 Heisenberg model in a random magnetic field. In order to access properties at varying energy densities across the entire spectrum for system sizes up to L=22 spins, we use a spectral transformation which can be applied in a massively parallel fashion. Our results allow for an energy-resolved interpretation of the many body localization transition including the existence of a many-body mobility edge. The ergodic phase is well characterized by Gaussian orthogonal ensemble statistics, volume-law entanglement, and a full delocalization in the Hilbert space. Conversely, the localized (non-ergodic) regime displays Poisson statistics, area-law entanglement and signs of multifractality in the Hilbert space where a true localization never occurs. We perform finite size scaling to extract the critical edge and exponent of the localization length divergence.
10:24AM S24.00013 Chiral spin density wave order on frustrated honeycomb and bilayer triangular lattice Hubbard model at half-filling, KUN JIANG, YI ZHANG, Department of Physics, Boston College, Chestnut Hill, MA 02467, USA, SEN ZHOU, State Key Laboratory of Theoretical Physics, Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100080, CHINA, ZIQIANG WANG, Department of Physics, Boston College, Chestnut Hill, MA 02467, USA — We study the ground state properties of the Hubbard model on the honeycomb lattice with nearest-neighbor $t_1$ and second nearest-neighbor hopping $t_2$, which is isomorphic to the bilayer triangular lattice. We show that, at half-filling, chiral spin-density wave ($\chi$-SDW) order emerges due to on-site Coulomb interaction $U$ in a wide range of $t_2/t_1$ where both the two-sublattice antiferromagnetic order for small $t_2/t_1$ and the decoupled three-sublattice 120° magnetic order are strongly frustrated. For fixed $t_2/t_1$, we find that increasing $U$ leads to a continuous transition from a $\chi$-SDW semimetal with anomalous Hall effect to a topological chiral Chern insulator exhibiting quantum anomalous Hall effect, which undergoes a first order transition into a $\chi$-SDW insulator with zero total Chern number but anomalous AC Hall effect. We obtain the rich phase diagram and discuss the novel magnetic and topological properties.

10:36AM S24.00014 Summing parquet diagrams via the functional renormalization group: x-ray problem revisited, COLIN WEST, ARTUR SAEZ-GARCIA, TZU-CHIEH WEI, Yang Institute for Theoretical Physics, Stony Brook University, WEI GROUP TEAM — We present a numerical scheme for efficiently extracting the higher-order moments and cumulants of various operators on spin systems represented as tensor product states, for both finite and infinite systems. These quantities can be useful in the evaluation of phase transitions. Of particular interest is the application of this method to calculate the so-called Binder’s Cumulant, which can be used to detect critical points even with small finite numerical calculations.

1This work was supported in part by the National Science Foundation.

Thursday, March 5, 2015 8:00AM - 11:00AM –
Session S25 DMP: Focus Session: Search for New Superconductors I 203B - Chenglin Zhang, Rice University

8:00AM S25.00001 Superconductivity in single-layer films of FeSe with a transition temperature above 100 K, JINFENG JIA, Shanghai Jiao Tong University — Recent experiments on FeSe films grown on SrTiO3 (STO) suggest that interface effects can be used as a means to reach superconducting critical temperatures (Tc) of up to 80 K. This is nearly ten times the Tc of bulk FeSe and higher than the record value of 56 K for known bulk Fe-based superconductors. Together with recent studies of superconductivity at oxides heterostructure interfaces, these results rekindle the long-standing idea that electron pairing at interfaces between two different materials can be tailored to achieve high temperature superconductivity. Subsequent angle-resolved photoemission spectroscopy measurements of the FeSe/STO system revealed an electronic structure distinct from bulk FeSe, with an energy gap vanishing at around 65 K. However, ex situ electrical transport measurements have so far only detected zero-resistance - the key superconductivity. Subsequent angle-resolved photoemission spectroscopy measurements of the FeSe/STO system revealed an electronic structure distinct from these results rekindle the long-standing idea that electron pairing at interfaces between two different materials can be tailored to achieve high temperature superconductivity. Together with recent studies of superconductivity at oxides heterostructure interfaces, these results rekindle the long-standing idea that electron pairing at interfaces between two different materials can be tailored to achieve high temperature superconductivity.

1In cooperation with Jian-Feng Ge, Zhi-Long Liu, Canhua Liu, Chun-Lei Gao, Dong Qian, Qi-Kun Xue, Ying Liu

8:36AM S25.00002 Superconducting property of Sn1-xInxTe compounds, KA-RYEONG KIM, Kyung-Hee Univ. — SnTe has been known as a topological crystalline insulator (TCI). TCI is produced by the inversion symmetry of crystal, instead of time-reversal symmetry and Z2 invariance. Recently, the superconducting properties were discovered in In-doped Sn1-xInxTe compounds, which is believed to be the first superconductor with TCI. We synthesized Sn1-xInxTe ($x = 0.1, 0.2, 0.3, 0.4, 0.5, 0.6$ and $0.7$ ) single like crystals by the flux method. From the electrical resistivity, magnetization, and heat capacity measurements, we obtained superconducting properties such as the critical temperature, upper-critical magnetic fields, coherence length, and Ginzburg-Landau parameters with respect to In-doping concentrations of Sn1-xInxTe in terms of Ginzburg-Landau and Bardeen-Cooper-Shrieffer (BCS) theory.

10:48AM S25.00003 Magnetic Structure of Superconducting FeTeOx Films by Neutron Scattering, L.K. NARANGAMMAMA, ZHIWEI ZHANG, J.I. BUDNICK, W.A. HINES, University of Connecticut, Storrs, J.W. LYNN, Center for Neutron Research, NIST, CHRISTOF NIEDERMAYER, Paul Scherrer Institut Villigen, B.O. WELLS, University of Connecticut, Storrs — We present the temperature-dependent neutron diffraction studies of superconducting FeTeOx, and non-superconducting FeTe films grown by PLD in both cases we were able to get strong elastic, magnetic neutron peaks even though we were using film samples. Both samples had magnetic scattering similar to that of bulk Fe$_{1.05}$Te, indicating the coexistence of magnetism and superconductivity in the oxidized films. We will present a detailed analysis of the differences in magnetism between the superconducting and non-superconducting samples.

1Work supported in part by the National Science Foundation.

2This work was supported in part by the National Science Foundation.
9:00AM S25.00004 The local electronic structure of 1T-Ta(S_{1−x}Se_x)2 studied by scanning tunneling microscopy . XINTONG LI, PENG CAI, ZHENQI HAO, CUN YE, Tsinghua Univ, NAIZHOU WANG, XIANHUI CHEN, YAYU WANG, University of Science and Technology of China — The 1T-TaS_2 compound exhibits a series of complex charge density wave (CDW) transitions and an unexpected insulating ground state at low temperature. It is generally considered to be a Mott insulator, thus a rare example of strongly correlated transition metal dichalcogenide. When a sufficient amount of S is substituted by Se, the system becomes a superconductor. The evolution of the electronic structure and CDW order across the insulator and superconductor transition has attracted much attention. In this talk, we report scanning tunneling microscopy studies of the atomic scale electronic structure of 1T-Ta(S_{1−x}Se_x)2 with varied Se contents. In pristine 1T-TaS_2, we observe the √3 × √3 commensurate CDW order at low temperature, as well as a well-defined insulating energy gap. With increasing Se content, the commensurate CDW order becomes a nearly commensurate CDW order, and a finite electron density of state appears at the Fermi level. Spectroscopic imaging reveals close correlations between the electronic density of states at various energies. We will discuss the implications of these results on the local electronic structure of doped Mott insulators and superconductors in correlated transition metal dichalcogenides.

9:12AM S25.00005 ABSTRACT WITHDRAWN

9:24AM S25.00006 Engineering superconductivity in metal/spin ice heterostructures . JIAN-HUANG SHE, CHOONG HYUN KIM, CRAIG FENNIE, Cornell University, MICHAEL LAWLER, Binghamton University and Cornell University, EUN-AH KIM, Cornell University — How to understand and control unconventional superconductivity is among the most fundamental and pressing challenges in modern condensed matter physics. Although spin fluctuation induced pairing has long been discussed as a mechanism for unconventional superconductivity, it has been challenging to prove the mechanism or use such insight to control superconductivity. We propose an artificial heterostructure consisting of metallic layer deposited on top of quantum spin ice which could exhibit unconventional superconductivity mediated by the spin fluctuations in the spin ice. We will discuss material candidates that are amenable for film growth and their expected band structure as well as their potential for topological superconductivity.

9:36AM S25.00007 Is Sodium a Superconductor Under Pressure? . ROXANNE TUTCHTON, The Colorado School of Mines, XIAO-JIA CHEN, The Carnegie Institution of Washington, ZHI GANG WU, The Colorado School of Mines — Superconductivity has been discovered in compressed Li with a critical temperature (T_c) of 14 K. The other alkali metals are, theoretically, predicted to become superconductors under pressure. Sodium (Na) is the notable exception. Previous ab initio calculations considered superconductivity only in the BCC and FCC structures of alkali metals; however, Na goes through complicated, structural phase transitions at higher pressures until it becomes an insulator around 260 GPa. We have performed first-principles linear response calculations for four metallic phases (BCC, FCC, c116 and t119) of Na to compute lattice dynamics and the electron-phonon spectral function. The electron-phonon coupling parameter as well as T_c were then determined as functions of pressure. Our results suggest that the critical temperature for Na rises with increasing pressure to a maximum T_c of 1.2 K in the c116 phase, then it decreases rapidly to zero K at higher pressures.

9:48AM S25.00008 Searching for new superconductors using perspectives from both chemistry and physics1. ROBERT CAVA, Department of Chemistry, Princeton University — Although some may claim otherwise, the view from the lab bench is that it remains very difficult if not impossible to make reasonable predictions for what will be an entirely new superconducting material. This lends a considerable amount of drama to this field, as spectacular superconductors are periodically known to appear out of the blue sky. Nonetheless if ones business is to find new superconductors, a rational approach has to be taken to the discovery process. In our research we try both chemistry and physics-based perspectives to guide us. Mostly, our searches fail but sometimes we have discovered new superconductors, and not by accident. In this talk I will describe some examples of searches from our current work that have yielded new (Low Tc) superconductors based on both chemical and physical ideas. The postdoctoral fellows in my research group who have had primary responsibility for the searches that I will describe are Huixia Luo and Weiwei Xie.

1This research is supported by the US Department of Energy and the AFOSR MURI on superconductivity.

10:00AM S25.00009 Search for superconductivity and novel phenomena in natural minerals . REN XIONG WANG, XIANGFENG WANG, Department of Physics, University of Maryland College Park, J.R. JEFFRIES, Lawrence Livermore National Laboratory, S.R. SAHA, R.L. GREENE, J. PAGLIONE, Department of Physics, University of Maryland College Park, C. SANTELLI, J. POST, Department of Mineral Sciences, Smithsonian Museum of Natural History — In a unique venture in collaboration with the Smithsonian Institution’s National Museum of Natural History, we present ongoing work from a project focusing on the search for superconductivity in mineral specimens provided by the Department of Mineral Sciences, including magnetization and transport studies of Bornite(Cu_{5}FeS_{4}), Berthierite(FeS_{1}Te_{0.5}S_{3}), Nagyagite(Pb_{5}Au(Te,Sb){_{4}}S_{5-8}) and other related compounds, report low temperature physical properties and ab initio calculations of electronic structure of these compounds, including several unreported magnetic transitions and unconventional transport properties. We focus on an in-depth study of transport and structural properties of Sperrylite(ΠTaS_{2}) under high pressures up to 120 GPa utilizing a designer diamond anvil cell, as well as artificial synthesis using chemical substitutions to tune structural and electronic properties. We will discuss the evolution of resistivity, from semiconducting to metallic behavior as a function of applied pressure and substitution, with indications that superconductivity is induced at the highest pressures.

1This work was supported by the AFOSR under the grant number AFOSR F9550-14-1-0202.

10:12AM S25.00010 Search for Superconductivity in Extraterrestrial Materials: An Electromagnetic Phase Transition with Spin-Glass Characteristics1. S. GU ÉNON, PIT-Nano Optics, University of Tuebingen, Department of Physics and Center for Advanced Nanoscience, University of California San Diego, J.G. RAMIREZ, ALI C. BASARAN, J. WAMPLER, Department of Physics and Center for Advanced Nanoscience, University of California San Diego, S. TAYLOR, Cold Regions Research and Engineering Laboratory, Dartmouth College New Hampshire, M. THIEMENS, Department of Chemistry and Biochemistry, University of California San Diego, IVÁN K. SCHULLER, Department of Physics and Center for Advanced Nanoscience, University of California San Diego — We have established a very sensitive, selective, and non-destructive microwave absorption technique to screen a wide range of different materials for superconductivity. This technique allows for the detection of minute amounts of superconducting material in a non-superconducting matrix and it is an ideal tool for searching for superconducting phases in materials found in nature. Here, we report on electro-magnetic phase transitions in extraterrestrial materials formed under very extreme conditions difficult to replicate in a laboratory. Of particular interest is a phase with a transition temperature of 110 K. The associated field scans are characteristic of a frustrated system. Frustrated systems were reported in magnetic systems (spin glasses) as well as in granular high Tc superconductors (frustrated Josephson Junction networks). We will discuss a procedure to discriminate between those two cases.
10:24AM S25.00011 Material Specific Characterization Dataset (MSCD): A Novel Computational System for Searching for High-Tc Superconductors, MICHAEL SCHAEFFER, O’PAUL ISIKAKU-IRONKWE¹, RTS Technologies, San Diego, CA 92126 — The search for novel high-Tc superconductors, HTSCs, involves billions of potential permutations and combinations in over 80 potential elements with thousands of structures. The need arises therefore for a quick-search system with predictive power. Using correlations of superconductivity with electronegativity, valence electrons, atomic number, formula weight, number of atoms and number of elements in the stoichiometry of superconductors, we have developed a simple predictive computational system called MSCD: Material Specific Characterization Dataset. MSCD of a superconductor defines and describes its stoichiometric structure in terms of averages of electronegativity, valence electrons, atomic number, formula weight, atoms-to-element ratio, ionic radii, first ionization energy and other associated ratios. We found that when the valence electrons and atomic numbers are the same, the materials have close Tcs. Also when the electronegativity and valence electrons are the same, they share the same crystal structure. Conversely, by tuning a material’s stoichiometry to correspond to a known superconductor’s MSCD, the material will become superconducting with close enough Tc. We give many examples of MSCD of superconductors and demonstrate the quick-search predictive power of MSCD in the search for novel HTSCs.

¹The Center for Superconductivity Technologies (TCST), Michael Okpara University of Agriculture, Umudike, Abia State, Nigeria

10:36AM S25.00012 Generalized Periodic System (GPS) for Superconductors, O’PAUL ISIKAKU-IRONKWE¹, MICHAEL SCHAEFFER², RTS Technologies, San Diego, CA 92126. In the search for new superconductors, the need arises for a periodic classification system with predictive power that includes all classes, types and families of superconductors. Using the Mendeleevian model of the Periodic Table of elements, based on increasing mass per atom, we reduce all superconductors to “super-atoms, super-elements,” and classify them into the same seven periods as the periodic table. We discover that for both pure elements and multi-element superconductors, the highest Tcs occur in period 4 superconductors with an argon shell core. The key difference between low Tc and high-Tc superconductors (HTSCs) in Period 4 is the presence of anions in the HTSCs. We observe that superconductors in the other periods lacking anions have a maximum Tc of about 40K; also at least three elements, with an average electronegativity of 2.0 or higher in a material is required for Tcs above 40K. The detailed GPS for superconductors which we have developed has predictive power and should be a guide in the design and search for high-Tc superconductivity.

¹Consultant
²The Center for Superconductivity Technologies, Micheal Okpara University of Agriculture, Umudike, Abia State, Nigeria

10:48AM S25.00013 Tunable cobalt vacancies and related properties in LaCoxAs2, GANG WANG, SHUJIE SHEN, SHIFENG JIN, Institute of Physics, Chinese Academy of Sciences, QINGZHEN HUANG, NIST Center for Neutron Research, NIST, TIANPING YING, DANDAN LI, XIAOLONG CHEN, Institute of Physics, Chinese Academy of Sciences, QINGZHEN HUANG COLLABORATION — The ThCr2Si2-type structure, composed of covalently bonded transition metal-metalloid layers and the intermediate metals, is a common structure to around 1000 compounds. However the origin of transition metal vacancies and their effects on the properties of corresponding compounds have been poorly understood. Here we will report the investigation of structure, physical properties, and electronic structure for a series of nominal LaCoxAs2 (1.6 ≤ x ≤ 2.1). It is revealed that the Co occupancy can be tuned between 1.98(1) and 1.61(1). The structural analyses show that the existence of Co vacancies results from charge balance due to the formation of bond between As-As. These Co vacancies adjust the Curie temperature from 205 K to 47 K and increase the resistivity by more than 100%. First-principles calculations indicate that the Co vacancies weaken the spin polarization and reduce the density of states at the Fermi level, resulting in decreased Curie temperature and increased resistivity, respectively. The results address the importance of transition metal vacancies in ThCr2Si2-type structure and offer a reliable route to tune the magnetism of ThCr2Si2-type structure.

Thursday, March 5, 2015 8:00AM - 11:00AM –
Session S26 DCP: Focus Session: At the Interface of Molecules and Materials: IV

204A - Bruce Weisman, Rice University

8:00AM S26.00001 Variance Spectroscopy: A New Bridge between Ensemble and Single-Particle Studies, R. BRUCE WEISMAN, Rice University — We have developed a new experimental technique that probes variations in the spectra from small regions of heterogeneous bulk samples resulting from statistical variations in composition. The method is demonstrated using suspensions of single-walled carbon nanotubes (SWCNTs), which contain mixtures of distinct structural species emitting photoluminescence at characteristic short-wave infrared wavelengths. Using dilute SWCNT suspensions, focused excitation beams, multichannel detection, and quick data collection, we capture several thousand emission spectra representing different spatial regions of the sample. The data sets are analyzed to find emission mean and variance values as a function of wavelength. The combined mean and variance spectra contain information unavailable from conventional methods, including the abundances of different emissive species and their relative emission efficiencies. The variance data are also analyzed for correlations between intensity fluctuations at different wavelengths to give novel two-dimensional maps that reveal the spectra of homogeneous sub-populations within heterogeneously broadened bulk spectra. The off-diagonal features in these maps expose spatially correlated concentration variations for nanotubes of different types, which arise from earliest stages of aggregation. Variance spectroscopy should prove a powerful new experimental tool for characterizing nanoparticle samples.

8:36AM S26.00002 TBD, LIBAI HUANG, Notre-Dame University — No abstract available.

9:12AM S26.00003 Multiphoton Photoemission/Velocity Map Imaging Studies of Single Particle Plasmonics: A New Ultrafast Laser Microscopy Tool for Nanomaterials, DAVID NESBITT, JILA, University of Colorado — The ability to look with ultrafast laser microscopy at nanoparticles has lead to an explosion of novel research opportunities in chemistry, physics and engineering. By way of example, this talk will attempt to present recent “vignettes” from our group in ultrafast photoelectron studies of novel plasmonic nanomaterials. In particular, scanning photoionization microscopy (SPIM) and dynamics of Au, Ag plasmonic rods, cubes, nanoshells, nanostars, etc) have been investigated at the single nanoparticle level, exploiting ultrafast laser pulses tuned over the nanoparticle plasmon resonance features and monitored by time-resolved, coherent multiphoton electron photoemission and velocity map imaging methods. The focus will be on simple physical pictures that help explain and interpret the underlying chemical physics on the nanoscale level.

In collaboration with Andrej Grubisic, NASA and Jacob Pettine, JILA, University of Colorado.

9:48AM S26.00004 Femtosecond nanoplasmonic dephasing of individual silver nanoparticles, RICHA MITTAL, RACHEL GLENN, ILYAS SAYTASHEV, MARCOS DANTUS, Michigan State University — Localized surface plasmon emission from individual silver nanoparticles and cluster of 100nm silver nanoparticles are probed by 15fs laser pulse replica generated by a pulse shaper. The Fourier transform of the nanoplasmonic coherence oscillations reveals different frequency components, phases, and dephasing rates for each nanoparticle. We find broadly distributed coherence dephasing rates that correspond to the cluster size. Our results provide insight into inhomogenous and homogenous broadening mechanisms in nanoplasmonic spectroscopy.
10:00AM S26.00005 Flicker Noise as a Probe of Electronic Interaction at Metal-Organic Interfaces. OLGUN ADAK, Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY, ETHAN ROSENTHAL, Department of Physics, Columbia University, New York, NY, JEFFERY MEISNER, Department of Chemistry, Columbia University, New York, NY, ERICK ANDRADE, ABHAY PASPATHY, Department of Physics, Columbia University, New York, NY, COLIN NUCKOLLS, Department of Chemistry, Columbia University, New York, NY, MARK HYBERTSEN, Center for Functional Nanomaterials, Brookhaven National Labs, Upton, NY, LATHA VENKATARAMAN, Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY — Understanding the nature of the charge transport at metal-organic interfaces is fundamental for achieving functional organic electronic devices. The charge transport at such interfaces can be achieved by through-bond and through-space interaction. While through-bond interaction dominates the electronic coupling in most systems, through-space interaction plays important role when through-bond interaction is suppressed, for example, due to quantum interference. In this talk, we first shed light into the origin of the flicker noise phenomenon in single molecule junctions and show how it can be used to distinguish between through-bond and through-space interaction at metal-organic interfaces using a scanning-tunneling microscope based break junction technique.

10:12AM S26.00006 Dynamic Oxidation of Gallium Phosphide Surface Tracked by Near Ambient Pressure XPS1. SYLWIA PTASINSKA, XUEQIANG ZHANG, University of Notre Dame — Both from applied and fundamental points of view, it is important that we have a detailed molecular-level understanding of gas-solid interface interactions, especially under operational conditions. Recent progress in in-situ instrumentations (e.g., Near Ambient Pressure X-ray Photoelectron Spectroscopy—NAP XPS), has enabled us to explore the physicochemical processes at the gas-solid interface over a varied range of pressures (up to mbar range), bridging the gap in our knowledge of interfacial interactions. Our recent investigations have focused on dissociative adsorption of small gas-phase molecules onto III-V semiconductors, which leads to surface oxidation. In this work, we carried out a pressure- and temperature-dependent study of GaP(111) oxidation in an O2 environment. Dynamic changes in chemical evolutions at the O2/GaP(111) interface were reflected in Ga 2p, O 1s, and P 2p spectra. Different oxidation states were observed, involving Ga2O, Ga2O3 and GaPO4 formation. A “phase diagram” of GaP(111) oxidation under various O2 pressures and temperatures can help us visualize transition states and gain more insights into chemical pathways leading to the final products of GaP oxidation. Further, an estimation of work function changes of the oxidized GaP surface was obtained under near ambient conditions.

1This material is based upon work supported by the U.S. Department of Energy Office of Science, Office of Basic Energy Sciences under Award Number DE-FC02-04ER15533.

10:24AM S26.00007 One Dimensional Surface Phonon Polaritons in Boron Nitride Nanotubes: High Field Confinement and Localization1. XIAOJI XU, Lehigh University, Bethlehem, PA, USA, BEHNOOD GHAMSARI, University of Ottawa, Ottawa, Ontario, Canada, DMITRI GOLBERG, WPI-MANA Centre of National Institute for Materials Science, Tsukuba, Ibaraki, Japan, PIERRE BERINI, University of Ottawa, Ottawa, Ontario, Canada, GILBERT WALKER, University of Toronto, Toronto, Ontario, Canada — We report the direct observation of one dimensional surface phonon polaritons (SPhPs) in boron nitride (BN) nanotubes at the mid infrared frequencies. High spatial resolution infrared near-field microscopy is used to spatially map the distribution of SPhPs in BN nanotubes. The polaritonic wavelength is experimentally found to be tunable by the tubular diameter as well as the configurations of the conductive supporting substrate. Effective refractive index of the SPhPs is found to be as high as ~70 for a thin BN nanotube. Furthermore, strong field localization and mitigation of the polariton damping is achieved with the use of a rough gold substrate. The randomly spaced nanometer-sized gold grains on the substrate act as distributed reflectors for propagating SPhPs, and confined the surface waves in the one-dimension nanotube. Such geometry allows high field concentration at mid infrared frequencies for chemical sensing and nonlinear optics. Given the analogy between phonon polaritons and plasmon polaritons, BN nanotubes can be used for building blocks for nano-photonic devices in the mid infrared frequencies, with design principles learnt from well-established metallic plasmonics.

1NSERC, ONR, MEXT Japan

10:36AM S26.00008 Characterization of Size, Anisotropy, and Density Heterogeneity of Nanoparticles by Sedimentation Velocity2. BORRIES DEMELER, University of Texas Health Sciences Center San Antonio — A critical problem in materials science is the accurate characterization of the size dependent properties of colloidal inorganic nanocrystals. Due to the intrinsic polydispersity present during synthesis, dispersions of such materials exhibit simultaneous heterogeneity in density, molar mass, and particle diameter. The density increments with respect to diameter and molar mass of these nanoparticles, if known, can then provide important information about crystal growth and particle size distributions. For most classes of nanocrystals, a mixture of surfactants is added during synthesis to control their shape, size, and optical properties. However, it remains a challenge to accurately determine the amount of passivating ligand bound to the particle surface post synthesis. The presence of the ligand shell hampers an accurate determination of the nanocrystal diameter. Using CdSe and PbS nanocrystals, and the silver nanoparticle (M4Ag44(p-MBA)30), as model systems, we describe how appropriate parametrizations of the flow equation can be used to extract high resolution composition information for mixtures of solutes that are heterogeneous in two out of three hydrodynamic parameters when the third is known. We show how this approach can yield important detail to the understanding of solution composition.

10:48AM S26.00009 Design of photo-absorption properties of hybrid organic-inorganic halide perovskite photovoltaic devices by cation manipulation. OSCAR GRANAS, SEAS, Harvard University and Dept. of Physics and Astronomy, Uppsala University, DMITRY VINICHENKO, Dept. of Chemistry and Chemical Biology, Harvard University, EFTHIMIOS KAXIARAS, Dept. of Physics, Harvard University — Photovoltaic devices based on hybrid organic-inorganic halide perovskite materials have lately sailed up as one of the most promising technologies for cost effective harvest of solar energy. In just a few years the efficiency has surpassed that of both conventional dye-sensitized- and organic solar cells. In this study we investigate the influence of the size of the cationic π-system on the electronic and structural properties of the perovskite photo-absorbing material. Using theoretical simulations we investigate key quantities for photovoltaic efficiency, such as band-gap, electron- and hole mass. We show that by changing the cation the band-gap and effective masses can be controlled. Structural changes are addressed, where we can see an enhanced influence of dispersion interaction as the cation polarizability increases. The effects of spin-orbit coupling is considered for both structural and electronic properties.

2Support from VR, the Ingegerd Bergh foundation, SNIC and XSEDE is gratefully acknowledged

Thursday, March 5, 2015 8:00AM - 11:00AM — Session S27 DCP: Focus Session: Solvation of Ions and Electrons II 204B - James M. Lisy, University of Illinois at Urbana-Champaign
8:00AM S27.00001 Spectral signatures of large amplitude vibrations in solvated ions. What do the intensities tell us about structure, bonding and dynamics? ANNE MCDOY, Department of Chemistry and Biochemistry, The Ohio State University — In this talk, I will discuss recent work in our group in which we made connections between proton transfer processes and hydrogen bonding and vibrational frequencies and intensities. Due to the large amplitude motions associated with proton transfer along a hydrogen bond, the vibrational spectra of these systems contain features that cannot be understood by the usual harmonic description of molecular vibrations. The breakdown reflects both the anharmonicity along this coordinate and coupling between this mode and other low frequency modes in these systems. It also reflects changes in the electronic structure as molecules vibrate. The presentation will draw from reported vibrational spectra for systems either containing intra- or intermolecular hydrogen bonds. Both the theoretical approaches used to study these systems and the insights gained from the studies will be described. The theoretical approaches range from the introduction of higher order terms to the harmonic analysis to adiabatic treatments in which the high- and low-frequency modes are treated at different levels of approximation and diffusion Monte Carlo studies in the full dimensionality of the system of interest.

8:36AM S27.00002 Ion Microsolvation Probed by Cryogenic Ion Trap Vibrational Spectroscopy, KNUT R. ASMIS, Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Germany — How ions are solvated in solution has intrigued physical chemists since the development of the theory of electrolytic dissociation by Arrhenius at the end of the nineteenth century. A molecular-level understanding of ion solvation is not only important for understanding chemical processes in solution, but also plays an important role in understanding the surface speciation and reactivity of aerosols. Infrared photodissociation (IRPD) spectroscopy of mass-selected ions, thermalized to cryogenic temperatures, allows for a detailed characterization of the influence of the stepwise solvation of an ion on its properties, one solvent molecule at a time. Recent advances in the vibrational spectroscopy of atmospherically-relevant microsolvated ions are highlighted, with particular emphasis on using isomer-specific detection schemes and measuring IRPD spectra down into the terahertz region of the electromagnetic spectrum.

9:12AM S27.00003 Solvation of ions investigated by DFT-MD simulations: from gas phase to oxide/liquid water interfaces, MARIE-PIERRE GAIGEOT, Universite d'Evry val d'Essonne-Paris, LAMBE UMR8587 — We investigate the solvation of ions by means of DFT-based molecular dynamics simulations (DFT-MD): ions solvated in clusters and ions solvated at solid oxide/liquid water interfaces. DFT-MD simulations provide a detailed knowledge of the solution structural properties at finite temperature, and dynamical anharmonic vibrational spectra extracted from DFT-MD are used to detail the relationships between vibrational features and structures. We present recent results for ionic clusters, i.e. solvation of Li+ by water molecules in Li+(H2O)3+3, including dynamical anharmonic vibrational spectra calculations and comparisons to IR-PD (InfraRed Pre-Dissociation) experiments at different temperatures, also including the dynamical formation of these clusters as it occurs in the experiments and the understanding of how high energy conformers can be formed and probed in theses experiments. We also present solvation of electrolytes at the quartz/liquid water interfaces. Here also, not only do we use DFT-MD in order to unravel the structure of these electrolytes at the interface between the oxide and liquid water but we also extract dynamical vibrational spectra to be compared to SFG (Sum Frequency Generation) experiments. With this comparison we aim at a detailed description of the interfacial structure and its related vibrational signatures.

These works have been done in collaboration with Prof J.M. Lisy (USA), Prof M. Sprik (UK), Prof M. Sulpizi (Germany), Dr V. Brites, and M. Pfeiffer.

9:48AM S27.00004 Anomalous Vibrational Signatures of Ions and Solvation, RYAN STEELE, University of Utah — Vibrational spectroscopy has long served as one of the key experimental windows into the inner workings of molecules. Developments in recent decades have continued to expand these techniques toward exotic ions and biologically relevant systems. Such developments have unearthed a wealth of anomalous vibrational signatures, many of which challenge canonical computational approaches to the simulation of vibrational spectra. In this presentation, the vibrational spectra of particularly challenging ionic systems will be explained via new computational simulations and theoretical frameworks. Examples include (a) strongly anharmonic—yet characteristic—vibrations in protonated, misfolded DNA base pairs, as well as (b) signatures of electronic motion in the vibrational spectra of water oxidation intermediates. Both cases demonstrate strong coupling of a unique electronic structure to quantum mechanical molecular motion. New methodology to enable the interface of these two requirements will also be briefly discussed.

10:24AM S27.00005 Modeling ion solvation in ethylene carbonate and propylene carbonate, AYSE ARSLANARGIN, THOMAS BECK, University of Cincinnati — Lithium-ion batteries (LIBs) and supercapacitors are expected to have important roles in renewable energy generation and in electric vehicles as electrochemical storage systems. Non-aqueous solvents such as ethylene carbonate (EC) and propylene carbonate (PC) are widely used as liquid electrolytes in LIBs. The electrolyte structure affects the efficiency of the ion transport, and understanding the solvent structure is essential for battery performance enhancements. This work investigates the thermodynamics of ion solvation in EC and PC. Free energy and enthalpy of solvation calculations have been conducted employing different force fields. Simulated annealing calculations have been performed to fit classical ion-solvent dimer interaction energies to quantum data. Non-bonded energy parameters are altered during the fitting process. The new parameters result in good agreement with the experimental free energy of solvation values, while the enthalpy of solvation results show deviations from the experimental data. These results suggest that classical models often do not accurately predict basic interactions in ion-solvent systems.

We acknowledge the support of the NSF (Grant No. CHE-1266105) and the Ohio Computer Center for a grant of supercomputer time.

10:36AM S27.00006 Mechanisms of Li-ion transport in bulk electrolytes and through solid-electrolyte interphases (SEI), DMITRY BEDROV, ZHE LI, University of Utah, OLEG BORODIN, Army Research Laboratory — Performance of Li-ion batteries is strongly coupled to the mechanisms of Li+ transport in bulk electrolytes, its transition through electrolyte/SEI interface and its transport through glassy SEI matrix. We will discuss the results of extensive atomistic molecular dynamics (MD) simulations using APPLEP polarizable force field and that have focused on understanding of correlations between the Li+ local structure and the mechanisms of Li+ transport in these systems. Specifically, we will address: a) Li+ transport in ionic liquid based electrolytes and the influence of organic solvent additives (ethylene carbonate and acetone), b) Li-ion transport through model SEIs comprised of alkyl dicarbonate anions and the influence of SEI contamination by Mn2+ cations, and c) transition of Li+ ions through SEI/electrolyte interfaces.
10:48AM S27.00007 Understanding Complex Ion Dynamics in Lithium-Ion Battery Electrolytes from First Principles1, MITCHELL ONG, VINCENZO LORDI, Lawrence Livermore National Laboratory, TIMO BREMER, ATILLA GYULASSY, Lawrence Livermore National Laboratory, University of Utah, ERIK DRAEGER, Lawrence Livermore National Laboratory, HARSH BHATIA, Lawrence Livermore National Laboratory, University of Utah, JOHN PASK, Lawrence Livermore National Laboratory — Lithium-ion secondary batteries are commonly used to power many consumer devices such as handheld phones, laptops, portable music players, and even electric vehicles. One of the key properties that influence the performance of lithium-ion batteries is the ionic conductivity of the electrolyte. This is dependent on the mobility of the Li ion in solution and also related to their solvation structure. In this work, we have performed first-principle molecular dynamics of an LiPF6 salt solvated in different organic solvents such as ethylene carbonate (EC), ethyl methyl carbonate (EMC) and a mixture of the two. We observed that the diffusivity of Li+ is correlated to the degree of Li+ solvation. Corresponding analysis for PF6− shows greater diffusivity than Li+ associated with a weakly-bound, poorly defined first solvation shell. Using a recent analysis method to study the distribution of directional change from relative angles at successive time intervals, we also characterize the complex motion of these ions and find distinct patterns for each ion in different organic solvents. These results provide valuable insight that can be used to improve the cycling rate of Li-ion batteries and potentially lead to the design of new electrolytes for better overall battery performance.

1 LLNL-ABS-663883

Thursday, March 5, 2015 8:00AM - 11:00AM –
Session S28 GMAG DMP: Focus Session: Kagome Antiferromagnets I 205 - Steven White, University of California, Irvine

8:00AM S28.00001 Exotic behavior of the magnetization process of the S=1/2 kagome-lattice antiferromagnet at one-third height of the saturation, TORU SAKAI, JAEA, SPRing-8, HIROKI NAKANO, University of Hyogo — The magnetization process of the S=1/2 Heisenberg antiferromagnet on the kagome lattice is studied by the exact numerical diagonalization [1]. We successfully obtain a new result of the magnetization process of a 42-site cluster in the entire range. Our analysis clarifies that the critical behavior around one-third of the height of the saturation is different from the typical behavior of the well-known magnetization plateau in two-dimensional systems. We also examine the effect of the \( \sqrt{3} \times \sqrt{3} \)-type distortion added to the kagome lattice. We find at one-third of the height of the saturation in the magnetization process that the undistorted kagome point is just the boundary between two phases that show their own properties that are different from each other. Our results suggest a relationship between the anomalous critical behavior at the undistorted point and the fact that the undistorted point is the boundary. A similar behavior of the magnetization process was also predicted in some other frustrated systems [2,3].


8:12AM S28.00002 Measuring symmetry fractionalization in topological orders: application to Z2 spin liquids on kagome lattice, YUAN-MING LU, Ohio State Univ - Columbus, MICHAEL ZALETEL, Station Q, Microsoft Research - Santa Barbara, ASHVIN VISHWANATH, University of California - Berkeley — Mounting numerical evidence for a gapped Z2 spin liquid in the kagome Heisenberg model urges us to develop methods to measure the global and space group symmetry properties of fractional excitations. We show that the universal symmetry characterization of fractional quasiparticles, the projective symmetry group (PSG), can be measured by a dimensional reduction scheme, which relates two-dimensional (2d) symmetric topological orders to 1d symmetry protected topological phases. This general framework allows us to unify Z2 spin liquids in different slave-particle (parton) constructions on the kagome lattice. It is also directly applicable to numeric results obtained in 2d DMRG studies.

8:24AM S28.00003 Chiral and Critical Spin Liquids in Spin-1/2 Kagome Antiferromagnet1, DONGNING SHENG, WEI ZHU, SHOUSHU GONG, Department of Physics and Astronomy, California State University, Northridge, GROUP OF PROF. D. N. SHENG TEAM — The spin liquids (SL) and their phase transitions have attracted much attentions. The extended kagome antiferromagnet emerges as the primary candidate for hosting both time reversal symmetry (TRS) preserving and TRS breaking SLs based on DMRG simulations. To uncover the nature of the novel transition between them, we study a minimum XY model with the nearest-neighbor (NN) \( (J_{xy}) \), the second and third neighbor couplings \( (J_{xy} = J_{x'y} = J_{y'x}) \). We identify the chiral SL (CSL) with the turn on of a small perturbation \( J'_{xy} \approx 0.06J_{xy} \), which is characterized by topological Chern number and conformal edge spectrum as the \( \nu = 1/2 \) fractional quantum Hall state. On the other hand, the NN XY model \( (J_{yy} = 0) \) is shown to be a critical SL, characterized by the gapless spin singlet and vanishing small spin triplet excitations. The phase transition from the CSL to the critical SL is driven by the collapsing of singlet gap. By following the evolution of entanglement spectrum, we find the transition takes place through the coupling of the edge states with opposite chiralities, which merge into the bulk and become gapless neutral excitations. The effect of the NN spin-\( z \) coupling is also studied, which leads to a phase diagram with an extended regime for the gapless SL.

1 U.S. Department of Energy, Office of Basic Energy Sciences under grant No. DE-FG02-06ER46305 (W.Z., D.N.S.), the National Science Foundation through grants DMR-1408560 (S.S.G).

8:36AM S28.00004 Chiral spin liquid in the extended Heisenberg model on the Kagome lattice, WENJUN HU, WEI ZHU, California State University, Northridge, YI ZHANG, Stanford University, SHOUSHU GONG, California State University, Northridge, FEDERICO BECCA, SISSA, DONGNING SHENG, California State University, Northridge, DONNA SHENG TEAM — We investigate the extended Heisenberg model on the Kagome lattice by using Gutzwiller projected fermionic states and the variational Monte Carlo technique. In particular, when both second- and third-neighbor super-exchanges are considered, we find that a gapped spin liquid described by non-trivial magnetic fluxes and long-range chiral-chiral correlations is energetically favored compared to the gapless U(1) Dirac state. Furthermore, the topological Chern number, obtained by integrating the Berry curvature, and the degeneracy of the ground state, by constructing linearly independent states, lead us to identify this flux state as the chiral spin liquid with \( C = 1/2 \) fractionalized Chern number.
demonstrate our method on different exactly solvable quantum dimer models on the kagomé lattice, and show that it can also be applied to generic dimer and
Institute of Technology — In topological quantum spin liquid states, the crystal symmetry operations often act on fractionalized spinon excitations in a
We established a quantum phase diagram for 0 < J2 < 0.25J1 and 0 ≤ J3 ≤ J1, where we find a q = (0, 0) Neel phase, a chiral spin liquid (CSL), a cuboc1 phase that breaks both time-reversal and spin rotational
symmetries, and a valence-bond solid at the neighbor of the Heisenberg model, where a possible Z2 spin liquid has been previously identified. Interestingly, the
classical cuboc1 phase could survive in the spin-1/2 system with strong quantum fluctuations, and the CSL emerges between the q = (0, 0) and the cuboc1
phases. We discover that the CSL has the short spin correlation pattern consistent with the cuboc1 phase, but the chiral order structure is totally different. The
CSL might be understood as a result of the competition between the q = (0, 0) and the cuboc1 phases in the presence of strong quantum fluctuations. We
further studied the quantum phase transitions from the CSL to the magnetically ordered phases, and to the possible Z2 spin liquid of the Heisenberg kagome
model. Interestingly, the exotic continuous topological phase transition might be realized in the system.

Quantum dimer model for the spin-1/2 kagome Z2 spin liquid . IOANNIS
ROUSOCHATZAKIS1, Leibniz Institute for Solid State and Materials Research, IFW Dresden, and Max Planck Institute for the Physics of Complex Systems,
Dresden Germany, YUAN WAN, OLEG TCHERNYSHYOV, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, Maryland 21218,
FREDERIC MILA, Institute of Theoretical Physics, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland — We revisit the description of
the low-energy singlet sector of the spin-1/2 Heisenberg antiferromagnet on kagome in terms of an effective quantum dimer model. With the help of exact
diagonalizations of appropriate finite-size clusters, we show that the embedding of a given process in its kagome environment leads to dramatic modifications of
the amplitudes of the elementary loop processes, an effect not accessible to the standard approach based on the truncation of the Hamiltonian to the
nearest-neighbor valence-bond basis. The resulting parameters are consistent with a Z2 spin liquid rather than with a valence-bond crystal, in agreement with the
last density matrix renormalization group results.

Quantum dimer model for the spin-1/2 kagome Z2 spin liquid . IOANNIS
ROUSOCHATZAKIS1, Leibniz Institute for Solid State and Materials Research, IFW Dresden, and Max Planck Institute for the Physics of Complex Systems,
Dresden Germany, YUAN WAN, OLEG TCHERNYSHYOV, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, Maryland 21218,
FREDERIC MILA, Institute of Theoretical Physics, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland — We revisit the description of
the low-energy singlet sector of the spin-1/2 Heisenberg antiferromagnet on kagome in terms of an effective quantum dimer model. With the help of exact
diagonalizations of appropriate finite-size clusters, we show that the embedding of a given process in its kagome environment leads to dramatic modifications of
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last density matrix renormalization group results.

Novel magnetic orderings in the kagome Kondo-lattice model . GIA-WEI CHERN,
KIPFTON BARROS, Los Alamos National Laboratory, JORN VENDERBOS, Massachusetts Institute of Technology, CRISTIAN BATISTA, Los Alamos National
Laboratory — We consider the Kondo-lattice model on the kagome lattice and study its weak-coupling instabilities at band filling fractions for which the Fermi
surface has singularities. These singularities include Dirac points, quadratic Fermi points in contact with a flat band, and Van Hove saddle points. By combining
a controlled analytical approach with large-scale numerical simulations, we demonstrate that the weak-coupling instabilities of the Kondo-lattice model lead to
exotic magnetic orderings. In particular, some of these magnetic orderings produce a spontaneous quantum anomalous Hall state.

Gapless and gapped spin liquids in frustrated spin-1/2 models . FEDERICO
BECCA, Consiglio Nazionale delle Ricerche (CNR) and International School for Advanced Studies (SISSA) — We present our recent numerical calculations on the
Heisenberg model on various two-dimensional lattices, showing that gapped and gapless spin liquids may be stabilized in highly-frustrated regimes. The
magnetically disordered phases can be described by considering Abrikosov fermions coupled to gauge fields. This approach gives a flexible and transparent
representation of a myriad of states, ranging from valence-bond solids to spin liquids with different properties, including chiral order. For the Kagome lattice,
we find that a gapless U(1) spin liquid with Dirac cones is competitive with previously proposed gapped spin liquids [1,2] also when small second- (J2) and
third neighbor (J3) antiferromagnetic couplings are considered on top of the nearest-neighbor (J1) super-exchange [3-5]. For the J1 − J2 model on finite clusters, a
gapped Z2 spin liquid can be stabilized in presence of a finite J2 super-exchange, with a substantial energy gain with respect to the gapless U(1) Dirac spin
liquid. However, this energy gain vanishes in the thermodynamic limit [4]. The presence of J3 favors a chiral spin liquid with non-trivial magnetic fluxes and
C = 1/2 fractionalized Chern number [5].

Quantum Selection of Order in an XXZ Antiferromagnet on a Kagomé
Lattice1, ALEXANDER CHERNYSHEV, Univ of California - Irvine, MICHAEL ZHITOMIRSKY, CEA Grenoble — By advancing the non-linear 1/S
expansion and the real-space perturbation theory we investigate quantum order-by-disorder selection of the ground state of the nearest-neighbor XXZ
antiferromagnet on the kagomé lattice. The two methods unanimously favor q = 0 over √3 × √3 magnetic order in a wide range of the anisotropy parameter
0 ≤ Δ ≤ 0.72. We demonstrated that the order selection is generated by topologically non-trivial spin-flip processes, presented a strong evidence of the rare case
of quantum and thermal fluctuations favoring different ground states, proposed a tentative S−Δ phase diagram of the model, and suggested further studies.

Detecting crystal symmetry fractionalizations in Z2 spin liquids on kagomé
lattice — insights from quantum dimer models . YANG QI, Perimeter Institute for Theoretical Physics, LIANG FU, Massachusetts Institute of Technology — In topological quantum spin liquid states, the crystal symmetry operations often act on fractionalized spinon excitations in a
fractionalized way. These features are important for identifying the symmetry enriched topological orders of the spin liquid states. In this work we propose a
simple way to detect signatures of such crystal symmetry fractionalizations from the symmetry representations of the ground state wave function. We
demonstrate our method on different exactly solvable quantum dimer models on the kagomé lattice, and show that it can also be applied to generic dimer and
spin models. Particularly our method can be used to distinguish several proposed candidates of Z2 spin liquid states on the kagomé lattice.
10:24AM S28.00011 Chern-Simons theory for Heisenberg spins on the Kagome Lattice, KRISHNA KUMAR, University of Illinois at Urbana-Champaign, KAI SUN, University of Michigan, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — We study the problem of Heisenberg spins on the frustrated Kagome lattice using a 2D Jordan-Wigner transformation that maps the spins (hard-core bosons) onto a system of (interacting) fermions coupled to a Chern-Simons gauge field. This mapping requires us to define a discretized version of the Chern-Simons term on the lattice. Using a recently developed result on how to define Chern-Simons theories on a class of planar lattices, we can consistently study spin models beyond the mean-field level and include the effects of fluctuations, which are generally strong in frustrated systems. Here, we apply these results to study magnetization plateau type states on the Kagome lattice in the regime of XY anisotropy. We find that the 1/3 and 2/3 magnetization plateaus are chiral spin liquid states equivalent to a primary Laughlin fractional quantum Hall state of bosons with (spin) Hall conductivity $\frac{1}{3} e^2/h$ and semionic excitations. The $\frac{2}{3}$ plateau is a chiral spin liquid equivalent to the first Jain descendant. We also consider the spin-1/2 Heisenberg model on the Kagome lattice with a chirality-breaking term on the triangular plaquettes. This situation also leads to a primary Laughlin bosonic fractional quantum Hall type state with filling fraction 1/2.

10:36AM S28.00012 A discretized Chern-Simons gauge theory on arbitrary graphs and the hydrodynamic theory of fraction Chern insulators, KAI SUN, University of Michigan, KRISHNA KUMAR, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — In this talk, we study how to discretize the Chern-Simons gauge theory on generic planar lattices/graphs, with or without translational symmetries, embedded on arbitrary 2D closed orientable manifolds. We show that as long as a one-to-one correspondence between vertices and faces can be defined on the graph such that each face is paired up with a neighboring vertex (and vice versa), a discretized Chern-Simons theory can be constructed. We further verify that all the essential properties of the Chern-Simons gauge theory are preserved in the discretized setup. In addition, we find that the existence of such a one-to-one correspondence is not only a sufficient condition for discretizing a Chern-Simons gauge theory, but also a necessary one, if we want the discretized theory to be nonsingular and to preserve some key properties of this topological field theory. A specific example will then be provided, in which we discretize the Chern-Simons gauge theory on a tetrahedron. In addition, as one application of our discoveries, we present a hydrodynamic theory for (discrete) fractional Chern insulators.

10:48AM S28.00013 No-go constraints on topological order in symmetric Mott Insulators, MICHAEL ZALETEL, Stanford University, ASHVINISH VISHWANATH, University of California, Berkeley — The search for anyonic excitations in Mott insulators (quantum magnets with an odd number of $S = 1/2$ spins per unit cell) has an ally in the Hastings-Oshikawa-Lieb-Schultz-Mattis theorem, which guarantees that a symmetric, gapped Mott insulator must be topologically ordered. However, this theorem is silent on which topological orders are permitted. We point out a new class of symmetry induced constraints on the topological order of a Mott insulator. For example, we show that double semion topological order cannot be realized in a symmetric Mott insulator. An application of our result is to the Kagome lattice quantum antiferromagnet where recent numerical calculations of entanglement entropy indicate a ground state compatible with either toric code or double semion topological order. Our result rules out the latter possibility.

Thursday, March 5, 2015 8:00AM - 11:00AM — Session S29 GMAG: Correlated Electron Magnetism I 206A - William Ratcliff, National Institute of Standards and Technology

8:00AM S29.00001 Investigation of magnetic order in Sm$\text{Tr}_2\text{Zn}_20$ ($\text{Tr} = \text{Fe, Co, Ru}$) and Sm$\text{Tr}_2\text{Cd}_20$ ($\text{Tr} = \text{Ni, Pd}$), DUYGU YAZICI, B. D. WHITE, UC, San Diego, P.-C. HO, California State University, Fresno, N. KANCHANA-VATEE, K. HUANG, UC, San Diego, N. R. DILLEY, Quantum Design, M. B. MAPLE, UC, San Diego — Single crystals of the cage compounds Sm$\text{Tr}_2\text{Zn}_20$ ($\text{Tr} = \text{Fe, Co, Ru}$) and Sm$\text{Tr}_2\text{Cd}_20$ ($\text{Tr} = \text{Ni, Pd}$) have been investigated by means of electrical resistivity, magnetization, and specific heat measurements. The compounds SmFe$\text{Zn}_20$, SmRu$\text{Zn}_20$, and SmNi$\text{Cd}_20$ exhibit ferromagnetic order with Curie temperatures of $T_C = 47.4$ K, 7.6 K, and 7.5 K, respectively, whereas SmPd$\text{Cd}_20$ is an antiferromagnet with a Néel temperature of $T_N = 3.4$ K. No evidence for magnetic order is observed in SmCo$\text{Zn}_20$ down to 110 mK. The Sommerfeld coefficients $\gamma$ are found to be 57 mJ/mol-K$^2$ for SmFe$\text{Zn}_20$, 79.5 mJ/mol-K$^2$ for SmCo$\text{Zn}_20$, 258 mJ/mol-K$^2$ for SmRu$\text{Zn}_20$, 165 mJ/mol-K$^2$ for SmNi$\text{Cd}_20$, and 208 mJ/mol-K$^2$ for SmPd$\text{Cd}_20$. Enhanced values of Sommerfeld coefficients $\gamma$ and a quadratic temperature dependence of the electrical resistivity at low temperature for SmRu$\text{Zn}_20$ and SmPd$\text{Cd}_20$ suggest an enhancement of the quasiparticle masses due to hybridization between localized $4f$ and conduction electron states.

8:12AM S29.00002 Non-Fermi liquid behavior and the underscreened Kondo effect in Fe$_{1-x}$Co$_x$Si, YAN WU, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, 70803, BRAD FULLER, Department of Chemistry, Louisiana State University, Baton Rouge, 70803, JULIA CHAN, Department of Chemistry, The University of Texas at Dallas, Richardson, 75080, DAVID YOUNG, JOHN DITUSA, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, 70803 — Mn or Co substitutions into the narrow band-gap insulator FeSi introduce charge carriers, either holes or electrons, accompanied by an equal density of more localized magnetic moments resulting in an interesting insulator-to-metal transition (IMT). Mn doping of FeSi exhibits an IMT where the nascent metal displays intriguing field sensitive non-Fermi-Liquid (NFL) behavior due to the underscreening of $S = 1$ impurity moments by the spin-1/2 hole carriers. Here, we present the results of an investigation of Fe$_{1-x}$Co$_x$Si ($0 < y < 0.1$). Our magnetization and susceptibility measurements indicate that for $y = 0.03$ Co-impurities also introduce a $S = 1$ magnetic moment that have a tendency to form singlets whereas for larger $y$ ferromagnetic interaction that grows with $y$. We have discovered a NFL behavior for $y < 0.03$ that evolves into the standard disordered Fermi-liquid form either by applying a magnetic field or by increasing $y$. The results of specific heat measurements on Fe$_{1-y}$Co$_y$Si, performed to explore the underlying underscreened Kondo mechanism, to investigate its variation with field and composition, and to compare with our Fe$_{1-y}$Mn$_y$Si data will be presented.

8:24AM S29.00003 Kondo versus indirect exchange: the role of the lattice and the actual range of RKKY interactions in real materials, ANDREW ALLERDIT, Northeastern University, ADRIAN FEIGUIN, Department of Physics, Northeastern University, CARLOS BUSSER, Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, GEORGE MARTINS, Department of Physics, Oakland University, Rochester — Magnetic impurities embedded in a metal interact via an effective Ruderman-Kittel-Kasuya-Yosida (RKKY)coupled by the conduction electrons, which is commonly assumed to be long ranged, with an algebraic decay in the inter-impurity distance. However, they can also form a Kondo screened state that is oblivious to the presence of other impurities. We study the competition mechanisms between both effects on the square and cubic lattices by introducing an exact mapping onto an effective one-dimensional problem that we can solve with the density matrix renormalization group method (DMRG). We show a dramatic departure from the conventional RKKY theory, that can be attributed to the dimensionality and different densities of states, as well as the quantum nature of the magnetic moments. In particular, for dimension $d > 1$, Kondo physics dominates even at short distances, while the ferromagnetic RKKY state is energetically unfavorable. Our findings can have clear implications in the interpretation of experiments and for tailoring the magnetic properties of surfaces.
8:36AM S29.00004 Magnetism in CeRhIn$_5$ at high fields measured by NMR$^1$. A. M. MOUCHE, F. RONNING, E. D. BAUER, J. D. THOMPSON, Los Alamos National Laboratory, A. P. REYES, P. L. KUHNS, National High Magnetic Field Laboratory, Tallahassee, FL — De Haas-van Alphen measurements$^1$ of CeRhIn$_5$ at ambient pressure show an abrupt change in the Fermi surface volume at high fields, $H^*=30$ T, and low temperatures resulting in antiferromagnetic phases with a small Fermi surface at fields below $H^*$ and a large Fermi surface at fields $H$ such that $H^* < H < 50$ T. Nuclear magnetic resonance (NMR) is the ideal probe for these magnetic states as the microscopic details are still lacking. Our preliminary NMR measurements find the magnetic order for $H \parallel c$ is incommensurate up to 30 T as opposed to $H \perp c$ which transitions from incommensurate to commensurate at $H^*=2$ T.$^2$ Furthermore, we find that the magnetic moment decreases near 17 T for $H \parallel c$. These measurements provide an insight into the magnetic anisotropy of CeRhIn$_5$ and are a crucial step to studying its high field phases. $[1]$ L. Jiao et al., arXiv 1308.0294. $[2]$ S. Raymond et al., J. Phys. Cond. Matt. 19, 242204 (2007).

$^1$Work at Los Alamos was performed under the auspices of the U.S. DOE, Office of Basic Energy Science, Division of Materials and Engineering.

8:48AM S29.00005 The Kondo Temperature of Two-dimensional Electron Gas with Rashba Spin-orbit Coupling. LIANG CHEN, Mathematics and Physics Department, North China Electric Power University, JINHUA SUN, Department of Physics, Zhejiang University, HO-KIN TANG, Department of Physics, National University of Singapore, HAI-QING LIN, Beijing Computational Science Research Centre — We use the Hirsch-Fye quantum Monte Carlo method to study the single magnetic impurity problem in two-dimensional electron gas with Rashba spin-orbit coupling. We calculate the spin susceptibilities for different spin-orbit couplings, different Hubbard interactions, and different chemical potentials. The Kondo temperatures for different parameters are estimated by fitting the universal curves of spin susceptibilities. We find that the Kondo temperature is almost a linear function of the Rashba spin-orbit energy when the chemical potential is close to the edge of the conduction band, and when the chemical potential is far away from the band edge, the Kondo temperature is independent of the spin-orbit coupling. These results demonstrate that, for single impurity problem in this system, the most important reason to alter the Kondo temperature is the divergence of density of states near the band edge, and the divergence is induced by the spin-orbit coupling.

9:00AM S29.00006 Remarkably robust and correlated coherence and antiferromagnetism in (Ce$_{1-x}$La$_x$)Cu$_2$Ge$_2$ single crystals. H. HODOVANETS, S.L. BUD’KO, W.E. STRASZHEIM, V. TAUFOUR, E.D. MUN, H. KIM, P.C. CANFIELD, Ames Laboratory and Department of Physics & Astronomy, Iowa State University, Ames, IA — We present results of transport and thermodynamic measurements on La diluted Kondo lattice compound CeCu$_2$Ge$_2$. La-substitution suppresses $T_K$ in an almost linear fashion from $\sim 4$ K, for $x=0$, to below 0.6 K, for $x>0.8$. Curiously, the system also shows low temperature coherent scattering below $T_{coh}$, up to $\sim 0.9$ of La, indicating a small percolation limit $\sim 9\%$ of Ce that separates a coherent state from a single-ion Kondo impurity state. $T_{coh}(H)$ was found to have different functional dependencies in coherent and single-ion regimes. Surprisingly, $T_{coh}$ was found to be proportional to $T_N$ over wide range of $x$. For Ce concentrations, $y=1-x$, in the range $0.01 \leq y \leq 0.08$, $T_{coh}$ in the resistivity data is proportional to $y^{0.5}$ and field-dependent thermopower shows features as expected for the single-ion Kondo impurity. This work was supported by the Department of Energy, Basic Energy Sciences. Note CORP 0207CH11358 and the AFSOR-MURI grant No. FA9550-09-1-0603.

9:12AM S29.00007 Discovery of a 3d-transition-metal-based ferromagnetic Kondo lattice system$^1$. AHMAD US SALEHEEN, TAPAS SAMANTA, DANIEL LEPKOWSKI, ALOK SHANKAR, JOSEPH PRESTIGIACOMO, Louisiana State Univ - Baton Rouge, IGOR DUBENKO, ABDIEL QUETZ. Southern Illinois University, ROY MCDougALD JR., GREGORY MCCANDLESS, JULIA CHIAN, University of Texas at Dallas, PHILIP ADAMS, DAVID YOUNG, Louisiana State Univ - Baton Rouge, NAUSHAD ALI, Southern Illinois University, SHANE STADLER, Louisiana State Univ - Baton Rouge — The formation of a Kondo lattice results in a wide variety of exotic phenomena associated with the competition between the Kondo effect and the RKKY interaction, such as heavy fermions, non-Fermi liquid behavior, unconventional superconductivity, and so on. A quantum critical point (QCP) has been frequently observed at the boundaries of competing phases for antiferromagnetic materials. However, the existence of a ferromagnetic (FM) QCP is unclear. Moreover, FM Kondo lattices are rare. Here we report the discovery of a FM Kondo lattice system Mn$_{1-x}$Fe$_x$CoGe, which is the first example of a 3d-metal-based system (i.e., not rare-earth-based). Resistivity, magnetic susceptibility, heat capacity and thermopower studies on a single crystal sample indicate that the anisotropic FM kondo lattice has formed along c-axis. The signature of a spin density wave transition was also observed above the Kondo minimum, below which the resistivity follows a log(T) behavior.

$^1$This work was supported by the U.S. Department of Energy (Grant Nos. DE-FG02-13ER46946 and DE-FG02-06ER46291).

9:24AM S29.00008 Weak hybridization and isolated localized magnetic moments in the compounds CeT$_2$Cd$_20$ (T = Ni, Pd)$^1$. BENJAMIN WHITE, DUYGU YAZICI, Department of Physics, University of California, San Diego, PEI-CHUN HO, Department of Physics, California State University, Fresno, NORAVEE KANCHANAVATEE, NAVEEN POUSE, AARON FRIEDMAN, M. BRIAN MAPLE, Department of Physics, University of California, San Diego — Large Ce-Ce distances of 6.7-6.8 Å and weak hybridization between Ce 4f and itinerant electron states act to promote stable localized magnetic moments in the compounds CeT$_2$Cd$_20$ (T = Ni, Pd), but also conspire to severely limit the strength of the Ruderman-Kittel-Kasuya-Yosida (RKKY) magnetic exchange interaction that couples them. As a consequence, measurements of electrical resistivity, performed on single-crystalline samples of these new Cd-based compounds down to 0.138 K, were unable to resolve any evidence for magnetic order. In this presentation, we will compare measurements of the physical properties of CeT$_2$Cd$_20$ (T = Ni, Pd) under ambient and applied pressures with the reported properties of the isostuctural compounds CeT$_2$X$_20$ (T = transition metal; X = Al, Zn). We will use these comparisons to discuss the interplay of unit cell volume, hybridization, and the RKKY interaction and its role in establishing the ground states of the Ce-based “1-2-20” compounds.

$^1$Sample synthesis and physical properties measurements were supported by the U.S. DOE under grant no. DE-FG02-04ER46105. Measurements of electrical resistivity below 1 K were supported by the NSF under grants no. DMR-1206553 and no. DMR-1104544.

9:36AM S29.00009 Spin zero-point fluctuations in d-metals. VLADIMIR ANTROPOV, ANDREY KUTEPOV, Ames Laboratory, Ames, USA, KAY DEWHURST, SANGEETA SHARMA, MPI for Microstructure Physics, Halle, Germany — We analyze the structure and the magnetic systems at low temperatures.

Work at Los Alamos was performed under the auspices of the U.S. DOE, Office of Basic Energy Science, Division of Materials and Engineering.
9:48AM S29.00010 Itinerant magnetism in CaMn$_2$Al$_2$$_{}^1$, JACK SIMONSON, Farmingdale State College, LUCIA STEINKE, Brookhaven National Laboratory, SHELBY ZELLMAN, JEDEDIJA KISTNER-MORRIS, AKSHAT PURI, Stony Brook University, EVON ANDREWS, Farmingdale State College, MEAGAN ARONSON, Stony Brook University and Brookhaven National Laboratory — We report the synthesis and basic properties of CaMn$_2$Al$_2$, a new itinerant magnet that is nearly isosstructural with the known quantum critical compound YFe$_2$Al$_2$. Magnetic susceptibility measurements performed on single crystals reveal a cusp at 2 K. Electrical resistivity measurements similarly have a maximum at this temperature, and heat capacity measurements show a broad peak with total entropy of ~ 10%R ln 2. These results together with those of neutron diffraction measurements suggest that CaMn$_2$Al$_2$ is weakly magnetic and potentially close to a quantum critical point.

1Research supported by a DOD National Security Science and Engineering Fellowship via the AFOSR.

10:00AM S29.00011 Complex magnetism and strong electronic correlations in Ce$_x$PdGe$_2$, ANDREW GALLAGHER, TIGLET BESARA, NHMFL, Florida State Univ., JIFENG SUN, FAMU-FSU College of Eng., Dept. Chem. & Biomed. Eng., ORNL, JOE THOMPSON, FILIP RONNING, ANDREW GALLAGHER, TIGLET BESARA, NHMFL, Florida State Univ., JIFENG SUN, FAMU-FSU College of Eng., Dept. Chem. & Biomed. Eng., ORNL, ZHAO, Max Planck Institute for Chemical Physics of Solids, Dresden, 01069, Germany — We report structure/chemical results, magnetization, heat capacity, and electrical transport data for single crystals of the new tetragonal compound Ce$_x$PdGe$_2$. Single crystal X-ray diffraction shows that this material crystallizes in the space group P4$_2$/mmc — and is related to the $\alpha$-ThSi$_2$-type structure. Complicated magnetism, with a two-part antiferromagnetic phase transition at $T_{N,1} = 10.7$ K and $T_{N,2} = 9.6$ K and subsequent ferromagnetic ordering near $T_C \approx 2.25$ K is observed. The ordered ground state emerges from a lattice of Ce ions that are hybridized with the conduction electrons, as revealed by the enhanced effective moment of the specific heat $\gamma \approx 50$ mJ/mol-Ce-K$^2$ (extrapolated to $T = 0$ for $T < T_C$). Electrical structure calculations suggest that there is significant f-electron weight in the density of states near the Fermi energy, consistent with the enhanced specific heat, and that the Fermi surface includes sheets with distinct nesting vectors. We will discuss prospects for tuning the ferromagnetism to zero temperature to produce a ferromagnetic quantum phase transition: e.g., through applied pressure and/or chemical substitution.

10:12AM S29.00012 Transport and torque magnetometry measurements on CeAuSb$_2$, LISSHAN ZHAO, Max Planck Institute for Chemical Physics of Solids, Dresden, 10069, Germany, EDWARD YELLAND, University of St Andrews, Fife, KY16 9SS, UK, JAN BRUIN, High Field Magnet Laboratory, Toemooveld 7, 6525ED Nijmegen, the Netherlands, HIDE SAKAI, Department of Applied Physics, School of Engineering, University of Tokyo, 7-3-1 Hongo Bunkyo-ku, Tokyo 113-8656 Japan, ILYA SHEIKIN, LNCMI-Grenoble (Grenoble High Magnetic Field Laboratory), CNRS, Grenoble, France, ANDREW MACKENZIE, Max Planck Institute for Chemical Physics of Solids, Dresden, 10069, Germany — The tetragonal crystal CeAuSb$_2$ has a layered structure and orders antiferromagnetically at $T < 6K$. Under a c-axis magnetic field, the Néel temperature is gradually suppressed to zero at a possible field-tuned quantum critical point at about 6 T. Within this antiferromagnetic phase, between the QCP and about 2.8 T, there is an additional, novel phase. We report transport measurements on pure single crystals of CeAuSb$_2$, in fields of up to 35 T and from room temperature down to 100 mK. We also report torque magnetometry measurements. Unlike a recent report, we find single, sharp transitions into the novel phase. We discuss the nature of the novel phase.

The work presented is supported by TOPNES(Topological Protection and Non-Equilibrium States in Strongly Correlated Electron Systems research programme), the Engineering and Physical Sciences Research Council (EPSRC, UK) and Max Planck Institute for Chemical Physics of Solids(Dresden, Germany) etc.

10:24AM S29.00013 Effects of uni-axial strain on electronic nematic state in Sr$_2$RuO$_4$, DANIEL BRODSKY, MARK BARBER, University of St Andrews, Scotland and Max Planck Institute for Chemical Physics of Solids, Germany, CLIFFORD HICKS, Max Planck Institute for Chemical Physics of Solids, Germany, ROBIN PERRY, The University of Edinburgh, Scotland, ANDREW MACKENZIE, Max Planck Institute for Chemical Physics of Solids, Germany — Sr$_2$RuO$_4$ exhibits a novel electronic phase in the vicinity of a magnetic field-tuned quantum critical point. This phase shows strong anisotropy under weak symmetry-breaking fields, so it is thought to be intrinsically nematic. We study this phase under anisotropic strain, using a piezoelectric-based device that can both compress and tension samples. We find that the phase responds strongly to anisotropic strain, and discuss this result in the context of various theoretical models for the phase.

10:36AM S29.00014 Evidence of magnetic clusters in the disordered ferromagnet Ni-V close to the quantum critical concentration, RUIZHE WANG, S. UBAID-KASSIS, A. SCHROEDER, Kent State University, Kent, OH, P.J. BAKER, F.L. PRATT, ISIS Facility, U.K., S.J. BLUNDELL, T. LANCASTER, RUIZHE WANG, S. UBAID-KASSIS, A. SCHROEDER, Kent State University, Kent, OH, T. VOJTA, Missouri University of S & T, Rolla, MO — We report the results of muon spin relaxation ($\mu$SR) experiments in zero field (ZF) and transverse field (TF) as well as magnetization (M) data of Ni$_{1-x}$V$_x$ close to the critical vanadium concentration $x_c \approx 11.6$% where the onset of the ferromagnetic (FM) order is suppressed. This material features a prototypical disordered quantum phase transition (QPT) as seen in the temperature (T) and magnetic field (H) dependence of $M(H,T)$. In the paramagnetic phase (PM) above $x_c$, $M(H,T)$ is well described by non-universal power laws characterized by an exponent $\alpha(x-x_c)$, establishing a quantum Griffiths phase. Here, we focus on the FM side of the QPT below $x_c$. After subtracting the spontaneous magnetization $M_0$, we find that $M(H,T) - M_0$ also follows a power law in $H$ at low $T$ with an analogous non-universal exponent $\alpha(x_c-x)$. This is the first evidence of a quantum Griffiths phase within the FM phase in this disordered alloy. $\mu$SR in ZF recognized a broad field distribution below $x_c$, as evidence of magnetic spatial inhomogeneties in the FM phase. Different muon depolarization rates in TF and ZF reveal magnetic clusters already in the PM regime. These observed clusters are important generic ingredients of a disordered QPT.

1current: Durham University, U.K.
2current: ETH Zurich, CH

10:48AM S29.00015 CeCu$_2$Ge$_2$: Challenging our understanding of quantum criticality, BIN ZENG, QIU ZHANG, DANIEL RHODES, National High Magnetic Field Lab, YASUYUKI SHIMURA, Institute for Solid State Physics, University of Tokyo, Kashiwa, Japan, DAIKI WATANABE, Department of Physics, Kyoto University, Kyoto, Japan, RYAN BAUMBACH, National High Magnetic Field Lab, PEDRO SCHLOTTMANN, Department of Physics, Florida State University, Tallahassee, Florida, TAKAO EBIIHARA, Department of Physics, Graduate School of Science, Shizuoka University, Shizuoka, Japan, LUIS BALICAS, National High Magnetic Field Lab — Here, we unveil evidence for a quantum phase transition in CeCu$_2$Ge$_2$. For the H/$c$-axis, no experimental evidence for QC. But as H is rotated towards the a-axis, these $\mu$S increase considerably becoming undetectable for $\theta > 56^\circ$. Around $H \approx 30$ T the resistivity becomes $\propto T$ which, coupled to the divergence of $\mu$, indicates the existence of a field-induced QC point ($H = 0$ K). This observation, suggesting FS hot spots associated with the SDW nesting vector, is at odds with current QC scenarios for which the continuous suppression of all relevant energy scales at $H_c(\theta,T)$ should lead to a line of quantum-critical points in the H-$\theta$ plane. Finally, we show that the complexity of its magnetic phase diagram(s) makes CeCu$_2$Ge$_2$ an ideal system to explore field-induced quantum tricritical and QC end points.

2This work is supported by the National Science Foundation Cooperative Agreement No. DMR-1157490, the State of Florida, and the U.S. Department of Energy. L.B. is supported by DOE-BES through Award No. DE-SC0002613.
8:00AM S30.00001 Magnetic properties of Ce(Fe\textsubscript{1-x}Co\textsubscript{x})\textsubscript{11}Ti and effects of H and N doping\textsuperscript{1}, LIQIN KE, VLADIMIR ANTPEROPOV, Ames Laboratory — The intrinsic magnetic properties of Ce(Fe\textsubscript{1-x}Co\textsubscript{x})\textsubscript{11}Ti related systems have been studied using electronic structure calculations. Both CeFe\textsubscript{11}Ti and CeCo\textsubscript{11}Ti have uniaxial magnetic anisotropy. Calculations of the magnetic anisotropy of Ce(Fe\textsubscript{1-x}Co\textsubscript{x})\textsubscript{11}Ti show that the easy magnetization direction changes from uniaxial to in-plane and then back to uniaxial with increasing Co content. This provides an explanation for the interesting non-monotonic behavior of coercivity observed in experiments. The effects of H and N doping on intrinsic magnetic properties are also studied. Both H and N doping increase the magnetization and Curie temperature while N doping has a stronger effect than H doping. Calculated \textit{Tc} enhancements agree well with experiments and it is found that volume and chemical effects contribute nearly equally to the \textit{Tc} enhancement with N doping. The uniaxial magnetic anisotropy decreases as N doping increases which we believe is consistent with the change in\textit{Tc}. However, a rare-earth idiosyncrasy effect is not only due to the changing of the anisotropy of Ce atom as generally believed. Instead, the decrease of MAE is a collective effect that anisotropy contributions from transition metal sites are also changed with N doping.

\textsuperscript{1}This work is supported by “Novel High Energy Permanent Magnet Without Critical Elements” project by ARPA-E of U.S. Department of Energy.

8:12AM S30.00002 First principles study of doping effects in NdFe\textsubscript{11}Ti permanent magnet compound, YOSUKE HARASHIMA, NRI, “RICS,” AIST; ESICMM, NIMS, KIYOHISA TERAKURA, NRI, “RICS,” AIST; NIMS, HIROI KINO, MANA, NIMS; ESICMM, SHOJI ISHIBASHI, NRI, “RICS.” Green-Innovative Magnetic Material Research Center, AIST , TAKASHI MIYAKE, NRI, “RICS,” ESICMM, NIMS, Green-Innovative Magnetic Material Research Center, AIST — Permanent magnet compounds are required to have large magnetization and strong uniaxial magnetocrystalline anisotropy. NdFe\textsubscript{11}Ti which is one of the ThMn\textsubscript{12}-type rare-earth 3d-transition metal compounds has large magnetic moment due to its high content of Fe. The magnetization and magnetocrystalline anisotropy of the compound can be tuned by nitrogen doping at interstitial sites. NdFe\textsubscript{11}Ti is a good candidate for a permanent magnet compound. Then, it is interesting whether there is another dopant that enhances the magnetic properties. We have investigated doping effects of NdFe\textsubscript{11}Ti X where X=B, C, N, O, and F by using first principles calculation. These dopants increase the magnetization, and the increase is especially large for N, O, and F doping. The magnetocrystalline anisotropy is estimated from the crystalline electric field parameter \textit{<r>}. NdFe\textsubscript{11}Ti has negative value of \textit{<r>} that implies the compound has in-plane anisotropy. As the atomic number of the dopant increases from B to N, \textit{<r>} is increased, and NdFe\textsubscript{11}Ti has a large positive value, suggesting strong uniaxial anisotropy. Then, \textit{<r>} turns to decrease as the dopant is changed from N to O to F, and NdFe\textsubscript{11}Ti has a large negative value. In conclusion, we found that N is the most appropriate dopant among B, C, N, O, and F.

8:24AM S30.00003 Hyperfine fields of Fe in Nd\textsubscript{2}Fe\textsubscript{14}B and Sm\textsubscript{2}Fe\textsubscript{17}N\textsubscript{3}\textsuperscript{1}, HISAZUMI AKAI, Univ of Tokyo, MASAKO OGURA, Osaka Univ — High saturation magnetization of rare-earth magnets originates from Fe and the strong magnetic anisotropy stems from f-states of rare-earth elements such as Nd and Sm. Therefore, the hyperfine fields of both Fe and rare-earth provide us with important pieces of information: Fe and rare-earth anisotropy. Nd\textsubscript{2}Fe\textsubscript{14}B and Sm\textsubscript{2}Fe\textsubscript{17}N\textsubscript{3} enable us to detect site dependence of the local magnetic moment and magnetic anisotropy (Fe sites also contribute to the magnetic anisotropy) while rare-earth NQR directly give the information of electric field gradients (EFG) that are related to the shape of the f-electron cloud as well as the EFG produced by ligands. In this study we focus on the hyperfine fields of materials used as permanent magnets, Nd\textsubscript{2}Fe\textsubscript{14}B and Sm\textsubscript{2}Fe\textsubscript{17}N\textsubscript{3} from theoretical points of view. The detailed electronic structure together with the hyperfine interactions are discussed on the basis of the first-principles calculation. In particular, the relations between the observed hyperfine fields and the magnetic properties are studies in detail. The effects of doping of those materials by other elements such as Dy and the effects of N adding in Sm\textsubscript{2}Fe\textsubscript{17}N\textsubscript{3} will be discussed.

\textsuperscript{1}This work was supported by Elements Strategy Initiative Center for Magnetic Materials Project, the Ministry of Education, Culture, Sports, Science and Technology, Japan.

8:36AM S30.00004 Correlations, spin-charge separation, and magnetic anisotropy, RALPH SKOMSKI, PRIYANKA MANCHANDA, Department of Physics and Astronomy and NCMN, University of Nebraska, Lincoln, NE 68588 — Much of the physics of condensed matter reflects electron-electron correlations. On an independent-electron level, correlations are described by a single Slater determinant with broken spin symmetry. This approach includes Hund’s rule correlations as well as the LSDA and LSDA+U approximations to density-functional theory (DFT). However, from Kondo and heavy-fermion systems it is known that the independent-electron approach fails to describe spin-charge separation in strongly correlated systems, necessitating the use of two or more Slater determinants. Using first-principle and model calculations, we show that spin-charge separation strongly affects the leading rare-earth anisotropy contribution in top-end permanent magnet materials such as Nd\textsubscript{2}Fe\textsubscript{14}B and SmCo\textsubscript{5}. Explicit correlation results are obtained for two limiting cases. First, we derive the density functional for tripositive rare-earth ions in a Bethe-type crystal field. The potential looks very different from the LSDA\textsuperscript{+U} potentials, including gradient corrections. Second, we use a simple model to show that Kondo-type spin-charge separation yield a rare-earth anisotropy contribution in the independent-electron approach. This research is supported by DOE (DE-FG02-04ER46152).

8:48AM S30.00005 Dy-Free Nd-Fe-B Based Permanent Magnets, ARJUN PATHAK, MAHMUD KHAN, KARL GSCHEINZENER, JR., RALPH MCCALLUM, VITALIJ PECHARSKY, The Ames Laboratory, US DOE, Iowa State University, Ames, Iowa 50011-3020, USA — Nd\textsubscript{2}Fe\textsubscript{14}B based permanent magnets are currently the state-of-the-art for high performance magnets. The prototype crystalize in the \textit{P4}_2/\text{mmm} tetragonal crystal structure, where the Nd atoms occupy the 4f and 4g sites, Fe atoms occupy six different atomic sites (16\textit{k}, 16\textit{j}, 8\textit{j}, 8\textit{j}, 4\textit{e}, 4\textit{c}), and B occupies only the 4g site. The leading contribution to the magnetocrystalline anisotropy in Nd\textsubscript{2}Fe\textsubscript{14}B energy comes from the Nd ions, which strongly prefer a \textit{c}-axis alignment at ambient temperature. Nd\textsubscript{2}Fe\textsubscript{14}B permanent magnet has excellent magnetic properties at room temperature but has poor high temperature properties (\textit{T}_{\text{Curie}}>400 K). A small amount of Dy (up to 10\%) is substituted for Nd in Nd\textsubscript{2}Fe\textsubscript{14}B to increase the high temperature performance. Although Dy containing Nd\textsubscript{2}Fe\textsubscript{14}B magnets are desired for high temperature applications, the high price and limited supply of Dy urges the development of Dy-free permanent magnets. Here, we discuss the magnetic properties of several Dy-free Nd-Fe-B based nanostructured magnets and propose alternatives for Dy-based Nd\textsubscript{2}Fe\textsubscript{14}B permanent magnets for high temperature applications such as electric drive motors and wind turbines. This work was supported by the U.S.DOE, ARPA-E, Rare Earth Alternatives in Critical Technologies for Energy (REACT). The research was performed at the Ames Laboratory which is operated for the U.S. DOE by Iowa State University under contract #DE-AC02-07CH11358.
9:00AM S30.00006 Axial Magnetic Anisotropy from Two Systems Fe$_x$B and Co$_2$B with Planar Anisotropy , VALENTIN TAUFOUR, TEJ LAMICHHANE, SERGEY L. BUDKO, ANTON JESCHE, ALAN I. GOLDMAN, KEVIN W. DENNIS, R. WILLIAM McCALLUM, VLADIMIR ANTROPOV, PAUL C. CANFIELD, Ames Laboratory / Iowa State University, Ames, IA 50011, USA — Growth of single crystals of (Fe$_{1-x}$Co$_x$)$_2$B (0 ≤ x ≤ 1) and detailed characterization of their magnetic properties will be presented. Despite the fact that both Fe$_x$B and Co$_x$B show a planar anisotropy at room temperature, we observe a uniaxial anisotropy at intermediate doping which makes (Fe$_x$Co$_{1-x}$)$_2$B a promising system for permanent magnet applications in a system without rare-earth element. Comparison with recent band structure calculations will be presented. The temperature dependence of the anisotropy measured on single crystals from 2 K to 1000 K shows some unusual variations with an increase of the magnetic anisotropy with increasing temperature at some specific substitution.

This work is supported by the Critical Materials Institute, an Energy Innovation Hub funded by the US DOE and by the Office of Basic Energy Science, Division of Materials Science and Engineering. Ames Laboratory is operated for the US DOE by Iowa State University under Contract No. DE-AC02-07CH11358.

9:12AM S30.00007 Electronic structure calculations of the temperature dependence of magnetocrystalline anisotropy in (Fe$_{1-x}$Co$_x$)$_2$B alloys$^1$, IVAN ZHURAVEV, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, Nebraska 68588, USA, LIQIN KE, VLADIMIR ANTROPOV, Ames Laboratory, Ames, Iowa 50011, USA, KIRILL BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, Nebraska 68588, USA — A number of important magnetic systems exhibit anomalous temperature dependence of the magnetocrystalline anisotropy (MCA), such as a spin-reorientation transition or an MCA increasing with temperature. The mechanisms of such anomalies vary. In Nd-Fe-B magnets the spin-reorientation transition is likely due to the ordering of Nd spins, while in MnBi the MCA quickly increases with temperature due to thermal expansion. (Fe$_{1-x}$Co$_x$)$_2$B alloys present another example of highly anomalous temperature-dependent MCA. Our calculations show that these anomalies are not due to thermal expansion. We therefore study the effects of spin disorder on MCA and on the electronic structure of this system using our implementation of the vector disordered-local moment (DLM) method with spin-orbit coupling within the Green’s function-based linear muffin-tin orbital (LMTO) method. We also consider the influence on MCA of the spin moments of Fe and Co. The results show that the observed anomalies are associated with the effects of thermal spin fluctuations on the electronic structure.

$^1$Work at UNL supported by NSF Grant DMR-1308751

9:24AM S30.00008 Superparamagnetism in the martensitic phase of the magnetic shape-memory alloys Ni$_{50-x}$Co$_{10}$Mn$_x$Sn$_{10}$ , SHAOJIE YUAN, Florida state univ, National High Magnetic Lab, PHILIP KUHNS, MICHAEL HOCH, NHMFL, JAMES BROOKS, Florida state univ, National High Magnetic Lab, ARNEIL REYES, NHMFL, VIJAY SRIVASTAVA, Aerospace Engineering and Mechanics, university of Minnesota, DANIEL PHELAN, Aerospace Engineering and Mechanics at university of Minnesota, RICHARD JAMES, CHRIS LEIGHTON, Chemical Engineering and Materials Science at university of Minnesota, NHMFL TEAM, UNIVERSITY OF MINNESOTA TEAM — The Ni-Mn based shape magnetic memory alloys have attracted considerable attention because of their interesting magnetic properties, including intrinsic superparamagnetism and intrinsic exchange-bias effects, which are found in the martensitic phase of these materials. Here, we report on the results of zero-field $^{59}$Mn NMR measurements made on the alloys Ni$_{50-x}$Co$_{10}$Mn$_x$Sn$_{10}$ with x=7 and x=14. The results show that Co substitution not only changes the electronic configuration of a fraction of the Mn ions but also alters the magnetic interaction among these ions, leading to marked changes in the low temperature antiferromagnetic and ferromagnetic components compared to x=0. For both x=7 and x=14 our analysis shows that the Mn ions form a new ferromagnetic nanoclusters in small Co rich regions of the sample. Based on the temperature dependence of the NMR spectral features, we propose a method to estimate the superparamagnetic cluster size distribution.

9:36AM S30.00009 Huge Magnetocrystalline Anisotropy in UMn$_2$Ge$_2$ , DAVID PARKER, Oak Ridge National Laboratory, NIRMAL GHIMIRE, Los Alamos National Laboratory, RYAN BAUMBACH, National High Magnetic Field Laboratory, Florida State Univ., Tallahassee FL, ERIC BAUER, Los Alamos National Laboratory, LING LI, DAVID MANDRUS, Univ. of Tennessee, Knoxville TN, JOHN SINGLETON, Los Alamos National Laboratory, DAVID SINGH, Oak Ridge National Laboratory — We present an experimental finding, as predicted theoretically by one of the authors, of an anomalously high uniaxial magnetic anisotropy energy - approaching 15 MJ/m$^3$ in the extremely strong Uranium spin-orbit coupling and the sizable orbital moment (approaching 2$\mu_B$) for U. This work is supported by the Critical Materials Institute, an Energy Innovation Hub funded by the US DOE and by the Office of Basic Energy Science, Division of Materials Science and Engineering. Ames Laboratory is operated for the US DOE by Iowa State University under Contract No. DE-AC02-07CH11358.

9:48AM S30.00010 Magnetic Anisotropy in UMn$_2$Ge$_2$ , MORGANN BERG, University of Texas at Austin, ALEX DE LOZANNE, RYAN BAUMBACH, JEEHOON KIM, ERIC BAUER, JOE THOMPSON, FILIP RONNING, Los Alamos National Laboratory — We present an experimental finding, as predicted theoretically by one of the authors, of an extremely high uniaxial magnetic anisotropy energy - approaching 15 MJ/m$^3$ in the 122 actinide ferromagnet UMn$_2$Ge$_2$. This large MAE appears to originate in the extremely strong Uranium spin-orbit coupling and the sizable orbital moment (approaching 2$\mu_B$) on this atom. Implications for other 122 compounds are discussed.

$^1$Supported by NSF grant DMR-0810119

10:00AM S30.00011 Lattice Monte Carlo Simulation Study Atomic Structure of Alnico 5-7 Permanent Magnets , MANH CUONG NGUYEN, XIN ZHAO, CAI-ZHUANG WANG, KAI-MING HO, Ames Lab, U.S. DOE and Department of Physics and Astronomy, Iowa State University — The fluctuations and increases in price and the issues in supply recently of rare earth metals re-heated the sought for non-rare earth permanent magnets. Alnico permanent magnets have been considered as promising replacements for rare earth-based permanent magnets due to the superiors in the magnetic performance at high temperature and the abundances of the constituent elements. Using lattice Monte Carlo simulation in combination with cluster expansion method we study the atomic structure of alnico 5-7 permanent magnets. We observed the phase separation into FeCo-rich and NiAl-rich phases in alnico 5-7 at low temperature, which is consistent with experiment. The phase boundary between these two phases is quite sharp. Both FeCo-rich and NiAl-rich phases are in B2 ordering with Fe and Al sitting on 7-site and Ni and Co sitting on 7-site. The degree of order of NiAl-rich phase is quite higher than that of FeCo-rich phase and it decreases with temperature slower than that of FeCo-rich phase. We also observed a small and increasing with annealing temperature magnetic moment in NiAl-rich phase, implying that the magnetic properties of alnico 5-7 could be improved by lowering annealing temperature to diminish the magnetism in NiAl-rich phase.
applications in hybrid molecular nano-spintronics. Dip-pen nanolithography. This could open a new pathway to controlled nanoscale manipulation of magnetism in dilute magnetic semiconductors with potential preparation of the (Ga,Mn)As surface, self-assembled monolayer patterns of organic molecules with sub-75 nanometer linewidth were successfully created by molecular-beam epitaxy, and the organic molecules were deposited by solution-based self-assembly or vacuum thermal evaporation. Charge-transfer molecules coverage could modify the magnetism of the dilute ferromagnetic semiconductor thin films. Mn-doped GaAs thin films with various thicknesses were grown by We investigated the effects of electron and hole donor molecule species on the surface of (Ga,Mn)As thin films with a focus on elucidating how the molecular...magnetic properties of $\varepsilon$-$\text{Fe}_2\text{O}_3$$^1$. We acknowledged partial financial support from the Elemental Strategy Initiative Center for Magnetic Materials (ESICMM) under outsourcing project of MEXT. The computation was partly carried out on the K-computer (Grant No. hp120086).

First principles study of Al substituted strontium hexaferrite. We have studied the site occupancy and magnetic properties of Al substituted M-type Strontium hexaferrite, SrFe$_{12-x}$Al$_x$O$_{19}$ with $x = 0.5$ and $x = 1.0$ using density functional theory (DFT). For $x = 0.5$ case, an Al atom preferentially occupy the 2a site at T = 0 K, this trend endures up to 220 K beyond this temperature Al atom is more likely to occupy the 12k site. For the $x = 1.0$ case, the site preference probability is maximum when two Al atoms occupy the 2a and the 12k sites. We found that magnetic anisotropy of SrFe$_{12-x}$Al$_x$O$_{19}$ increases as the concentration of Al atoms increases, while there is a reduction in the magnetic moment per unit cell by 5µB and 10µB in the case of $x = 0.5$ and $x = 1.0$, respectively. Our results agree with the available experimental results on Al substituted hexaferrite.
8:12AM S31.00002 Different symmetry of the magnetization-direction dependence between the impurity band and valence band in GaMnAs1, IRiya Muneta, Toshiki Kanaki, Shinobu Ohya, Masaki Tanaka. The University of Tokyo — In semiconductors with heavily doped with nonmagnetic shallow acceptors, an impurity band (IB) is formed around the valence band (VB) top and merged with VB. As a result, the parabolic VB top is strongly deformed in a non-parabolic dispersion. In GaMnAs, however, the VB top keeps the parabolic dispersion though there is energy overlap between VB and IB [1-3], which is completely different from the conventional nonmagnetic semiconductors. Here, we measure tunneling anisotropic magnetoresistance on GaMnAs tunnel devices in a spectroscopic way [4-6], analyze the magnetization-direction and energy dependence of the density of states (DOS), and investigate the different symmetry between VB and IB to clarify the mysterious overlap between the two bands. We find that the magnetization-direction dependence of VB DOS is mainly four-fold symmetry along [100] which is the same as the crystal symmetry, while that of IB DOS is mainly two-fold symmetry along [110] unlike the crystal symmetry. These results reveal the unique band structures of Mn-doped III-V ferromagnetic semiconductors. [1] S. Ohya et al., Nat. Phys. (2011). [2] I. Muneta et al., APL (2013). [3] M. Kobayashi et al., PRB (2014). [4] C. Gould et al., PRL (2004). [5] H. Saito et al., PRL (2005). [6] L. Gao et al., PRL (2007).

1This work was partly supported by Grant-in-Aids for Scientific Research including Specially Promoted Research, J.M. thanks the JSPS research fellowship program for Young Scientists.

8:24AM S31.00003 Anisotropic magnetic dynamics in (Ga,Mn)As film1, Xiang Li, Sinjing Dong, Tahee Yoo, Sergio Mello, Xinyu Liu, Jacek Furdyna, Margaret Dobrowolska, Department of Physics, University of Notre Dame — (Ga,Mn)As shows excellent magnetic properties which are usually described by a single-domain model. In this study, we perform a systematic investigation of ac magnetic susceptibility in (Ga,Mn)As films as a function of temperature and field carried out in parallel with dc magnetization measurements. A single ac susceptibility peak is observed close to T_C for the field along [1-10] orientation; a single peak is seen close to 22 K along [110]; and both peaks are observed along [100]. Detailed analysis indicates that the peak near T_C is related to the para-ferromagnetic transition. And the ferromagnetic domains nucleate with their easy axis aligned with [1-10] direction, involving 180° interaction along the easy axis. The peak near 22 K, on the other hand, originates from magnetization switching between two biaxial easy axes separated by a small angle, which is induced by the competition between uniaxial and cubic anisotropy. Dynamic properties emerging from the distinct frequency dependences of the ac susceptibility in these two temperature regions, such as magnetic relaxation times, have been analyzed using various models. Investigations in patterned films will be carried out as well.

1This work is supported by the National Science Foundation Grant DMR1400432.

8:36AM S31.00004 Theory of the Novel Mn-doped II-IV-V Dilute Magnetic Semiconductors. James Glasbrenner, NRC/NRL — A recently discovered magnetic semiconductor Ba_{1-x}K_x(Zn_{1-y}Mn_y)As_2, with its decoupled spin and charge doping, provides a unique opportunity to elucidate the microscopic origin of the magnetic interaction and ordering in dilute magnetic semiconductors (DMS). We show that (i) the conventional density functional theory (DFT) accurately describes this material, and (ii) the magnetic interaction emerges from the competition of the short-range superexchange and a longer-range interaction mediated by the itinerant As holes, coupled to Mn via the Schrieffer-Wolff ρ-d interaction representing an effective Hund’s rule coupling, J_H^{ρd}. The key difference between the classical double exchange and the actual interaction in DMS is that an effective J_H^{ρd}, as opposed to the standard Hund’s coupling J_H, depends on the Mn d-band position with respect to the Fermi level, and thus allows tuning of the magnetic interactions. The physical picture revealed for this transparent system may also be applicable to more complicated DMS systems.

9:12AM S31.00005 Annealing studies of ion-beam irradiated GaMnAs thin films, Segio L.A. Mello, M.M. Sant’Anna, C.F.S. Codeço, Universidade Federal do Rio de Janeiro, Brazil, S. Dong, T. Yoo, X. Li, X. Liu, J.K. Furdyna, University of Notre Dame — We have studied the effect of ion-beam irradiation on GaMnAs films by means of systematic transport and magnetization measurements. Both the magnetization and the conductivity of such samples decrease as a result of increase of disorder and defects in the system caused by the irradiation process. In this study we investigate the recovery of such irradiated samples, by measuring their magnetization and transport properties before and after annealing. Our preliminary transport measurements on annealed-irradiated samples show significant enhancement of the transport properties of the films (revealed by the increase of conductivity and of the critical temperature). Samples comparison of resistivity curves ρ(T) of annealed-irradiated and annealed-non-irradiated samples indicates that most defects created by low fluences of ion beams are similar to those created while growing the samples. This is evidenced by the fact that low ion-fluence irradiation ρ(T) curves of annealed-irradiated and annealed-non-irradiated samples nearly match. For high ion-fluence, however, the sample properties cannot be fully recovered by annealing. This suggests that the nature of a minor fraction of irradiation-created defects is different from those created during sample growth.

9:24AM S31.00006 Spin relaxation time dependence on optical pumping in GaAs:Mn, Veronika Burobina, University of California, San Diego, Christian Binek, University of Nebraska-Lincoln — We analyze the dependence of electron spin relaxation time on optical pumping in a partially-compensated acceptor semiconductor GaAs:Mn using analytic solutions for the kinetic equations of the charge carrier concentrations [1]. Our results are applied to previous experimental data of spin-relaxation time vs. excitation power for magnetic concentrations of approximately 10^17cm^{-3} [2]. The agreement of our analytic solutions with the experimental data supports the mechanism of the earlier-reported atypically long electron-spin relaxation time in the magnetic semiconductor.


9:36AM S31.00007 Visible-light electroluminescence in Mn-doped GaAs light-emitting diodes, Daiki Maruo, Department of Electrical Engineering and Information Systems, University of Tokyo, Pham Nam Hai, Department of Physical Electronics, Tokyo Institute of Technology, Masaaki Tanaka, Department of Electrical Engineering and Information Systems, University of Tokyo — We demonstrate visible-light electroluminescence (EL) due to d-d transitions in GaAs:Mn based LEDs. We design p-n junctions with a p^+GaAs:Mn layer, in which at a reverse bias voltage (-3 to -6 V), an intense electric field builds up in the depletion layers of the p^-n junctions. Holes are injected to the depletion layer by Zener tunneling from the conduction band or by diffusion of minority holes from the valence band of the n-type layer. These holes are accelerated by the intense electric field in the depletion layer, and excite the d electrons of Mn in the p^+ GaAs:Mn layer by impact excitations. We observe visible-light emission at E_1 = 1.89 eV and E_2 = 2.16 eV, which are exactly the same as the 4T_1 → 4A_1 and 4A_2 → 4T_1 transition energy of Mn. The threshold voltage for observation of visible-light EL is -4 V, corresponding to -(E_1 + E_2)/e. This indicates that the impact excitation is most effective for the one step excitation from the ground state 4A_1 to the highest excited state 4A_2.
10:00AM S31.00008 Magnetic Circular Dichroism (MCD) Studies on MOVPE Grown InMnSb and InMnAs 1, 2. M.A. MEEKER, B.A. MAGILL, G.A. KHODAPARAST, Virginia Tech, D. SAHA, C.J. STANTON, University of Florida, S. MCGILL, National High Magnetic Field Laboratory, Florida, B.W. WESSELS, Northwestern University — Carrier-induced ferromagnetism in magnetic III-V semiconductors has opened up several opportunities for device applications as well as for fundamental studies of a material system in which itinerant carriers interact with the localized spins of magnetic impurities. The origin of the carrier-induced ferromagnetism is still an open and exciting question. In order to understand the hole mediated ferromagnetism, probing the band structure in these material systems is crucial. Here we present magnetic circular dichroism (MCD) studies on MOVPE grown InMnSb and InMnAs, both with Curie temperatures above 300K. The measurements were performed on samples with different Mn contents, with the laser excitation energy tuned from 0.92-1.45eV, and external magnetic fields ranging up to 31 Tesla. The measurements are compared with MCD calculations based on an 8 band Pidgeon-Brown model. Comparison of the experimental results with the theoretical calculations provides a direct method to estimate the spin-polarization of the electron in the semiconductor. 

1 This work was supported by the NSF through grant: DMR-0846834 Career Award, DMR-1105437, and DMR -1305666. Also supported by the Institute of Critical Technology and Applied Sciences (ICTAS) at Virginia Tech.

10:12AM S31.00010 Ge doping of FeGa 1,2. J.C. ALVAREZ-QUICENO, M. CABRERA-BAEZ, UFABC, Brazil, J. MUNÉVAR, H. MICKLITZ, E.M. BITTAR, E. BAGGIO-SAITOVITCH, CBPF, Brazil, R.A. RIBEIRO, M.A. AVILA, G.M. DALPIAN, UFABC, Brazil, J.M. OSORIO-GUILLÉN, UdeA, Colombia — The intermetallic narrow-gap semiconductor FeGa is one of the few Fe-based diamagnetic materials. Experimentally, Ge doping induces a ferromagnetic (FM) state. The mechanism responsible for this FM response is still unestablished, but there are proposals of itinerant magnetism to explain this behavior. Our DFT simulations show that inserting holes induces a delocalized FM response, while inserting electrons induces a localized FM response around some Fe atoms. We also modeled different distributions of Ge substitution and observe that the FM response depends on the Ge concentration and also on the Ge distribution on the Ga sites. We observed that the extra electrons become localized in some specific Fe atoms, rather than delocalized over the entire crystal lattice, as expected from an itinerant model. For experimental probing of this scenario, we have performed 57Fe Mössbauer spectroscopy on flux-grown singlecrystalline samples. The resulting resonance peak shape supports a localized model for ferromagnetism, since it is possible to resolve the presence of two distinct Fe isomer shifts (despite a single crystallographic site), expected to correspond to Fe atoms with high and low magnetic moments.

1 The authors thank Capes, CNPQ and FAPESP for financial support.

10:24AM S31.00011 Ge:Mn Dilute Magnetic Semiconductor. LAILA OBIED, Brock University, SJORED ROORDA, University of Montreal, DAVID CRANDELS, Brock University — This work aims to develop Ge:Mn dilute magnetic semiconductor and study the fundamental origin of ferromagnetism in this system. Using ion implantation at 77 K, a single crystal Ge wafer was doped with magnetic Mn ions. The implantation was done at ion energy of 4.76 MeV with a fluence of 2 x 10^{15} ion/cm². X-ray diffraction (XRD) of the as-implanted sample showed that the implanted layer was amorphous. Therefore, different samples were annealed at 200 °C, 330 °C and 600 °C in a tube furnace to achieve a solid phase epitaxial regrowth of the implanted layer. XRD of the sample annealed at 330 °C for 33 hours showed a polycrystalline layer. The depth profile of Mn in the as-implanted sample and the post-annealed sample at 330 °C was determined using secondary ion mass spectroscopy (SIMS) and it was found that some Mn diffused to the surface during the annealing. XRD of the sample annealed at 600 °C for 35 minutes showed peaks corresponding to an unknown phase in addition to peaks from amorphous and polycrystalline Ge. The sample annealed at 200 °C for 168 hour showed no evidence of solid phase epitaxy. A SQUID was used to measure the magnetic properties of all samples. At low temperature, the as-implanted sample showed a paramagnetic behaviour. A magnetic hysteresis at 5K and up to 200K was observed for the samples annealed at 330 °C and 200 °C. The 600 °C annealed sample showed no ferromagnetic response and a significant reduction in the paramagnetic response at low temperature as compared to the as-implanted sample.
the strain-induced changes in spin-orbit coupling on the Re-atoms. This interplay between structural deformations and magnetism leads to a giant MCA (LSAT), SrTiO$_3$.

Magnetocrystalline anisotropy (MCA) has significant implications in a range of applications such as power generation and magnetic data storage. We report the results of using first-principles electronic structure calculations, I show how this electrostatic chemical strain (ECS) effect can be used to tune both crystal field energies and the frontier orbital structure in correlated (La, A)NiO$_3$. Oxygen ligands, which alter the M cation’s $d$-orbital occupancies and spin state, thereby imparting desirable electronic functionality. In this talk, I describe an atomistic engineering approach that makes use of long-range electrostatic interactions between atomic metal-monoxide planes ($\Lambda\Theta$ and $\Lambda\Theta'$) in naturally occurring superlattices, e.g., Ruddlesden-Popper (RP), phases, to tune interlayer atomic structure, orbital degeneracies, and magnetic properties. Using first-principles electronic structure calculations, I show how this electrostatic chemical strain (ECS) effect can be used to tune both crystal field energies and the frontier orbital structure in correlated (La, A)NiO$_3$ RP phases at fixed stoichiometry. I describe how to enhance the Ni $e_g$ orbital polarization, resulting in NiO$_6$ units that exhibit a single $d(\Delta^2 - 5\zeta^2)$ band at the Fermi level—electronic features similar to the layered superconducting cuprates. This approach is generic in construction, making it applicable to any layered topology supporting heterovalent cation substitutions. I conclude by showing it is a realistic strategy to tailor the electronic properties of known materials, and discover yet-to-be realized novel functional oxides without resorting to complex assembly of multi-component heterostructures.

1 Funding for this work is provided by the Defense Advanced Research Projects Agency (DARPA), grant no. N00001-12-4224 and performed in collaboration with P. Balachandran and A. Cammarata.

8:12AM S32.00002 Effects of Ferroelectric Polarization and Strain on Magneto-Crystalline Anisotropy of SrRuO$_3$. JEEVAKA WEERASINGHE, TULA R. PAUDEL, EVGENY Y. TSYMBAL, Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, Nebraska 68588, USA — Magnetoelastic properties of materials have recently been extensively investigated due to their potential application in magnetic data storage, spintronics and high-frequency magnetic devices. Among these properties is the strain effect on magneto-crystalline anisotropy (MCA) which allows the control of magnetization orientation and thus has a direct relevance to magnetic memory applications. In this work, we explore the magneto-crystalline anisotropy of ferromagnetic metal oxide SrRuO$_3$ using first-principles density functional calculations. Due to the presence of Ru atoms, this material has a relatively strong spin-orbit coupling resulting in high MCA. We investigate how epitaxial compressive and tensile strain affect the bulk anisotropy of this material. We also explore epitaxial SrRuO$_3$/BaTiO$_3$ heterostructures where ferroelectric polarization of BaTiO$_3$ affects the interface MCA energy and thus may be used as a control parameter to switch the magnetization orientation. We discuss the physical origins of the effects predicted in terms of the modulation of the electronic structure of SrRuO$_3$ by polarization strain and strain.

8:24AM S32.00003 Control strain of magnetic structure in layered iridates via strong orbital-lattice coupling. CHOONG HYUN KIM, CRAIG FENNIE, Cornell Univ — We have studied from first principles the structural, electronic, and magnetic properties of the layered-perovskite iridates $\text{A}_2\text{IrO}_3$ and $\text{A}_2\text{Ir}_2\text{O}_7$ ($\text{A}=$Sr,Ba) as a function of epitaxial strain. In most of perovkite iridates, due to their large spin-orbit coupling and cubic crystal field, ground state could be described by an effective total angular momentum state $J_{\text{tot}}=1/2$ within $I_{2g}$ manifold. In contrary to what is usually assumed, we find that $d_{2z^2-r^2}$ orbital plays a crucial role to determine a magnetic ground state of iridates if the cubic crystal field is not big enough compared to bandwidth. For instance Ba$_2$IrO$_3$ with tensile strain induces a situation in which magnetization is reversed. Our first-principles results show how A-site cation, dimensionality, and strain are correlated with the band width and crystal field to control magnetic ground states.

8:36AM S32.00004 Electrostatic Chemical Strain: An Approach to Electronic Structure Engineering in Layered Oxides. JAMES RONDONELLI, Northwestern University — Traditional approaches to create and control functional electronic materials have focused on new phases in previously unknown bulk minerals. More recently, interlayer physics has spawned interest in known materials in unexplored atomic scale geometries, especially in complex transition metal oxides (TMO), where heterostructures and superlattices with abrupt interfaces can be created on demand. The interfaces between TMOs often give rise to directional electronic features similar to the layered superconducting cuprates. This approach is generic in construction, making it applicable to any layered topology supporting heterovalent cation substitutions. I conclude by showing that it is a realistic strategy to tailor the electronic properties of known materials, and discover yet-to-be realized novel functional oxides without resorting to complex assembly of multi-component heterostructures.

9:12AM S32.00005 First principles study of the origin of Strain-tunable extraordinary magnetocrystalline anisotropy in Sr$_3$CrReO$_6$ epitaxial films. M.R. BALL, The Ohio State University. J.M. LUCY, O.D. RESTREPO, OSU, A.J. HAUSER, UC, Santa Barbara, J.R. SOLIZ, OSU, J.W. FREELAND, Argonne National Lab, P.M. WOODWARD, W. WINDL, F. Y. YANG, OSU — Magnetocrystalline anisotropy (MCA) has significant implications in a range of applications such as power generation and magnetic data storage. We report the discovery of extraordinarily large anisotropy fields and strain-tunable MCA in Sr$_3$CrReO$_6$ epitaxial films. These films grown on (LaAlO$_3$)$_{0.7}$(Sr$_2$AlTaO$_6$)$_{0.3}$(LSAT), SrTiO$_3$, and SrCr$_5$Nb$_3$O$_{17}$/LSAT substrates undergo dramatic changes in MCA shown by a shift in easy axis from in-plane to out-of-plane. To find the origin of this, we determine the strain-induced distortions and octahedral rotations by performing density functional theory (DFT) calculations using VASP. Correlation effects were treated within GGA+$U$. In DFT, the change in easy axis under strain seen in experiment can be examined through the difference in total energies for magnetic orientation along different crystal axes known as the magnetic anisotropy energy (MAE). The MAE is directly related to the moment anisotropy which is the difference between hard- and easy-axis orbital moments. When a sign change in the moment anisotropy is present, a change in easy axis is indicated. We indeed find this sign change with increasing c/a ratio which is in agreement with experiments. The origin of the MAE resides in the strain-induced changes in spin-orbit coupling on the Re-atoms. This interplay between structural deformations and magnetism leads to a giant MCA.
9:24AM S32.00006 Depth-resolved magnetic and structural analysis of relaxing epitaxial Sr$_2$CrReO$_6$ films. JEREMY LUCY, FENG-YUAN YANG, The Ohio State University, ADAM HAUSER, University of California, Santa Barbara, YAO-HUA LIU, HUA ZHOU, YONGSEONG CHOI, SUZANNE G.E. TE VELTHUIS, DANIEL HASKEL, Argonne National Laboratory — Structural relaxation in a Sr$_2$CrReO$_6$ epitaxial film, with strong spin-orbit coupling, leads to depth-dependent magnetism. We combine a couple of depth-resolved synchrotron x-ray techniques, including two-dimensional reciprocal space mapping and x-ray magnetic circular dichroism experiments, to demonstrate this effect. An 800 nm film of Sr$_2$CrReO$_6$, grown with tensile epitaxial strain on SrCr$_{0.5}$Nb$_{0.5}$O$_3$, relaxes away from the Sr$_2$CrReO$_6$/SrCr$_{0.5}$Nb$_{0.5}$O$_3$ interface. Grazing incidence x-ray diffraction measurements of the film elucidate the in-plane strain relaxation while depth-resolved x-ray magnetic circular dichroism at the Re L$_3$ edge reveals the magnetic contributions of the Re site. This demonstrates a significant change in the magnetic system. This provides an interesting and powerful way to probe the depth-varying structural and magnetic properties of a complex oxide with synchrotron-source x-ray techniques.

1Work supported by the NSF, Grant No. DMR-1420451.

9:36AM S32.00007 Effects of Strain and Buffer Layer on Interfacial Magnetization in Sr$_2$CrReO$_6$ Films. YAOHUA LIU, S.G.E. TE VELTHUIS, Materials Science Division, Argonne National Laboratory, A. GLAVIC, H. AMBAYE, V. LAUTER, Quantum Condensed Matter Division, Oak Ridge National Laboratory, J.M. LUCY, F.Y. YANG, Department of Physics, The Ohio State University — Magnetic double-perovskite Sr$_2$CrReO$_6$ (SCRO) has several functional properties including a T$_C > 500$ K, high spin polarization, large spin-orbit interaction, and semiconducting behavior in highly ordered films. However, fabrication of highly ordered films is still challenging, and progress toward device applications requires an in-depth understanding of the electronic and magnetic properties, especially at interfaces. We have investigated how the Cr/Re antisite disorder and strain affect the interfacial magnetization in SCRO films via x-ray and polarized neutron reflectometry. We find that the magnetization of SCRO films is reduced near the interface with the substrate. The width of this interfacial layer weakly depends on the strain and decreases when a SrCr$_0$O$_3$ buffer layer is used to reduce the antisite disorder. Interestingly, for the SCRO film deposited on a SCNO buffer layer, the region with reduced magnetization is wider than the antisite disorder region at the SCRO/SCNO interface, suggesting that antisite disorder is not the only mechanism reducing the magnetization.

3Work at ANL was supported by the DOE-BES, MSE, at OSU by the Center for Emergent Materials, a NSF MRSEC (DMR-1420451), at ORNL by DOE-BES, Scientific User Facilities Division.

9:48AM S32.00008 Strong Enhancement of Magnetization in Fully Strained SrRuO$_3$ films on Sr$_2$RuO$_4$ single crystal substrates. SEUNGGRAN LEE, Y.J. SHIN, M.C. LEE, C.H. SOHN, S.J. KANG, CCES-IBS & Seoul Nat’l Univ., M.S. ANWAR, Y. SUGIMOTO, S. YONEZAWA, Y. MAENO, Kyoto University, T.W. NOH, CCES-IBS & Seoul Nat’l Univ. — We have investigated epitaxial growth and magnetic properties of SrRuO$_3$ (SRO113) films on single crystal Sr$_2$RuO$_4$ (SRO214) substrates. X-ray diffraction shows only SRO113(001) peaks indicating epitaxial deposition; rocking scan of SRO112(002) indicates a sharp curve with a full width at half maximum of <0.05° implying high crystallinity of our films. Transmission electron microscopy further verifies fully strained of SRO113 films with sharp interface. Surprisingly, the magnetic properties of SRO113/SRO214 show strong enhancement of magnetization (M > 3 μ$_B$/Ru), which has never found in SRO113(001) material systems. In addition, the Curie temperature of our films is identical to that of a bulk SRO113. Magnetic properties of SRO113 films are known to decrease under strain, attributed to Ru06 octahedral distortion. In comparison with varying strain of SRO113 films employing various perovskite substrates, we also found such enhancement is not coming from strain effect; M does not exceed 2 μ$_B$/Ru consistent with previous results due to the low spin configuration nature of SRO113. Possible origins of unique magnetic properties of SRO113/214 will be further discussed.

10:00AM S32.00009 Strain dependence of interfacial antiferromagnetic coupling in La$_{0.7}$Sr$_{0.3}$MnO$_3$/SrRuO$_3$ superlattices. SUJIT DAS, Institute for Physics, MLU Halle-Wittenberg, Germany, ANDREAS HERKLOTZ, Oak Ridge National Lab., Oak Ridge, 37830 TN, USA, ECKHARD PIPPEL, Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany, EP. JIU GUO, Institute for Physics, Johannes-Gutenberg University Mainz, 55128 Mainz, Germany, DIANA RATA, KATHRIN DORR, Institute for Physics, MLU Halle-Wittenberg, Germany — We have investigated the magnetic response of La$_{0.7}$Sr$_{0.3}$MnO$_3$/SrRuO$_3$ superlattices to biaxial in-plane strain applied in-situ. Superlattices grown on piezoelectric substrates of 0.72PbMg$_{1/3}$Nb$_{2/3}$O$_3$/0.28PbTiO$_3$ (PMN-PT) show strong antiferromagnetic coupling of the two ferromagnetic components. The coupling field of μ$_B$HAP = 1.8 T is found to change by μ$_B$δHAP/δε ~ 520 mT%$^{-1}$ under reversible biaxial strain (ε) at 80 K in a [La$_{0.7}$Sr$_{0.3}$MnO$_3$(22 Å)/SrRuO$_3$(55 Å)]$_{15}$ superlattice. This reveals a significant strain effect on interfacial coupling. The applied in-plane compression enhances the ferromagnetic order in the manganese layers which are under as-grown tensile strain. It is thus difficult to disentangle the contributions from strain-dependent antiferromagnetic Mn-O-Ru interface coupling and Mn-O-Mn ferromagnetic double exchange near the interface, since the enhanced magnetic order of Mn spins leads to a larger net coupling of SrRuO$_3$ layers at the interface. We discuss our experimental findings taken into account both the strain-dependent orbital occupation in a single-ion picture and the enhanced Mn order at the interface.

3This work was supported by the DFG within the Collaborative Research Center SFB 762 “Functionality of Oxide Interfaces.”

10:12AM S32.00010 Epitaxial strain induced atomic ordering in stoichiometric LaCoO$_3$ thin films. WOO SEOK CHOI, Sungkyunkwan University, JI-HWAN KWON, Seoul National University, HYOUNGJEEN JEEN, Oak Ridge National Laboratory, GEORGE A. SAWATZKY, University of British Columbia, VLADIMIR HINKOV, Max Planck-UBC Centre for Quantum Materials, MIYOUNG KIM, Seoul National University, HO NYUNG LEE, Oak Ridge National Laboratory. — Heteroepitaxial strain imposed in complex transition metal oxide thin films is recognized as an effective tool for identifying and controlling emergent physical phenomena. Stoichiometric LaCoO$_3$ is particularly interesting, since the thin film form of the material exhibits a robust macroscopic ferromagnetic ordering, while the bulk form of the material is a zero spin, nonmagnetic insulator. In this work, we show that the ferromagnetic ordering observed in LaCoO$_3$ thin films is related to a lattice modulation in the atomic scale, originating from the epitaxial strain. The possibility of oxygen vacancies have been carefully ruled out using various macroscopic and microscopic spectroscopic techniques, and an unconventional strain relaxation behavior identified by strip-like lattice modulation pattern was responsible for the non-zero spin ground state of Co$^{3+}$ ions [1,2]. We further note that the unconventional strain relaxation did not involve any uncontrolled misfit dislocations.

1W. S. Choi et al., Nano Lett. 12, 4966 (2012).
Effect of periodicity on order parameters of multiferroic superlattices\footnote{NSF Grant EPS-01002410}.

SHALINI KUMARI, NORA ORTEGA, Department of Physics and Institute for Functional Nanomaterials, University of Puerto Rico, San Juan, PR 00931-3334, USA — Superlattice (SL) structures with alternating perovskite oxide layers have attracted enormous attention due to their fascinating physics and technology. The half-metallic oxide La$_{0.67}$Sr$_{0.33}$MnO$_3$ (LSMO) and multiferroic Pb$_{2/3}$Zr$_{0.2}$Ti$_{0.8}$O$_{2}$ (F23) materials have been chosen to fabricate SLs by pulsed laser deposition technique on cubic LSAT substrates with LSMO or LaNiO$_3$ as bottom electrodes. X-ray diffraction studies revealed superlattice structure with satellite peaks modulated around main peaks. Atomic force microscopy studies disclosed a systematic decrease in grain size with decrease of modulation periodicity ($\Lambda$) in SLs. Piezo force microscopy studies of SL films confirmed ferroelectricity at a nanoscale level. XPS studies of SLs with $\Lambda=5$ nm confirmed the existence of all elements in the films. A relatively small reduction in saturation magnetization from 28 to 20 emu/cm$^3$ at $H=5$ kOe, remanant polarization from 21 to 10 $\mu$C/cm$^2$ and increase in dielectric constant from 530 to 743 were observed with decrease of $\Lambda$. The observed features will be explained in context of finite size, interfaces, stress, lattice distortion, and grain sizes effects.

Electric-field control of magnetization in (Co(t)/Pt)n/Pb(Mg1/3Nb2/3)$_{1-x}$TiO$_3$ multiferroic heterostructures.

YING SUN, YONGGANG ZHAO, AITIAN CHEN, YAN LIU, Department of Physics, Tsinghua University, Beijing 100084, China, LVKUAN ZOU, XIAOLI ZHENG, QINTONG ZHANG, JIANWANG CAI, XIUFENG HAN, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, WENBO WANG, WEIDA WU, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — A promising way to control magnetism via electric fields is using the converse magnetoelectric effect (CME) in heterostructures composed of ferromagnetic and ferroelectric materials. So far there are few reports on electric-field (E) control of magnetic materials with perpendicular magnetic anisotropy (PMA) which is important in information storage because of its high density and thermostability. In this work, we have systematically studied the CME in heterostructures formed by growing (Co(t)/Pt)n multilayers with different Co thicknesses and n on (011)-oriented ferroelectric Pb(Mg1/3Nb2/3)$_{1-x}$TiO$_3$ substrates. By tuning Co thickness to the vicinity of the spin reorientation critical thickness, samples with PMA, in-plane magnetic anisotropy and crossover were obtained. They showed dramatic different behaviors of E control of magnetization. The results can be understood by considering the interaction between the piezoelectric induced magnetic anisotropy and Co thickness-dependent magnetic anisotropy.

Manipulation of magnetic phase separation and orbital occupancy in manganese by strain engineering and orbital effect.

BIN CUI, CHENG SONG, FENG PAN, Tsinghua Univ, KEY LABORATORY OF ADVANCED MATERIALS (MOE) TEAM — The modification of electronic phases in correlated oxides is one of the core issues of condensed matter. We report the reversible control of ferromagnetic phase transition in manganese films by ionic liquid gating, replicating the La$_{1-x}$Sr$_x$MnO$_3$ (LSMO) phase diagram. The formation and annihilation of an insulating and magnetically hard phase in the soft magnetic matrix, which randomly nucleates and grows across the film, is directly observed under different gate voltages ($V_{G}$). The realization of reversible metal-insulator transition in colossal magnetoresistance materials can lead to the development of four-state memories. (Adv. Funct. Mater. DOI: 10.1002/adfm.201402007) The orbital occupancy and magnetic anisotropy of LSMO films are manipulated by $V_{G}$ in a reversible and quantitative manner. Positive and negative $V_{G}$ increases and reduces the occupancy of the orbital and magnetic anisotropy that were initially favored by strain (irrespective of tensile and compressive), respectively. This finding fills in the blank of electrical manipulation of four degrees of freedom in correlated system. (Adv. Funct. Mater. (revised))

Thursday, March 5, 2015 8:00AM - 11:00AM — Session S33 DBIO DPOLY: Focus Session: Conformations and Dynamics of Biopolymers I

Comparison of the Single Molecule Dynamics of Linear and Circular DNAs in Planar Extensional Flows\footnote{Texas Tech University John R. Bradford Endowment}.

YANFEI LI, Texas Tech University, KAI-YEN HSIAO, CHRISTOPHER BROCKMAN, University of Illinois at Urbana-Champaign, DANIEL YATES, GREGORY MCKENNA, Texas Tech University, CHARLES SCHROEDER, University of Illinois at Urbana-Champaign, MICHAEL SAN FRANCISCO, Texas Tech University, JULIE KORNFIELD, California Institute of Technology, RAE ANDERSON, University of San Diego — Chain topology has a profound impact on the flow behaviors of single macromolecules [1]. The absence of free ends separates circular polymers from other chain architectures, i.e., linear, star, and branched. In the present work, we study the single chain dynamics of large circular and linear DNA molecules by comparing the relaxation dynamics, steady state coil-stretch transition, and transient molecular individualism behaviors for the two types of macromolecules. To this end, large circular DNA molecules were biologically synthesized [2] and studied in a microfluidic device that has a cross-slot geometry to develop a stagnation point extensional flow [3]. Although the relaxation time of rings scales in the same way as for the linear analog, the circular polymers show quantitatively different behaviors in the steady state extension and qualitatively different behaviors during a transient stretch. The existence of some commonality between these two topologies is proposed. [1] M. Kapnistos et al., Nat. Mater. 7, 997 (2008). [2] S. Laib et al., Macromolecules 39, 4115 (2006). [3] M. Tanyeri et al., Lab Chip 11, 1786 (2011).

Ratchet rectification effect on the translocation of a flexible polyelectrolyte chain induced by spatial asymmetry of the channel.

DEBASISH MONDAL, MURUGAPPAN MUTHUKUMAR, University of Massachusetts — We report a three dimensional Langevin dynamics simulation of a uniformly charged flexible polyelectrolyte, translocating through a symmetric narrow channel with periodically varying cross-sections, under the influence of a periodic external electric field. When reflection symmetry of the channel is broken, rectification effect is observed with a favored direction for the chain translocation. For a given volume of the channel unit and polymer length, the rectification occurs only after a threshold frequency of the external periodic driving. We also observe that the extent of the rectification depends on the length of the polyelectrolyte, geometric parameters of the channel governing the spatial asymmetry, and the strength of the external periodic driving field. The observed rectification process is interpreted in terms of an effective asymmetric periodic potential along the direction of the polymer translocation.

Comparison of Translocations of Ring and Linear Polymers.

NING OU YANG, MURUGAPPAN MUTHUKUMAR, University of Massachusetts — We compare the translocation dynamics of ring and linear polymer chains (pertinent to circular and linear DNA) through a nanopore under a driving force, using the Fokker-Planck formalism and scaling arguments. We report qualitatively different dynamics between these topologies arising from the conformational entropy of the polymer and pore-polymer interaction.
8:36AM S33.0004 Increasing polymer diffusivity by increasing the contour length: The surprising effect of YOYO-1 on DNA dynamics

SEUNGHWAN SHIN, KEVIN DORFMAN, XIANG CHENG, Univ of Minn — Double-stranded DNA (dsDNA) labeled with cyanine dyes such as YOYO-1 has been extensively used as a model to study equilibrium and dynamic properties of semiflexible polyelectrolytes. The ability to directly visualize the polymer dynamics is an attractive feature of these experiments, but positively charged cyanine dyes affect the physical properties of dsDNA, distorting the double helix and counterbalancing the intrinsic negative charge of the backbone. A variety of studies have been conducted to reveal the effect of the dye on the contour length and the persistence length of dsDNA. However, fewer efforts have been made to directly quantify the effect of dye on the diffusion behavior of dsDNA. In order to resolve this issue, we measured the in-plane diffusion coefficient of unconfined dsDNA using confocal microscopy. Although there is widespread consensus that intercalation increases the contour length of dsDNA, we find that increasing the dye-base pair ratio for YOYO-1 actually enhances the diffusion of dsDNA. This enhancement is more significant at lower ionic strengths, which implies that the increase in the diffusion coefficient by dye-DNA intercalation is mainly due to a reduction of excluded volume effect resulting from charge neutralization on the backbone.

8:48AM S33.0005 Using an effective dimensionality to map the force-extension relation for a semi-flexible polymer in a nanoslit

HENDRICK DE HAAN, University of Ontario Institute of Technology — The force-extension relation for a semi-flexible polymer is well described by the Marko-Siggia equation in both two and three dimensions. However, while of interest for experimental systems such as DNA in nanotubes, the behaviour between these limiting dimensionalities is less understood. We will present results from simulations of a polymer subject to a stretching force \( F \) and confining geometry \( L \times 1 \times h \), with \( h \ll L \). The relevant persistence length are shown to change. This observation leads to the definition of an effective dimensionality, \( d_{eff} \), to characterize the system. At low \( F \), using \( d_{eff} \) in a generalized form of the Marko-Siggia relation provides good agreement with the simulation curves. However, at high \( F \), \( d_{eff} \) drifts back towards \( d = 3 \). The reason behind this \( F \) dependence is discussed. Semi-empirical forms for strong and weak confinement regimes will be presented and shown to give good agreement across all slit heights and stretching forces. \( d_{eff} \) is thus dependent on \( h \) and \( F \) and provides a cohesive physical picture for all regimes.

9:00AM S33.0006 Correlated Fluctuations of DNA Between Nanofluidic Traps

EXANDER KLOTZ, LYNDON DUONG, MIKHAIL MAMAEV, WALTER REISNER, McGill Univ — Nanofluidic polymer physics has been the subject of intense investigation, and experimental efforts have focused almost exclusively on quantifying equilibrium confined chain conformation in simple nanoslits (2D) and nanochannel (1D) geometries. Complex nano environments, defined as spaces composed of interlinked nanoscale regions of varying confinement and dimensionality, are also technologically significant and have qualitatively distinct physics. Here, a single DNA molecule is suspended between two adjacent nanocavities structures embedded in an open nanoflat. A portion of the molecule occupies each cavity with a third linker segment connecting the two. Contour fluctuations between the cavities give rise to novel correlations. Cross-correlation of the time-dependent cavity intensities enables a noise insensitive measurement of the relaxation times for the segmental transfer modes. We explore how these relaxation times scale with cavity width and spacing and compare our results to a simple free energy model incorporating a slend termed linker spring energy and cavity self-exclusion cost.

9:12AM S33.0007 Metastable Tight Knots in DNA

LIANG DAI, Singapore-MIT Alliance for Research and Technology, C. BENJAMIN RENNER, PATRICK DOYLE, Department of Chemical Engineering, Massachusetts Institute of Technology — Knotted structures can spontaneously occur in polymers such as DNA and proteins, and the formation of knots affects biological functions, mechanical strength and rheological properties. In this work, we calculate the equilibrium size distribution of trefoil knots in linear DNA using off-lattice simulations. We observe metastable knots on DNA, as predicted by Grosberg and Rabin. Furthermore, we extend their theory to incorporate the finite width of chains and show an agreement between our simulations and the modified theory for real chains. Our results suggest localized knots spontaneously occur in long DNA and the contour length in the knot ranges from 600 to 1800 nm.

9:24AM S33.0008 Translocation of a Polymer Chain Through a Nanopore Starting From a Confining Nanotube: The Limit of high Peclet Numbers

GARY W. SLATER, DAVID SEAN, University of Ottawa, HENDRICK DE HAAN, University of Ontario Institute of Technology — We use Langevin Dynamics simulations to study a scenario where a confining nanotube is used as a way to limit the range of conformations available to a polymer chain prior to driven translocation. We find that the tube not only reduces the variance in translocation times (a useful result for practical applications), but also that the elongated polymer conformations yield longer translocation times (also a useful result) that can be dominated by the post-propagation process when the diameter of the nanotube is smaller than a universal critical value. We adapt the tension propagation theory for this geometry and find agreement with the simulations using a single friction parameter to model the roles of both the nanotube and the modified theory for real chains. Our results suggest localized knots spontaneously occur in long DNA and the contour length in the knot ranges from 600 to 1800 nm.

9:36AM S33.0009 Dynamics of a fluctuating semi-flexible membrane

NATHANIEL TUKDARIAN, AIQUN HUANG, RAMESH ADHIKARI, ANIKET BHATTACHARYA, University of Central Florida — We report our preliminary studies of conformations and dynamics of a fluctuating semi-flexible membrane. Our membrane is a 2D lattice with linear segments (i.e., rods) of length \( L \) and \( n_b \) excluded volume beads connected by anharmonic springs. The stiffness of the membrane is controlled by adjusting the strength \( k_b \) of the bending potential \( \mathcal{U}_b = k_b (1 - n_i - n_j) \) between adjacent elementary plaquettes consisting of three beads at the corners connected by bonds and characterized by normal unit vectors \( \hat{n}_i \) and \( \hat{n}_j \). We study the conformations and dynamic fluctuations of the membrane using Brownian dynamics simulation. We show how the radius of gyration scales with \( N \) and \( k_b \), and study characteristics of the transverse fluctuations, the root-mean-square displacement of the center of mass, and the dynamics of the end monomers at each corner.

9:48AM S33.0010 Expanded experimental parameter space of semiflexible polymer assemblies through programmable nanomaterials

DAVID SMITH, CARSTEN SCHULDT, JESSICA LORENZ, TERESA TSCHIRNER, MAXIMILIEN MOEBIUS-WINKLER, Fraunhofer Institute for Cell Therapy and Immunology, JOSEF KAES, MARTIN GLASER, TINA HAENDLER, JOERG SCHNAUSS, University of Leipzig, Institute for Soft Matter Physics — Biologically evolved materials are often used as inspiration in the development of new materials as well as examinations into the physical principles governing their behavior. For instance, the biopolymer constituents of the highly dynamic cellular cytoskeleton such as actin have inspired a deep understanding of soft polymer-based materials. However, the molecular toolbox provided by biological systems has been evolutionarily optimized to carry out the necessary functions of cells, and the inability modify basic properties such as biopolymer stiffness hinders a meticulous examination of parameter space. Using actin as inspiration, we circumvent these limitations using model systems assembled from programmable materials such as DNA. Nanorods with comparable, but controllable dimensions and mechanical properties as actin can be constructed from small sets of specially designed DNA strands. In entangled gels, these allow us to systematically determine the dependence of network mechanical properties on parameters such as persistence length and crosslink strength. At high concentration of the presented attractive forces, we see a transition to highly-ordered bundled and “aster” phases similar to those previously characterized in systems of actin or microtubules.

# Abstracts
well structure. Are described, in addition to, the temperature dependent hot carrier dynamics and phonon mediated thermalization coefficient for the InAs/AlAsSb quantum
excitation spot size, which was compared with experiment by measurements using variable diameter pinholes to determine beam radius. Here, these techniques
laser spot size is important in order to determine the absorbed power density. Simulations were performed based on our PL geometry in order to calculate the
of the power density, penetration depth, diffusion, and recombination rates using a combination of simulation and empirical methods. A precise measurement of
is investigated using continuous wave photoluminescence (PL). The
occurred at temperatures between about 775 and 825
Delaware — To better assess the potential of cobalt oxide for thermal energy storage (TES), the Co3O4/CoO oxidation/reduction reaction has been studied by
top 1000 molecules for use as photovoltaic materials based on their optical absorption properties obtained via time-dependent density functional theory. This
a molecular library of more than 2.6 million candidate compounds based on their performance as possible OPV materials. Here, we present a ranking of the
cost is potentially lower. The Harvard Clean Energy Project, using a cheminformatic approach of pattern recognition and machine learning strategies, has ranked
MARIO BORUNDA, SHUO DAI, Oklahoma State University, ROBERTO OLIVARES-AMAYA, Princeton University, CARLOS AMADOR-BEDOLLA, UNAM,
Q SANGEETHA VIJEYARAGUNATHAN, TETSUYA D. MISHIMA, MICHAEL B. SANTOS, IAN R. SELLERS, University of Oklahoma — We present an investi-
gation of hot carriers in InAs/AlAsSb quantum wells as a practical candidate for a hot carrier solar cell absorber. The thermalization coefficient (Q)
S20
National Lab — Recent discoveries of two novel phases of silicon, Si
S24
, CHIN SHEN ONG, SANGKOOK CHOI, STEVEN G. LOUIE, Department of Physics, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, UK, FLORIAN REHFE LD, CHRISTOPH F. SCHMIDT, Third Institute of Physics-Biophysics, Georg August University, Goettingen — Molecular stress generation in cells is spatially and temporally organized in complex patterns to drive meso-scale active processes such as intracellular transport, cell migration or cell division. To quantitatively understand how these processes are driven, it is necessary to map local
stresses inside cells, which is hard due to the lack of appropriate probes. We have designed a molecular-scale probe consisting of a self-assembled DNA hairpin
with a fluorophore - quencher pair that responds to small forces (pN) applied to its ends. We demonstrate the working of this force sensor in vitro and explore
possibilities for in vivo application to map local stress fields in cells.

10:12AM S33.00012 AFM Studies of Conformational Changes in Proteins and Peptides, NICOLETA
PLOS CARIU, PINA KUK SUTHANKAR, JOHN TOMICH, ROBERT SODZIEKIVCI, Kansas State University — Here, we present estimates of molecular
stiffness and mechanical energy dissipation factors for some examples of proteins and peptides. The results are obtained from AFM force spectroscopy
measurements. To determine molecular stiffness and mechanical energy dissipation factors we developed a model based on measuring several resonance
frequencies of an AFM cantilever in contact with either single protein molecule or peptides adsorbed on arbitrary surface. We used compliant AFM cantilevers
with a small aspect ratio - a ratio of length to width - in air and in liquid, including biologically relevant phosphate buffered saline medium.

1Department of Physics
2Department of Biochemistry and Molecular Biophysics
3Department of Biochemistry and Molecular Biophysics
4Department of Physics

10:24AM S33.00013 Reptation Theory and Many Body Effects in Semiflexible Polymer Dy-
namics, ERWIN FREY, Univ Muenchen — No abstract available.

Thursday, March 5, 2015 8:00AM - 11:00AM –
Session S34 GERA: Biofuels, Solar Fuels and Artificial Photosynthetic Systems 210A -

8:00AM S34.00001 Computational assessment of organic photovoltaic candidate compounds,
MARIO BORUNDA, SHUO DAI, Oklahoma State University, ROBERTO OLIVARES-AMAYA, Princeton University, CARLOS AMADOR-BEDOLLA, UNAM,
ALAN ASPURU-GUZIK, Harvard University — Organic photovoltaic (OPV) cells are emerging as a possible renewable alternative to petroleum based resources
and are needed to meet our growing demand for energy. Although not as efficient as silicon based cells, OPV cells have as an advantage that their manufacturing
cost is potentially lower. The Harvard Clean Energy Project, using a cheminformatic approach of pattern recognition and machine learning strategies, has ranked
a molecular library of more than 2.6 million candidate compounds based on their performance as possible OPV materials. Here, we present a ranking of the
top 1000 molecules for use as photovoltaic materials based on their optical absorption properties obtained via time-dependent density functional theory. This
computational search has revealed the molecular motifs shared by the set of most promising molecules.

8:12AM S34.00002 Thermogravimetric, Calorimetric, and Structural Studies of the Co3O4/CoO
Oxidation/Reduction Reaction, KARL UNRUH, RONALD CICHOCKI, BRIAN KELLY, GERALD POIRIER, Univ of Delaware — To better assess the potential of cobalt oxide for thermal energy storage (TES), the Co3O4/CoO oxidation/reduction reaction has been studied by
thermogravimetric (TGA), calorimetric (DSC), and x-ray diffraction (XRD) measurements in N2 and atmospheric air environments. TGA measurements showed
an abrupt mass loss of about 6.6% in both N2 and air, consistent with the stoichiometric reduction of Co3O4 to Co and structural measurements. The onset
temperature of the reduction of Co3O4 in air was only weakly dependent on the sample heating rate and occurred at about 910 °C. The onset temperature for
the oxidation of CoO varied between about 850 and 875 °C for cooling rates between 1 and 20 °C/min, but complete re-conversion to Co3O4 could only be
achieved at the slowest cooling rates. Due to the dependence of the rate constant on the oxygen partial pressure, the oxidation of Co3O4 in a N2 environment
occurred at temperatures between about 775 and 825 °C for heating rates between 1 and 20 °C/min and no subsequent re-oxidation of the reduced Co3O4
was observed on cooling to room temperature. In conjunction with a measured transition heat of about 600 J/g of Co3O4, these measurements indicate that
cobalt oxide is a viable TES material.

8:24AM S34.00003 Electronic and Optical Properties of Novel Phases of Silicon and Silicon-
Based Derivatives, CHIN SHEN ONG, SANGKOOK CHOI, STEVEN G. LOUIE, Department of Physics, UC Berkeley and Lawrence Berkeley National Lab — Recent discoveries of two novel phases of silicon, Si320 and Si324, lead to promises of quasi-direct band gap silicon crystals that are capable
of complementing indirect-gap diamond cubic silicon for use in the solar cell industry. This work studies the quasiparticle excitations and optical spectra of
these two structures, Si320 and Si324, assessing their suitability for use as photovoltaic materials. We carry out ab initio GW and GW-BSE calculations for the
quasiparticle excitations and optical spectra, respectively, including self-energy and electron-hole interaction effects. This work was supported by NSF grant
No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley
National Laboratory’s NERSC facility.

8:36AM S34.00004 Accurate determination of the temperature dependent thermalization coeffi-
cient (Q) in InAs/AlAsSb quantum wells, HAMIDREZA ESMAILPOURJ, JINFENG TANG, VINCENT R. WHITESIDE, SANGEETHA VIJEYARAGUNATHAN, TETSUYA D. MISHIMA, MICHAEL B. SANTOS, IAN R. SELLERS, University of Oklahoma — We present an investiga-
tion of hot carriers in InAs/AlAsSb quantum wells as a practical candidate for a hot carrier solar cell absorber. The thermalization coefficient (Q) of the sample
is investigated using continuous wave photoluminescence (PL). The Q is accurately determined through transfer matrix calculations of the absorption, analysis
of the power density, penetration depth, diffusion, and recombination rates using a combination of simulation and empirical methods. A precise measurement of
laser spot size is important in order to determine the absorbed power density. Simulations were performed based on our PL geometry in order to calculate the
excitation spot size, which was compared with experiment by measurements using variable diameter pinholes to determine beam radius. Here, these techniques
are described, in addition to, the temperature dependent hot carrier dynamics and phonon mediated thermalization coefficient for the InAs/AlAsSb quantum
well structure.
8:48AM S34.00005 Improved performance due to selective passivation of nitrogen clusters in GaInNAs solar cells1. MIWA FUKUDA, VINCENT R. WHITESIDE, University of Oklahoma, MOHAMED AL KHALIFI, MATHIEU LEROUX, CRHEA-CNRS, France, KHALID HOSSAIN, Amethyst Research Inc., IAN R. SELLERS, University of Oklahoma — While GaInNAs has the potential to be a fourth-junction in multi-junction solar cells it has proved to be difficult to incorporate due to the low solubility of nitrogen in these materials. Specifically, mid-gap states attributed to nitrogen clusters have proved prohibitive for practical implementation of these systems. Here, we present the selective passivation of nitrogen impurities using a UV-activated hydrogenation process, which enables the removal of defects while retaining substitution nitrogen. Temperature dependent photoluminescence measurements of a GaInNAs p-n junction cell show a classic “s-shape” associated with localization prior to hydrogenation, while after hydrogenation no sign of the “s-shape” is evident. This passivation of nitrogen centers is reflected in improved performance of solar cell structures relative to reference, unpassivated devices presenting a potential route to practical implementation of GaInNAs solar cells.

1The authors acknowledge support through Oklahoma Center for the Advancement of Science and Technology under the Oklahoma Applied Research Support Grant No. AR12.2-040

9:00AM S34.00006 Amorphous carbon for photovoltaics1. FRANCESCA RISPLENDI, JEFFREY C. GROSSMAN, Massachusetts Inst of Tech-MIT, Materials Science and Engineering dept. — All-carbon solar cells have attracted attention as candidates for innovative photovoltaic devices. Carbon-based materials such as graphene, carbon nanotubes (CNT) and amorphous carbon (aC) have the potential to present physical properties comparable to those of silicon-based materials with advantages such as low cost and higher thermal stability. In particular a-C structures are promising systems in which both sp2 and sp3 hybridization coordination are present in different proportions depending on the specific density, providing the possibility of tuning their optoelectronic properties and achieving comparable sunlight absorption to aSi. In this work we employ density functional theory to design suitable device architectures, such as bulk heterojunctions (BJH) or pn junctions, consisting of a-C as the active layer material. Regarding BHJ, we study interfaces between aC and C nanostructures (such as CNT and fullerene) to relate their optoelectronic properties to the stoichiometry of aC. We demonstrate that the energy alignment between the a-C mobility edges and the occupied and unoccupied states of the CNT or C60 can be widely tuned by varying the aC density to obtain a type II interface. To employ aC in p-n junctions we analyze the p- and n-type doping of a-C focusing on an evaluation of the Fermi level and work function dependence on doping. Our results highlight promising features of aC as the active layer material of thin-film solar cells.

9:12AM S34.00007 Highly Selective Photocatalytic CO2 Reduction on TiO2-Passivated InP in Ionic Liquids1. GUANGTONG ZENG, JING QIU, SHERMIN ARAB, ZHEN LI, STEPHEN CRONIN, University of Southern California — Lowering the overpotential required to drive the photocatalytic reduction of CO2 to useful products is a very important challenge. In this article, we use an ionic liquid [EMIM][BF4] as co-catalyst to improve the selectivity and efficiency of CO2 reduction to CO on TiO2-passivated InP. Here, the InP surface is passivated using a thin film of TiO2 deposited by atomic layer deposition (ALD), which improves the photocorversion efficiency by as much as 17X compared to bare InP. We believe there are three mechanisms of enhancement in this photocatalytic system. Firstly, the TiO2 deposited by ALD is n-type due to oxygen vacancies, and forms a pn-junction with the underlying p-type InP photocathode, resulting in a built-in potential which reduces electron-hole recombination through charge separation. Secondly, the Ti4+ active sites formed on the TiO2 surface lower the energy of the CO2− intermediate through the formation of an intermediate complex. Thirdly, the [EMIM]+ ions in solution also stabilize the CO2− intermediate, further lowering the energy barrier of this reaction. Here, we use a non-aqueous ionic liquid solution, which prohibits hydrogen formation and enables highly selective CO2 reduction with a Faradaic efficiency of 46%. This general approach of passivating narrower band gap semiconductors with TiO2 and utilizing a non-aqueous ionic liquid solution allows a wide range of materials to be considered for photocatalysis, enabling more efficient photocatalysts to be developed.

9:24AM S34.00008 High-throughput search for photoabsorbers for solar fuels1. SLOBODAN MITROVIC, Caltech, Joint Center for Artificial Photosynthesis, EEARL CORNELL, Lawrence Berkeley National Laboratory, PAUL NEWHOUSE, JOEL HABER, RYAN JONES, JOHN GREGOIRE, Caltech, Joint Center for Artificial Photosynthesis — We present the suite of instrumentation developed specifically to search for light absorber materials for solar hydrogen and carbon-based fuels. A pre-screening method utilizes colorimetric image analysis to search for positive and negative metrics for electronic bandgap, isolate materials not suitable for further screening and identify phase clusters in the compositional space of combinatorial material libraries. Then, two highly-automated instruments screen for photocurrent, by performing incident-photon conversion efficiency measurement in a redox couple, and absorption properties via UV-Vis-NIR spectroscopy. Finally, we present a new instrument for multispectral microscopic imaging of material libraries. We will discuss the challenges in automated data analysis from large datasets and multispectral data-cubes.

1This material is based upon work performed by the Joint Center for Artificial Photosynthesis, a DOE Energy Innovation Hub, supported through the Office of Science of the U.S. Department of Energy under Award Number DE-SC000499.

9:36AM S34.00009 First-principles study of MnNiO3 as an alkaline oxygen-evolution photocatalyst1. JIE YU, Joint Center for Artificial Photosynthesis, Lawrence Berkeley National Laboratory, QIMIN YAN, Molecular Foundry, Lawrence Berkeley National Laboratory, WEI CHEN, ANUBHAV JAIN, Environmental Energy Technologies Division, Lawrence Berkeley National Laboratory, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, KRISTIN PERSSON, Environmental Energy Technologies Division, Lawrence Berkeley National Laboratory — We present a first-principles study of MnNiO3, a promising oxygen-evolution photocatalyst. Using density functional theory with the screened hybrid functional of Heyd, Scuseria, and Ernzerhof (HSE), we compute and analyze the ground-state geometry and electronic structure. We find that MnNiO3 is a ferrimagnetic semiconductor with an indirect band gap, consistent with experimental observations. We also predict that MnNiO3 has promising band edge positions relative to the vacuum, with potential to straddle the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) redox potentials in aqueous solution. A detailed analysis of the band structure and density of states provides a clear explanation why MnNiO3 is promising for OER. Pourbaix diagram calculations suggest that MnNiO3 is stable in alkaline solution at potentials relevant for oxygen evolution. This work was supported by the Department of Energy through the Joint Center for Artificial Photosynthesis.

9:48AM S34.00010 Energy requirements for CO2 capture from ambient air (DAC) competitive with capture from flue-gas (PCC)1. CHRISTOPH MEINRENKEN, Columbia University — Capture of CO2, whether from a flue gas source (PCC) or from distributed sources via ambient air (DAC), is a key enabling technology to provide carbon for sustainable synthetic energy carriers such as solar fuels. Based on thermodynamic minimum considerations, DAC is often expected to require about 3 times more energy (per ton CO2 captured) than PCC because CO2 in ambient air is more dilute. Here, we calculate the energy required for a humidity swing-based DAC installation that uses an anionic exchange resin as sorbent. The calculation uses recently measured equilibrium CO2 loadings of the sorbent as function of partial CO2 pressure, temperature, and humidity. We calculate the installation’s electricity consumption to be about 45 kJ per mole of pure CO2 at 1 bar (scenario-dependent). Furthermore, we estimate the amount of heat provided by ambient air and thus provide context of the overall energy and entropy balance and thermodynamic minimum views. The electricity consumption is competitive with typical parasitic loads of PCC-equipped coal-fired power plants (40-50 kJ per mole at same pressure) and significantly lower than predicted for other DAC installations such as Na(OH) sorbent-based systems. Our analyses elucidate why DAC is not always more energy-intensive than PCC, thus alleviating often cited concerns of significant cost impediments.

1Financial support by ABB for research presented herein is gratefully acknowledged.
10:00AM S34.00011 MIS Solar Cell Devices Based on a Cu2O Substrate Utilizing h-BN as an Insulating and Passivating Layer1. ONUR ERGEN, ASHLEY GIBB, OSCAR VAZQUEZ-MENA, WILL REGAN, ALEX ZETTL, University of California at Berkeley — We demonstrate Cu2O based metal insulator semiconductor Schottky (MIS-Schottky) solar cells with efficiencies exceeding 3%. A unique direct growth technique is employed in the fabrication, and hexagonal boron nitride (h-BN) serves simultaneously as a passivation and insulation layer on the active cuprous oxide (Cu2O) layer. The devices are the most efficient of any Cu2O based MIS-Schottky solar cells reported to date.

1Department of Physics, University of California at Berkeley, Berkeley, California 94720, USA. 2Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA.

10:12AM S34.00012 Electronic properties of BiI3 using hybrid functionals1. PATRICK M. MCBRIDE, ANDERSON JANOTTI, CHRIS G. VAN DE WALLÉ, Univ of California - Santa Barbara — BiI3 has recently gained interest as a high-efficiency light-output scintillator material, but limited research has been done to investigate its electronic structure. Most theoretical investigations have been limited to using density functional theory (DFT) within the local density approximation (LDA) or the generalized gradient approximation (GGA), which are known to give an incorrect electronic band gap. Furthermore, these studies ignore van der Waals (vdW) interactions, even though BiI3 has a layered structure held together by vdW forces. In this talk we present results of hybrid functional calculations, including the effects of spin-orbit coupling, for the electronic and structural properties of BiI3. We will address effects of including vdW interactions and spin-orbit coupling on the nature of the band gap, electron and hole effective masses, and the band edge positions with respect to vacuum level and other relevant semiconductors. We will also discuss the suitability of BiI3 as a photovoltaic material.

1This work was funded by the Bonderson Fellowship

10:24AM S34.00013 Quantitative model of EBIC for CdTe, PAUL HANEY, HEAYOUNG YOON, National Institute for Standards and Technology, PRAKASH KOIRALA, ROBERT COLLINS, U. Toledo, NIKOLAI ZHITENEV, National Institute for Standards and Technology — Electron beam induced current (EBIC) is a powerful characterization technique which offers the high spatial resolution needed to study polycrystalline solar cells. In an EBIC experiment, a beam of high energy electrons excites electron-hole pairs, some fraction of which are collected by contacts. Ideally, an EBIC measurement reflects the spatially resolved quantum efficiency of the device. However, experiments on polycrystalline CdTe solar cells reveal that the EBIC collection efficiency is substantially lower than the quantum efficiency of the device under optical excitation. In order to reliably extract intrinsic material properties from EBIC signals, this difference must be reconciled. Two important differences between an EBIC experiment and normal device operation are: 1. the high generation rate density associated with the electron beam, and 2. the substantial effect of the exposed surface in an EBIC experiment. By developing numerical and analytical models which account for both of these effects, the difference in the material response under EBIC and normal device operation conditions can be understood. Comparison between the model and experiment show good agreement between quantities such as maximum EBIC collection efficiency versus charge generation rate.

10:36AM S34.00014 Studying Anomalous Open-Circuit Voltage Drop-Out in Concentrated Photovoltaics Using Computational Numerical Analysis, MARGARET STEVENS, CHANDLER DOWNS, THOMAS VANDERVELDE, SCOTT MAC'LACHLAN, JAMES ADLER, Tufts University — Under high solar concentration, an anomalous open-circuit voltage drop-out has been observed experimentally, but not understood theoretically. This anomaly has often been attributed to various thermal effects, but the effect is also observed in flash testing, where thermal effects do not have time to accumulate. We discuss our theoretical examination of semiconductor performance under high optical generated carrier injection. Under these conditions, the number of optically generated charge carriers increase past the number of equilibrium charge carriers. The effect of dynamically changing charge carrier compositions on fundamental electrical properties, such as open-circuit voltage, has yet to be explored in detail. Using the Newton-Raphson method, we solved the carriers continuity equations for the optically generated charge carriers as a function of material depth in bulk III-V semiconducting materials. Ultimately, we implemented these carrier concentration functions in our simulations of the p-n band structures to characterize the impact of solar concentration on the electrical behavior of photovoltaic devices.

10:48AM S34.00015 Polymer-directed Hybrid Nanostructures for Enhanced Electrocatalytic Activity and Solar Fuel Generation, DONG HA KIM, YOON HEE JANG, JI-EUN LEE, LI NA QUAN, YU JIN JANG, EWHA Woman's Univ, POLYMER NANOHYBRID MATERIALS LAB TEAM — In this presentation, we introduce a comprehensive approach to the design and fabrication of hybrid nanostructures directed by functional polymers for photovoltaic, pholectricchemical and electrocatalytic properties. A unique strategy to generate core-shell nanoparticles based on AuNPs decorated with PANI shell with uniformly distributed alloy metal NPs in the PANI shells was developed. We systematically investigate the structural alteration during the sequential synthetic process and compared the electrocatalytic performance with respect to Pt-decorated AuNP-PANI structures in terms of the oxygen reduction reaction. Aimed for an alternative photoanodes, hierarchical mesoporous carbon-TiO2 inverse opal nanostructures were synthesized by complementary colloid and block copolymer (BCP) self-assembly, where the triblock copolymer P123 acts simultaneously as template and carbon source. Analytical studies show that incorporation of carbon moieties into TiO2 creates a new energy level above the valence band of TiO2, resulting in an effective decrease in the band gap. A significant enhanced visible light photocatalytic activity was demonstrated in terms of the degradation of p-nitrophenol (~79 %) and photoelectrochemical water splitting.

Thursday, March 5, 2015 8:00AM - 11:00AM – Session S35 DAMOP: Optomechanics, Hybrid Systems and Macroscopic Systems at the Quantum Limit 210B - Chen-Lung Hung, Purdue University

8:00AM S35.00001 Anthracene Crystals Doped with Dibenzoterrylene Molecules in Optical Fibre Microcavities, K.D. MAJOR, E.A. HINDS, ALEX S. CLARK, C. POLLISENI, S. GRANDI, Y.H. LIEN, Imperial College London, QUANTUM NANOPHOTONICS, CENTRE FOR COLD MATTER, QUANTUM OPTICS AND LASER SCIENCE GROUP TEAM — Dibenzoterrylene molecules placed in an anthracene crystal are stable emitters resistant to photobleaching and with a high quantum efficiency and low phonon coupling. Placing dibenzoterrylene doped anthracene crystals within a optical fibre microcavity can lead to enhanced emission of radiation into the modes of the optical cavity. The optical fibre microcavities are already coupled to a optical photon source. By selecting the correct cavity mirror reflectivities, the emission can be preferentially directed down the optical fibre. Excitation of the dibenzoterrylene molecules leads to the emission of single photons and can then be used as a micron-scale fibre coupled single photon source.
8:12AM S35.00002 Optomechanical Levitation of Tethered Dielectrics in a Cavity, TINA MÜLLER, CHRISTOPH REINHARDT, BODGAN PIČIU, ABEER BARASHEED, SIMON BERNARD, ALEXANDRE BOURASSA, XINYUAN ZHANG, CHRISTOPHER MCNALLY, JACK SANKEY, McGill University, MCGILL OPTOMECHANICS LAB TEAM — Optically supporting dielectric materials has the potential to increase their mechanical quality factors far beyond the limits set by material dissipation. As the mechanical frequency $\omega$ increases due to the applied optical spring, the quality factor increases as $\omega^2$, meaning that the overall dissipation rate decreases and the mass experiences less force noise from the environment. However, a major limitation when trapping weakly tethered dielectrics is the mode mixing with the low-$\omega$ mechanical modes of the tethers, occurring when the frequency of the trapped element becomes degenerate with the tether mode frequencies. In addition, the maximum trap strength is limited by the maximum optical power a dielectric can be exposed to before breakdown. Here, we describe an optimal system to overcome these limits, based on a straightforward cavity levitation scheme and controlling the position and angle of the mechanical element via its tethers. We also show progress towards trapping a SiN tethered membrane with our scheme, and discuss implementations based on other materials.

8:24AM S35.00003 Optomechanics in a Millikelvin Environment, BRADLEY HAUER, ALLISON MACDONALD, GREG POPOWICH, PAUL KIM, ARON FREDRICK, XAVIER ROJAS, JOHN DAVIS, University of Alberta — As advances in technology continue to improve the quality and reduce the size of nanofabricated devices, we edge closer and closer to the prospect of observing quantized motion of a mesoscopic mechanical resonator. Measurements of such devices, which consist of dozens to tens of nanometers, would provide an excellent test of the scales at which quantum mechanics is applicable. However, due to their relatively large effective masses, these devices must be cooled to $\text{mK}$ temperatures to reach their quantum ground state. The field of cavity optomechanics, which has already achieved quantum limited measurement sensitivity, provides a promising avenue for performing such measurements. To this end, we have designed a tapered fiber optomechanical coupling apparatus, with full 3D control and real time imaging of the coupling environment, on the base plate of a dilution refrigerator. This experiment is capable of passively cooling devices to temperatures below 10 mK, at which oscillators with resonance frequencies as low as 150 MHz will be cooled to single phonon occupancy. In this talk, I will present preliminary measurements from this cutting edge system.

8:36AM S35.00004 Optomechanical applications of optically levitated nanoparticles, LEVI NEUKIRCH, Department of Physics and Astronomy, University of Rochester, NICK VAMIVAKAS, Institute of Optics, University of Rochester — Optomechanics experiments performed in vacuum with optically levitated oscillators offer mechanical quality factors unmatched by clamped resonators. Single-beam gradient force traps have been proven capable of stably levitating nanoscale dielectric spheres in high vacuum, and parametric modulation of the trap stiffness has been demonstrated as an efficient way to cool the center of mass motion. We present our optical levitation and cooling apparatus, and characterize its performance. We discuss several applications which extend control to degrees of freedom beyond the three-dimensional translational motion of the particle.

8:48AM S35.00005 Analytic Solution of the Equation of Motion for an Optically-Torqued, Overdamped Nanorod, W.C. KERR, H. NASIF, S. RAYNOR, Wake Forest Univ. — Shelton et al.[1] performed an experiment to drive a nanorod, immersed in a viscous medium, by an optical field with rotating polarization. The nanorod had a length of about 5 microns, was held in an optical trap and placed in water, which provided a frictional torque. A linearly polarized optical beam was incident on the rod, and its polarization plane was rotated by passing it through a rotating half-wave plate. The rod’s polarization tensor was anisotropic, so its induced dipole moment was not parallel to the field; thus a driving torque was exerted on the rod. A simplified equation was written in terms of an auxiliary variable proportional to the nanorod’s angle in a rotating frame, the equation was the same as that of a damped, driven pendulum. We find that this ODE is amenable to analytic solution. The solution identifies a certain critical angular frequency such that the inertial term of the equation of motion can be ignored. When this simplified equation was written in terms of an auxiliary variable proportional to the nanorod’s angle in a rotating frame, the equation was the same as that of a damped, driven pendulum. We find that this ODE is amenable to analytic solution. The solution identifies a certain critical angular frequency, such that qualitatively different motions occur when the light polarization rotation frequency is less than or greater than the critical frequency. All features of the analytic solution agree quantitatively with the experiment.

1 Supported by the the Office of Naval Research award number N000141410442

8:00AM S35.00006 Dark-field Spectroscopy of Plasmonic Nanodevices with Nanometer Scale Features, DAVID FRENCH, STEPHEN BAUMAN, DESALEGN DEBU, CAMERON SAYLOR, JOSEPH HERZOG, University of Arkansas — Plasmonic nanodevices are metallic structures that exhibit plasmonic effects when exposed to light, causing scattering and enhancement of that light. These plasmons makes it possible for light to be focused below the diffraction limit. Dark-field spectroscopy has been used to capture scattering spectra of these structures, in order to examine the scattering and resonant frequencies of the plasmons provided by the devices. Dark-field spectroscopy is particularly well suited to this task because it is inexpensive to set up and it functions well with low signals. This paper examines the relation between the geometries of the devices and the spectral intensity of the scattered light. We study geometric parameters including device thickness and adhesion layer effects. Additionally we plan to investigate nanostructures fabricated with novel fabrication technique with device dimensions that are below 10 nm, both gap width and structure width. These devices are modeled computationally as well as manufactured and characterized experimentally.

9:00AM S35.00007 Probing emitter-cavity dressed states through environmental transitions, JAKE ILES-SMITH, Blackett Laboratory, Imperial College London, London, SW7 2AZ, UK, AHSAN NAZIR, Photon Science Institute and School of Physics & Astronomy, The University of Manchester, Oxford Road, Manchester M13 9PL, UK — In this work we explore the effect of phonons on the emission properties of a cavity QED system in several important parameter regimes — the semi-classical intermediate coupling, Fano, and strong coupling regime. Specifically, we examine the effect of phonon interactions on the emission spectrum of a quantum dot in a high-Q optical cavity, focusing in particular on a micropillar type setup. We demonstrate that the quantum mechanical nature of the phonon environment, and short timescales over which phonons processes occur, allows one to probe the joint eigenstates of the cavity and TLS even in a semi-classical regime. Not only does this demonstrate a failure of the traditional quantum optics treatment, but also challenges the notion that phonons decohere such a system to a more classical description. Furthermore, we demonstrate that the behaviour we predict may be observed in a straightforward fashion by considering the cavity reflectivity, associated phase shift, or the cavity emission spectra.

9:12AM S35.00008 Near-analytic solutions to the PMD equations in Periodically Spun Fiber using Differential Transform Method, VINOD MISHRA, US Army Research Laboratory — Periodically spun optical fibers have been found to reduce Polarization Mode Dispersion (PMD) in propagating optical modes [1]. The resulting coupled ordinary differential equations are usually solved numerically. To gain better physical understanding and dependence of PMD Change Factor (PCF) on relevant parameters, analytical solutions are to be preferred. The current work uses Differential Transform Method to derive analytical solutions to the original equations as a series and investigates their properties.

9:36 AM S35.00009 Manipulation of Light Propagation in Photonic Crystal  . ZHIYUAN YANG, Department of Physics, UNT; AMITABH JOSHI, Department of Physics and Institute for Quantum Studies, Texas A&M University, YURI ROSTOVTSEV, Department of Physics, UNT — A propagation of probe electromagnetic waves have been investigated in a heterostructure formed by linear and nonlinear layers. The appearance of a forbidden band gap for a probe electromagnetic field induced by another control electromagnetic field has been shown to lead to trapping of a probe pulse inside structure. Switching off the control field leads to resuming the propagation of the probe pulse. Implementation of nonlinear layer has been suggested.

9:48 AM S35.00010 Quantum Friction in Different Regimes1. JULIANE KLATT, STEFAN BUHMANN, Albert-Ludwig University, Freiburg, Germany — Quantum friction is the velocity-dependent force between two polarizable objects in relative motion, resulting from field-fluctuation mediated transfer of energy and momentum between them. Due to its short-ranged nature it has proven difficult to observe experimentally. Theoretical attempts to determine the precise velocity-dependence of the quantum drag experienced by a polarizable atom moving parallel to a surface arrive at contradicting results. Scheel and Barton predict a force linear in relative velocity $v$ — the former using the quantum regression theorem and the latter employing time-dependent perturbation theory. Intravaia, however, predicts a $v^3$ power-law starting from a non-equilibrium fluctuation-dissipation theorem. In order to learn where exactly the above approaches part, we set out to perform all three calculations within one and the same framework: macroscopic QED. In addition, we include contributions to quantum friction from Doppler shift and Röntgen interaction, which play a role for perpendicular motion and retarded distances, respectively, and consider non-stationary states of atom and field.

1 DFG Emmy-Noether Program

10:00 AM S35.00011 Friction forces on atoms after acceleration. DIEGO DALVIT, Los Alamos National Laboratory, FRANCESCO INTRAVAIA, Max Born Institute, Germany, VANIK MKRTCHIAN, Institute for Physical Research, Armenia, STEFAN BUHMANN, University of Freiburg, Germany, STEFAN SCHHEEL, University of Rostock, Germany, CARSTEN HENKEL, University of Postdam, Germany — We revisit the calculation of atom-surface quantum friction in the formulation based on perturbation theory. We show that the power dissipated into field excitations and the associated friction force depend on how the atom is boosted from being initially at rest to a configuration in which it is moving at constant velocity parallel to the planar interface. In addition, we point out that there is a subtle cancellation between the one-photon and part of the two-photon dissipating power, resulting in a leading order contribution to the frictional power which goes as the fourth power of the velocity.

10:12 AM S35.00012 Parametric mechanical pumping in graphene membranes , ROBERTO DE ALBA, ISAAC STORCH, THANNIYIL SEBASTIAN ABHILASH, Department of Physics, Cornell University, FRANCESCO MASSEL, Department of Physics, University of Jyväskylä, PAUL L. MCEUEN, Department of Physics, Cornell University, HAROLD G. CRAIGHED, School of Applied & Engineering Physics, Cornell University, JEEVAK M. PARPIA, Department of Physics, Cornell University — We demonstrate tension-mediated mechanical mode coupling in suspended graphene membranes. These nonlinear effects arise due to graphene’s large elastic modulus and large deflections. We show experimentally that these mode-mode interactions can be utilized to parametrically amplify or cool mechanical motion, and that the coupled system obeys similar physics to optical-cavity-coupled mechanical systems. This enables all-electrical parametric control of the resonator dynamics, including self-oscillation. Mechanical pumping can thus enhance the performance of graphene-based force sensors, or supplement traditional cooling schemes to probe coupled mechanical systems approaching the quantum regime.

10:24 AM S35.00013 Aging and annealing of ultrahigh quality factor silicon resonators1. THOMAS METCALF, XIAO LIU, Naval Research Laboratory — At liquid helium temperatures, resonators fabricated from single crystal silicon can have remarkably high quality factors, exceeding 50 million. However, the quality factors are still far from the limits predicted from known loss mechanisms, indicating the possibility of future improvement and increased sensitivity. Measurements of the baseline quality factor after a sequence of annealing and aging steps have shown that there are at least two loss mechanisms that contribute, one of which reappears with megasecond aging. The relation between these loss mechanisms and the resonator fabrication processing steps is considered, with implications for the ultimate sensitivity of resonator-based devices and in the phonon transport properties of silicon-based devices.

1 Work supported by the Office of Naval Research

10:36 AM S35.00014 Mechanical mode coupling and nonlinearity in as-grown GaAs nanowires , FLORIS BRAAKMAN, DAVIDE CADEDDU, University of Basel, GOZDE TUTUNCUOGLU, FEDERICO MATTEINI, DANIEL RÜFFER, ANNA FONTCUBERTA I MORRAL, École Polytechnique Fédérale de Lausanne, MARTINO POGGIO, University of Basel — We demonstrate coupling and nonlinear behavior of transverse mechanical modes of as-grown GaAs nanowires. Because of their small dimensions and potentially defect-free growth, nanowire cantilevers are promising as ultrasensitive force transducers for scanning probe microscopy. Furthermore, nanowire heterostructures can combine functionalities in one integrated structure which makes them attractive as hybrid systems. The observed nonlinearity is used to demonstrate mechanical mixing of two excitation frequencies, as well as to amplify a signal at a frequency close to the mechanical resonance of the nanowire oscillator. The mode coupling is observed both in a pump-probe experiment, where the resonance of one mode is shifted to higher frequencies by pumping the other mode, and in a time-resolved manner in a ringdown experiment, in which case a clear beating pattern with frequency equal to the frequency difference between the two modes is present. Sufficiently strong coupling forms the basis for phenomena such as phonon-cavity physics, mechanically induced transparency and synchronization. Furthermore, the nonlinearity and mode coupling can be used in various amplification schemes for enhancing sensitivity in force microscopy.

10:48 AM S35.00015 Room Temperature Experiments with a Macroscopic Sapphire Mechanical Oscillator . JEREMY BOURHILL, EUGENE IVANOV, MICAHEL TOBAR, UWA — We present initial results from a number of experiments conducted on a 0.53 kg sapphire “dumbbell” crystal. Mechanical motion of the crystal structure alters the dimensions of the crystal, and the induced strain changes the permittivity. These two effects frequency modulate resonant microwave whispering gallery modes, simultaneously excited within the crystal. A novel microwave readout system is described allowing extremely low noise measurements of this frequency modulation with a phase noise floor of -160 dBc/Hz at 100 kHz, near our modes of interest. Fine-tuning of the crystal’s suspension have allowed for the optimisation of mechanical Q-factors in preparation for cryogenic experiments, with a value of 8 x 10^7 achieved so far. Finally, results are presented that demonstrate the excitation of mechanical modes via radiation pressure force. These are all important steps towards the overall goal of the experiment; to cool a macroscopic device to the quantum ground state.
8:00AM S36.00001 Non-equilibrium dynamics of atomic Fermi and Bose gas under lattice geometry transformation, CHEN-YEN LAI, CHIH-CHUN CHIEN, Univ of California - Merced — The tunability of ultra-cold atom experiments has provided a new arena of exploring quantum effect in both bosonic and fermionic system in and out of equilibrium. According to recent experiments [Phys. Rev. Lett. 108, 045305 (2012)], a triangular lattice can be dynamically tuned into a square or kagome lattice by adjusting frequency and focus point of laser beams. We simulate the dynamical properties of single component fermions and weakly interacting bosons under various transformation processes, including different ramping time scales, different ramping functions, and more importantly into different types of lattice geometry. A non-equilibrium steady state, which is not thermalized, is found in single component fermion system under different particle densities in both small size system and in the thermodynamic limit. In contras, weakly interacting bosons do not exhibit observable steady state behavior. This opens new opportunities of research on dynamical multi-band effects.

8:12AM S36.00002 Spatio-temporal correlations in the Bose Hubbard model after a quantum quench1, MATTHEW FITZPATRICK, MALCOLM KENNEDY, Simon Fraser University — The dynamics of the Bose Hubbard model after a quantum quench have attracted much recent attention. Theoretically, it has proven challenging to describe spatio-temporal correlations in dimensions higher than one. We use the Schwinger-Keldysh technique and a strong coupling expansion to develop a two particle irreducible formalism that allows the study of correlations in time and space in both superfluid and Mott insulating regimes after a quantum quench. We obtain equations of motion for two-time correlation functions and relate our results to recent cold-atom experiments.

8:24AM S36.00003 Trap-induced scales in non-equilibrium dynamics of strongly interacting bosons, RAJDEEP SENSARMA, Tata Institute of Fundamental Research, ANIRBAN DUTTA, KRISHNENDU SENGUPTA, Indian Association for Cultivation of Sciences — We use a time-dependent hopping expansion technique to study the non-equilibrium dynamics of strongly interacting bosons in an optical lattice in the presence of a harmonic trap characterized by a force constant $K$. We show that after a sudden quench of the hopping amplitude $J$ across the superfluid (SF)-Mott insulator (MI) transition, the SF order parameter $\Delta$ displays a novel non-monotonic spatial profile. Both these phenomena can be explained as consequences of trap-induced time and length scales affecting the dynamics and can be tested by concrete experiments.
10:12AM S36.00010 Controlling the condensate in driven optical lattices , ALBERTO NOCERA, ADRIAN FEIGUIN, Department of Physics, Northeastern University, Boston, Massachusetts 02115, USA — We study the one-dimensional attractive Hubbard model under the influence of a periodic driving potential with the time-dependent density matrix renormalization group showing that the system can be driven in an unconventional paired state characterized by a condensate made of Cooper-pairs with a finite center-of-mass momentum similar to a Fulde-Ferrell state. We obtain results both in the laboratory and the rotating reference frames demonstrating that the momentum of the condensate can be finely tuned by changing the ratio between the amplitude and the frequency of the driving. In particular, by quenching the above ratio to the value giving suppression of the tunneling and putting the Coulomb interaction strength to zero, we are able to “freeze” the condensate. We finally study the effects of different initial conditions, and compare our numerical results to those obtained from a time-independent Floquet theory in the large frequency regime. Our work offers the possibility of engineering and controlling unconventional paired states in fermionic condensates.

10:24AM S36.00011 Dissipative effects in dipolar, quantum many-body systems 1, ARGHAVAN SAFAVI-NAINI, JILA, CU Boulder, BARBARA CAPOGROSSO-SANSONE, University of Oklahoma, ANA MARIA REY, JILA, CU Boulder — We use Quantum Monte Carlo simulations, by the Worm algorithm, to study the ground state phase diagram of two-dimensional, dipolar lattice bosons where each site is coupled, via density operators, to an external reservoir. A recent related study of the XXZ model with ohmic coupling to an external reservoir reported the existence of a bath-induced Bose metal phase in the ground state phase diagram away from half filling, and a Luttinger liquid and a charge density wave at half-filling [1]. Our work extends this methodology to higher dimensional systems with long-range interactions. In the case of hard-core bosons, our method can be applied to experimental systems featuring dipolar fermionic molecules in the presence of losses. This work utilized the Janus supercomputer, which is supported by the NSF (Award No. 1412194) and the University of Colorado Boulder, and is a joint effort with the University of Colorado Denver and the National Center for Atmospheric Research, as well as OU Supercomputing Center for Education and Research (OSCER) at the University of Oklahoma.

10:36AM S36.00012 ABSTRACT WITHDRAWN —

10:48AM S36.00013 Evolutionary games of condensates in driven and dissipative bosonic systems 1, JOHANNES KNEBEL, MARKUS F. WEBER, TORBEN KRÜGER, ERWIN FREY, Ludwig Max Univ Muenchen — Condensation is a collective behavior of particles observed in both classical and quantum physics. For example, when an equilibrated, dilute gas of bosonic particles is cooled to a temperature near absolute zero, the ground state becomes macroscopically occupied (Bose-Einstein condensation). Whether novel condensation phenomena occur far from equilibrium is a topic of vivid research. Only recently has it been proposed that a driven and dissipative gas of bosons can condense not only into a single, but also into multiple non-degenerate states. This phenomenon may occur when a system of non-interacting bosons is weakly coupled to a reservoir and is driven by an external time-periodic force (Floquet system). Coherence becomes negligible and the condensation is described by a Pauli master equation, which also arises in the evolutionary dynamics of classical agents. In our work, we apply concepts from evolutionary dynamics to determine the states that become condensates. This condensate selection is guided by the vanishing of relative entropy production. We find that the system of condensates never comes to rest: The occupation numbers of condensates oscillate, which we demonstrate for a rock-paper-scissors game of condensates.

1 Deutsche Forschungsgemeinschaft (SFB-TR12), German Excellence Initiative (Nanosystems Initiative Munich), Center for NanoScience Munich, Studienstiftung des Deutschen Volkes

Thursday, March 5, 2015 8:00AM - 11:00AM —

Session S37 GQI: Semiconductor Qubits - Gated Dots and Impurities I

8:00AM S37.00001 Dispersive measurement of electron spin states in Coulomb-confined silicon double quantum dots, MATTHEW HOUSE, TAKASHI KOBAYASHI, BENT WEBER, SAM HILE, SVEN ROGGE, MICHELLE SIMMONS, Centre for Quantum Computation and Communication Technology, University of New South Wales — We use radio frequency reflectometry with a resonant circuit to probe the electronic spin state. We map the ground state transition between singlet and triplet states as a function of electric and magnetic fields, which shows that the exchange energy can be tuned over an order of magnitude (about 10 to 100 eV) or more in this device. We apply high frequency pulses to induce an excited spin state and observe that the dispersive measurement can detect the excited spin state in addition to the ground state.

8:12AM S37.00002 Bias Triangles Presented in Chemical Potential Space, JUSTIN PERRON, Joint Quantum Institute, M.D. STEWART, JR, NEIL M. ZIMMERMAN, NIST - Natl Inst of Stds & Tech — Readout of spins in solid state electronic devices requires some form of spin-to-charge conversion. Through analysis of the data we are able to present spin resolvability on a single plot in chemical potential space. The presentation will allow comparisons between different biasing directions to be made in a clean and straightforward manner. This ability will be useful for investigating into PSB where these comparisons are paramount.

8:24AM S37.00003 Single-electron regime and Pauli spin blockade in a silicon metal-oxide-semiconductor double quantum dot 1, SOPHIE ROCHELLE, Université de Sherbrooke, GREGORY A. TEN EYCK, TAMMY PLUYM, MICHAEL P. LILLY, MALCOLM S. CARROLL, Sandia National Laboratories, MICHEL PIORO-LADRiÈRE, Université de Sherbrooke — Silicon quantum dots are promising candidates for quantum information processing as spin qubits with long coherence time. We present electrical transport measurements on a silicon metal-oxide-semiconductor (MOS) double quantum dot (DQD). First, Coulomb diamonds measurements demonstrate the one-electron regime at a relatively high temperature of 1.5 K. Then, the 8 mK stability diagram shows Pauli spin blockade with a large singlet-triplet separation of approximately 0.40 meV, pointing towards a strong lifting of the valley degeneracy. Finally, numerical simulations indicate that by integrating a micro-magnet to those devices, we could achieve fast spin rotations of the order of 30 ns. Those results are part of the recent body of work demonstrating the potential of Si MOS DQD as reliable and long-lived spin qubits that could be ultimately integrated into modern electronic facilities.

1 Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
8:36AM S37.00004 Tunable Radio-frequency Quantum Point Contact, ANNE-MARIE ROY, OLIVIER SAINT-JEAN RONDEAU, JULIEN CAMIRAND-LEMYRE, MICHEL PIORO-LADRIÈRE, Université de Sherbrooke — Manipulating the spin of single electrons in quantum dots is a promising avenue for quantum information processing. As the readout of the spins is performed via spin-to-charge conversion, establishing a charge sensing technique[1] that is fast and highly sensitive is crucial. For this reason, radio-frequency quantum point contact charge sensors have become widespread[2]. Here we present a tunable quantum point contact charge sensor using a cryogenic variable capacitor[3], tunable from 2 to 12 pF. We obtain optimal impedance matching for different quantum dot devices over a frequency range from 125 to 210 MHz. The flexibility of our setup allows the integration of radio-frequency charge sensors to a variety of nanostructures.


8:48AM S37.00005 Measurement, modeling, and simulation of cryogenic SiGe HBT amplifier circuits for fast single spin readout, TROY ENGLAND, Sandia National Laboratories, MATTHEW CURRY, CQUC and Department of Physics and Astronomy, University of New Mexico, STEVE CARR, BRIAN SWARTZENTRUBER, MICHAEL LILLY, NATHAN BISHOP, MALCOLM CARROL, Sandia National Laboratories — Fast, low-power quantum state readout is one of many challenges facing quantum information processing. Single electron transistors (SETs) are potentially fast, sensitive detectors for performing spin readout of electrons bound to Si:P donors. From a circuit perspective, however, their output impedance and nonlinear conductance are ill suited to drive the parasitic capacitance typical of coaxial conductors used in cryogenic environments, necessitating a cryogenic amplification stage. We will discuss calibration data, as well as modeling and simulation of cryogenic silicon-germanium (SiGe) heterojunction bipolar transistor (HBT) circuits connected to a silicon SET and operating at 4 K. We find a continuum of solutions from simple, single-HBT amplifiers to more complex, multi-HBT circuits suitable for integration, with varying noise levels and power vs. bandwidth tradeoffs. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a Lockheed-Martin Company, for the U. S. Department of Energy under Contract No. DE-AC04-94AL85000.

9:00AM S37.00006 Giant valley splitting in Si/oxide: discriminating Fang-Howard or Tamm-Shockley interface states, AMINTOR DUSKO, BELITA KOILLER, Instituto de Física - UFRJ, ANDRÉ SARAIVA, UFRJ / University of Wisconsin - Madison — The conduction band of silicon presents six inequivalent degenerate minima, or valleys. The presence of an abrupt interface lifts this degeneracy by a few 0.1 meV, an energy scale that may directly affect spin qubits. Experiments reporting splittings over 20 meV[1] cannot be explained by this mechanism. Extended Si/oxide interface (Tamm-Shockley) states may account for this enhancement[2]. We present a renormalization solution for the 1D tight-binding (TB) model of this interface state[2], so that the full range of TB parameters is readily accessible[3]. The renormalization language naturally reveals the role played by the chemical bond of atoms across the interface. Our approach eliminates the need for a supercell calculation[2], proving the formation of intrinsic interface states regardless of electric field. Moreover, the rectification rate of convergence provides quantitative estimates for the localization lengths of these states. We compare these interface states to the usual field-bound Fang-Howard states, suggesting capacitance measurements to differentiate them[3].


9:12AM S37.00007 Interface roughness mediated phonon relaxation rates in Si quantum dots, RIFAT FERDOUS, YULONG HSUEH, GERHARD KLIMECK, RAJIB RAHMAN, Purdue University — Si QDs are promising candidates for solid-state quantum computing due to long spin coherence times. However, the valley degeneracy in Si adds an additional degree of freedom to the electronic structure. Although the valley and orbital indices can be uniquely identified in an ideal Si QD, interface roughness mixes valley and orbital states in realistic dots. Such valley-orbit coupling can strongly influence the charge carrier relaxation. Recent experimental measurements of various relaxation rates differ from previous predictions of phonon relaxation in ideal Si QDs. To understand how roughness affects these relaxation rates, for example spin relaxation due to spin-valley coupling, which is a byproduct of spin-orbit and valley-orbit coupling, we need to understand the effect of valley-orbit coupling on valley relaxation first. Using a full-band atomistic tight-binding description for both the system's electron and electron-phonon Hamiltonians, we analyze the effect of atomic-scale interface disorder on phonon induced valley relaxation and spin relaxation in a Si QD. We find that, the valley splitting dependence of valley relaxation rate governs the magnetic field dependence of spin relaxation rate. Our results help understand experimentally measured relaxation times.

9:24AM S37.00008 Theory of 1- and 3-electron g-factors in Si quantum dots for spin-qubit manipulation, RUSKO RUSKOV, CHARLES TAHAN, Laboratory for Physical Sciences, MICHAEL E. FLATTE, University of Iowa, MENNO VELD-HORST, ANDREW DZURAK, University of New South Wales — Although the spin-orbit interaction in silicon is very weak, it is possible to map out the electron spin resonance (ESR) frequency with high precision in MOS quantum dot (QD) qubits by using isotopically purified silicon[1]. Using this method, the g-factor with 1 and 3 electrons in the dot has been measured with an in-plane magnetic field and as a function of the applied electric field perpendicular to the interface (along the growth direction [001]) [2]. Here, we present a theoretical model of the electron g-factor in Si QDs. We show that the results could be explained with the effect of an electron envelope function deformation in the confining interface region. Since the QD orbital splitting is much larger than the valley splitting at the interface, the system with 1 or 3 electrons probes the valley states at the interface, and the sign and size of the g-factor renormalization (order of tens of MHz in the chosen range of the electric field) could be explained via the spin-orbit 2D interaction induced at the interface. Electrical g-factor control opens the possibility of fast and all-electric manipulation of a few electron spin-qubit, without the need of a nanomagnet or a nuclear spin-background.


9:36AM S37.00009 Counted Sb donors in Si quantum dots, MEENAKSHI SINGH, JOSE PACHECO, EDWARD BIELEJEJ, DANIEL PERRY, GREGORY TEN EYCK, NATHANIEL BISHOP, JOEL WENDT, DWIGHT LUHMAN, MALCOLM CARROLL, MICHAEL LILLY, Sandia National Laboratories — Deterministic control over the location and number of donors is critical for donor spin qubits in semiconductor based quantum computing. We have developed techniques using a focused ion beam and a diode detector integrated next to a silicon MOS single electron transistor to gain such control. With the diode detector operating in linear mode, the numbers of ions implanted have been counted and single ion implants have been detected. Poisson statistics in the number of ions implanted have been observed. Transport measurements performed on samples with counted number of implants have been performed and regular coulomb blockade and charge offsets observed. The implications for various gates are found to be in agreement with QCAD simulations for an electrostatically defined dot. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE Office of Basic Energy Sciences user facility. The work was supported by Sandia National Laboratories Directed Research and Development Program. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a Lockheed-Martin Company, for the U. S. Department of Energy under Contract No. DE-AC04-94AL85000.
9:48AM S37.00010 Development of Linear Mode Detection for Top-down Ion Implantation of Low Energy Sb Donors, JOSE PACHECO, MEENAKSHI SINGH, EDWARD BIELEJEIC, MICHAEL LILLY, MALCOLM CARROLL, Sandia Nat Labs — Fabrication of donor spin qubits for quantum computing applications requires deterministic control over the number of implanted donors and the spatial accuracy to within which these can be placed. We present an ion implantation and detection technique that allows us to deterministically implant a single Sb ion (donor) with a resulting volumetric distribution of <10 nm. This donor distribution is accomplished by implanting 30keV Sb into Si which yields a longitudinal straggle of <10 nm and combined with a <50 nm spot size using the Sandia Nanolplantrameter (nl). The ion beam induced charge signal is collected using a MOS detector that is integrated with a Si quantum dot for transport measurements. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE Office of Basic Energy Sciences user facility. The work was supported by Sandia National Laboratories Directed Research and Development Program. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a Lockheed-Martin Company, for the U. S. Department of Energy under Contract No. DE-AC04-94AL85000.

10:00AM S37.00011 Long-lived spin coherence and nuclear modulation effects of the silicon vacancy in 4H-SiC at room temperature, SAMUEL CARTER, ONEY SOYKKAL, SOPHIA ECONOMOU, EVAN GLASER, Naval Research Laboratory — The silicon vacancy in silicon carbide is currently being considered for applications in quantum information and sensing, with several studies showing room temperature spin polarization and manipulation. We perform room temperature optically-detected magnetic resonance and spin echo measurements on an ensemble of silicon vacancies to better characterize the nature of this system and determine the spin coherence properties. The spin coherence time is shown to be dependent on magnetic field, varying from a few ms at low fields to longer than 30 µs at 50 mT. Strong spin echo modulation that varies with magnetic field is also observed. The modulation is attributed to the interaction with nearby nuclear spins and is well-described by a theoretical model.

10:12AM S37.00012 Oxygen-Boron Vacancy Defect in Cubic Boron Nitride: A Diamond NV−Isoelectronic Center, TESFAYE ABTEW, WEIWEI GAO, University at Buffalo, State University of New York, XIANG GAO, Beijing Computational Science Foundation under Grant No. DMR-0946404. Work at Beijing CSRC is supported by the National Natural Science Foundation of China (Grant No. 11328401).

10:24AM S37.00013 Observation of a single rare-earth ion in a crystal by electric-field-modulation spectroscopy for a readout of a nuclear-spin qubit, KOUCI CHIMURA, HAYATO GOTO, SATORI KAMAKURA, MAMIKO KUJRIAKA, Frontier Research Laboratory, Corporate Research & Development Center, Toshiba Corporation — Nuclear spin states of rare-earth-metal ions in crystals are known as good candidates for qubits in solids because of their long coherence time and their good controllability by lights. In the frequency-domain quantum computer (FDQC), nuclear spin states of the ions are employed as qubits defined in a frequency domain, and interaction between the qubits is mediated by a single cavity mode. In FDQC we can use adiabatic passage with dark states to perform single-qubit gates and two-qubit gates [1], and a single-qubit gate using adiabatic passage has been demonstrated [2]. For two-qubit gates, quantum states of qubit ions need to be read out and operated individually. In order to observe a single ion in a crystal, we studied modulated signals due to ions in a cavity-mode spectrum of a monolithic optical cavity made of Pr3+:Y2SiO5. Owing to the cavity enhancement and the electric-field-modulation spectroscopy, signals which are likely due to individual ions (statistical fine structure in an inhomogeneously broadened optical transition) were observed.


10:36AM S37.00014 Wavefunction dynamics in a quantum-dot electron pump under a high magnetic field, SUNGGUEN RYU, KAIST, MASAYA KATAOKA, NPL, United Kingdom, HEUNG-SUN SIM, KAIST — A quantum-dot electron pump, formed and operated by applying time-dependent potential barriers to a two-dimensional electron gas system, provides a promising redefinition of ampereme. The pump operation consists of capturing an electron from a reservoir into a quantum dot and ejecting it to another reservoir. The capturing process has been theoretically understood by a semi-classical treatment of the tunneling between the dot and reservoirs. But the dynamics of the wavefunction of the captured electron in the ejection process has not been theoretically addressed, although it is useful for enhancing the pump accuracy and for utilizing the pump as a single-electron source for mesoscopic quantum electron devices. We study the dynamics under a strong magnetic field that leads to magnetic confinement of the captured electron, which dominates over the electrostatic confinement of the dot. We find that the wave packet of the captured electron has the Gaussian form with the width determined by the strength of the magnetic field, and that the time evolution of the packet follows the classical drift motion, with maintaining the Gaussian form. We discuss the possible signatures of the wave packet dynamics in experiments.

1. V. Kashcheyevs, B. Kaestner, PRL 104, 186805 (2010)

10:48AM S37.00015 Semiconducting nanodimer as a photonic cavity: Large and well-defined Rabi splitting, MITSUHARU UEMOTO, Graduate School of Engineering Science, Osaka University, HIROSHI AJIKI, Photon Pioneers Center, Osaka University — A metallic nanodimer acts as a photonic cavity because a strong light field appears at the gap region due to a surface plasmon resonance. In this talk, we propose a photonic cavity consisting of a semiconducting nanodimer with a small gap, and theoretically demonstrate large and well-defined vacuum Rabi splitting of a two-level emitter placed at the photonic cavity. A light field is strongly enhanced at the gap region of the semiconducting nanodimer due to an exciton resonance. The interaction between the enhanced light and the emitter is significantly larger than that in a conventional photonic cavity, because the semiconducting nanodimer has a small cavity-mode volume beyond the diffraction limit as well as the metallic nanodimer. In contrast to the metallic nanodimer, the exciton decay rate at low temperature is very small, and as a result, the quality factor reaches Q ~ 10^8 which is about 100 times larger than that of the metallic nanodimer. Consequently, the large Rabi splitting energy (~ 1.7 meV) appears for the small dipole moment (~ 25 Debye) of the emitter, and the splitting energy is two times larger than the spectral width. Such a well-defined Rabi splitting is highly suited for both fundamental researches and applications.
from the effect of mode-mode coupling. The shape of the spectrum depends on the interrelation between the nonlinear coupling strength and the decay rates of the modes. The characteristic of the coupling-induced frequency fluctuations being non-Gaussian, it is possible to average over them in a path-integral formulation and thus to find the power due to the oscillator decay. We show that the mode coupling can be easily identified from the change of the spectrum due to weak resonant driving. Despite their decay coming from the coupling to (THz) light in free-space optical cavities and to microwave (GHz) fields in superconducting circuits. Exploiting this parametric coupling to realize quantum information transfer between these domains entails construction of devices with challenging requirements. These devices must integrate the membranes with superconducting circuits operating at cryogenic temperatures in proximity of free space optical photons while meeting demands for various quantum and coupling requirements. Here we show how to construct such “hybrid quantum devices” by microfabricating and assembling chip-based structures that can be inserted into high-finesse optical cavities compatible with low temperatures. We include an overview of recent fabrication improvements of membranes mechanically isolated from environment by phononic band-gap crystals.

This work is supported by awards from DARPA, NSF, JSPS (Japan), MOST (Taiwan) and NTU (Taiwan).

DAN HU, School of Natural Sciences, Univ of California, Merced. SHANG-YU HUANG, Dept. of Physics, National Taiwan Univ. JIE-QIAO ZHOU, CEMS, RIKEN, Japan. LIN TIAN, School of Natural Sciences, Univ of California, Merced. HSI-SHENG GOAN, Dept. of Physics, National Taiwan Univ. — Optomechanical systems with ultrastrong coupling could demonstrate nonlinear optical effects such as photon blockade. The system-bath couplings in these systems play an essential role in observing these effects. In this work, we use a dressed-state master equation approach to study the quantum coherence of an optomechanical system. In this approach, the system-bath couplings are decomposed in terms of the eigenbasis of the optomechanical system. The mode-dependent decay rates and mode-dependent coupling terms are included. Compared with the standard master equation, our master equation includes photon-number-dependent terms that induce dephasing. We calculate cavity dephasing, second-order photon correlation, and two-cavity entanglement using the dressed-state master equation. At high temperature, our master equation predicts faster decay of the quantum coherence than with the standard master equation. The second-order photon correlation derived with our master equation shows less antibunching than that with the standard master equation.

This work is funded by AFOSR and MURI.

8:24AM S38.00003 Improving integration of high-Q silicon nitride membrane resonators into electro-opto-mechanical devices for hybrid quantum systems. 
K. CICAK, NIST - Boulder, R.W. ANDREWS, P.-L. YU, R.W. PETERSON, T.P. PURDY, P.S. BURNS, C.A. REGAL, K.W. LEHNERT, JILA: University of Colorado and NIST, Boulder, R.W. SIMMONDS, NIST - Boulder. — Macroscopic high-stress silicon nitride membranes can be implemented as ultra-high-quality-factor mechanical resonators operating in the quantum regime with average phonon occupancy below one quantum. Mechanical motion of these resonators can be engineered to simultaneously couple both to (THz) light in free-space optical cavities and to microwave (GHz) fields in superconducting circuits. Exploiting this parametric coupling to realize quantum information transfer between these domains entails construction of devices with challenging requirements. These devices must integrate the membranes with superconducting circuits operating at cryogenic temperatures in proximity of free space optical photons while meeting demands for various quantum and coupling requirements. Here we show how to construct such “hybrid quantum devices” by microfabricating and assembling chip-based structures that can be inserted into high-finesse optical cavities compatible with low temperatures. We include an overview of recent fabrication improvements of membranes mechanically isolated from environment by phononic band-gap crystals.

8:36AM S38.00004 Coherent mechanically-mediated state transfer between a superconducting qubit and a cavity. 
HUGO RIBEIRO, Department of Physics, McGill University, Montreal, Quebec H3A 2T8, Canada. YING-DAN WANG, Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190, China. AASHISH CLERK, Department of Physics, McGill University, Montreal, Quebec H3A 2T8, Canada. — We study coherent state transfer between a superconducting qubit and a cavity coupled via a nanomechanical resonator. There are two major challenges relating to state transfer of such systems. First, the duration of the protocol needs to be shorter than the shortest time-scale associated with dissipation (qubit relaxation, mechanical damping, cavity decay ...). This constraint implies that most of the well-known adiabatic transfer protocols cannot be used as is. Second, a fast double swap protocol, where the state of the qubit is first transferred to the mechanical degree of freedom and then to the cavity, is the most sensible scheme to mechanical dissipation. Here, we present some protocols that take into account both constraints and optimize the fidelity of the coherent state transfer.

8:48AM S38.00005 Phonon mechanisms of nonlinear decay and dephasing of mesoscopic vibro-mechanical systems. 
JUAN ATALAYA, Michigan State University. THOMAS W. KENNY, Stanford University. MARK I. DYKMAN, Michigan State University. — The frequencies and the decay rates of mesoscopic oscillators depend on vibration amplitudes. Nonlinear decay has been seen recently in various nano- and micro-mechanical systems. Here we consider a microscopic mechanism of nonlinear decay, the nonlinear coupling of the vibrational mode of interest, for example, a flexural mode, to other vibrations. Typically, the modes of interest have low eigenfrequencies \( \omega_0 \). Their decay comes from the coupling to acoustic-phonon type vibrations with much higher frequency and density of states. Thus, nonlinear decay requires quartic anharmonic coupling or cubic anharmonicity in the higher order. We find the decay rate for the inverse lifetime of the involved phonons, which is determined by the internal nonlinearity and the boundary scattering, being either much larger or smaller than \( \omega_0 \). The results extend the thermo-elastic, Akhiezer, and Landau-Rumer decay theory to nonlinear decay of mesoscopic modes and make specific predictions on the temperature and frequency dependence of the decay rate for different types of systems. We show that nonlinear decay is invariably accompanied by dephasing. We also show that in nano-electro-mechanical systems the decay rate can be electrostatically controlled.

9:00AM S38.00006 Spectra of mesoscopic oscillators with dispersive mode-mode coupling. 
YAXING ZHANG, MARK DYKMAN, Michigan State University. — Mesoscopic vibrational systems typically have several nonlinearly coupled modes with different frequencies and with long lifetime. Examples are provided by flexural modes of carbon nanotubes, graphene sheets, and nanobeams. We consider the power spectrum of one of these modes, which we call an oscillator. Thermal fluctuations of the amplitudes of the modes coupled to the oscillator lead to fluctuations of its frequency and thus to the broadening of its spectrum. However, the coupling-induced broadening is partly masked by the broadening due to the oscillator decay. We show that the mode coupling can be easily identified from the change of the spectrum due to weak resonant driving. Despite the coupling-induced frequency fluctuations being non-Gaussian, it is possible to average over them in a path-integral formulation and thus to find the power spectrum. The shape of the spectrum depends on the interrelation between the nonlinear coupling strength and the decay rates of the modes. The characteristic features of the spectrum are analyzed in the limiting cases. We also find that the spectral effect of the internal nonlinearity of the oscillator differs substantially from the effect of mode-mode coupling.

This Research is funded by AFOSR and MURI.
9:12AM S38.00007 Improving the cooling performance of a mechanical resonator with two-level-sstem defects. TIAN CHEN, XIANG-BIN WANG, Tsinghua University — We study cooling performance of a realistic mechanical resonator containing defects. The normal cooling method through an optomechanical system does not work efficiently due to those defects. We show by employing periodical $\sigma_+$ pulses, we can eliminate the interaction between defects and their surrounded heat baths up to the first order of time. Compared with the cooling performance of no $\sigma_+$ pulses case, much better cooling results are obtained. Moreover, this pulse sequence has an ability to improve the cooling performance of the resonator with different defects energy gaps and different defects damping rates.

3 We acknowledge financial support in part by the 10000 Plan of Shandong Province, by National High-Tech Program of China Grants No. 2011AA010800 and No. 2011AA010803, and by National Natural Science Foundation of China Grants No. 11174177 and No. 60725416.

9:24AM S38.00008 Determination of effective mechanical properties of a double-beam beam by means of a nano-electromechanical transducer. HAN HUEBL, FREDRIK HOCKE, MATTHIAS PERNPEINTNER, Walther-Meissner-Institut, Garching, Germany, XIAOQING ZHOU, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland, ALBERT SCHLIESDER, Niels Bohr Institute, Copenhagen, Denmark, TOBIAS J. KIPPPENBERG, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland, RUDOLF GROSS, Walther-Meissner-Institut, Garching, Germany. — In the field of optomechanics, the light field in an optical resonator dynamically interacts with a mechanical degree of freedom, enabling cooling and amplification of mechanical motion. This concept of light matter interaction can be transferred to the microwave (MW) regime combining superconducting MW circuits with nanometer-sized mechanical beams, establishing the class of circuit nano-electromechanics. To Taylor the mechanical properties of a vibrational element, double and multi-layer systems are of particular interest, e.g., the combination of highly tensile stressed SiN and metallic layers allow to increase the mechanical resonance frequency while maintaining a capacitive coupling scheme. Here, we investigate the mechanical properties of a doubly-clamped, double-layer nanobeam embedded into an electromechanical system. The nanobeam consists of a highly pre-stressed silicon nitride and a superconducting niobium layer. By measuring the mechanical displacement spectral density both in the linear and the nonlinear Duffing regime, we determine the pre-stress and the effective Young’s modulus of the nanobeam corroborating the analytical double-layer model expectations.

9:36AM S38.00009 Circuit Electromechanics with a Non-Metallized Nano-beam. MATTHIAS PERNPEINTNER, Walther-Meissner-Institut, Garching, Germany, T. FAUST, Center for NanoScience and Fakultät für Physik, Ludwig-Maximilians-Universität München, München, Munich, Germany, F. HOCKE, Walther-Meissner-Institut, Garching, Germany, J.P. KOTTHAUS, Center for NanoScience and Fakultät für Physik, Ludwig-Maximilians-Universität München, München, Munich, Germany, E.M. WEIG, Department of Physics, University of Konstanz, Konstanz, Germany, H. HUEBL, R. GROSS, Walther-Meissner-Institut, Garching, Germany. — In the field of cavity optomechanics, a motional degree of freedom is coupled to an optical cavity. This approach can be transferred to the solid state environment by combining a superconducting microwave cavity with a nanomechanical resonator. Typically, metallized mechanical resonators are used, coupling capacitively to the microwave cavity. In contrast, non-metallized nanomechanical beams provide higher quality factors and have therefore been employed for mechanical sensing devices. Here, we present an approach to integrate a pure, i.e. non-metallized nanobeam, into a nano-electromechanical device, which is based on the dielectric coupling between a superconducting coplanar waveguide microwave resonator and a tensile-stressed silicon nitride nanobeam. By making use of the Duffing nonlinearity of the strongly driven beam, we calibrate the amplitude spectrum of the mechanical motion and determine the electromechanical vacuum coupling. We find a quality factor of $480,000$ at a resonance frequency of $14$ MHz and $0.5K$. We deduce a vacuum coupling of $11.5 mHz$, which is in quantitative agreement with finite element based model calculations.

9:48AM S38.00010 Temporal and spectral mode conversion of microwave signals with a mechanical resonator. ADAM REED, REED ANDREWS, University of Colorado, Boulder/JILA/NIST, TAUNO PALOMAKI, University of Washington, KATARINA CICAK, JOHN TEUFEL, NIST Boulder, KONRAD LEHNERT, University of Colorado, Boulder/JILA/NIST. — Microwave fields are a powerful means for carrying information between separate quantum devices. Different devices, however, typically emit and capture fields with distinct frequencies and temporal envelopes. This spectral and temporal mismatch presents a challenge when wigning these elements into a fully functional information processing network. Here we show that this mismatch can be overcome by using an electromechanical circuit to arbitrarily alter the temporal envelope and center frequency of microwave signals, while at the same time acting as a storage medium. We demonstrate a protocol that shifts the frequency of $7$ GHz microwave signals by $250$ MHz, and converts an exponentially decaying temporal envelope into a Gaussian envelope. To characterize our signal conditioner in the quantum regime, we inject signals with a few quanta of energy to extract the total added noise and storage lifetime of the conditioner.

10:00AM S38.00011 Reservoir engineering in microwave cavity optomechanics. FLORENT LECOCQ, JEREMY CLARK, JOSE AUMENTADO, RAYMOND SIMMONDS, JOHN TEUFEL, NIST Boulder — Microwave cavity optomechanics is an architecture in which a freely suspended membrane modulates the frequency of a superconducting microwave resonant circuit. The resulting parametric interactions influence both the mechanical degree of freedom and the microwave light emerging from the cavity. Even at cryogenic temperatures, the mechanical oscillator resonating at $10$ MHz is typically dominated by its thermal reservoir, washing out any quantum behavior. However, in the presence of coherent drives to the cavity, the bare mechanical properties can be overwhelmed by the strong opto-mechanical interactions from the light field. By choosing wisely the frequency and amplitude of the drives, one can engineer the environment seen by the mechanical oscillator, a technique known as “reservoir engineering”. From an experimentalist point of view, we will discuss how using two-tone driving schemes, we exploit correlations in the vacuum noise to: (1) eliminate the backaction imparted on the mechanical quadrature being measured, a technique so-called Back-Action Evasion, or (2) strongly couple the mechanical mode to a squeezed microwave bath.

10:12AM S38.00012 Microwave electromechanics on suspended piezoelectric membranes. G. PEAIRS, K. J. SATZINGER, A. VAINSENCHER, UC Santa Barbara, A. N. CLELAND, University of Chicago — Nanomechanical resonators with microwave frequency resonances have been operated in the quantum regime, and are attractive for hybrid electro- and opto-mechanical schemes. We characterize a class of electromechanical devices using propagating phonons in two dimensions, operating at frequencies compatible with both superconducting qubits and optomechanical resonators. We use interdigitated transducers on suspended aluminum nitride membranes to launch and detect traveling acoustic waves. We demonstrate resonances localized to the transducers, as well as transmission across membranes and extended resonances in the acoustic cavities formed by the edges of the suspended membranes. We compare these measurements to analytic as well as finite-element models to determine key parameters, including the electromechanical coupling and propagation loss.

10:24AM S38.00013 Building a quantum interface between microwave and optical photons. A. VAINSENCHER, G. PEAIRS, K.J. SATZINGER, UC Santa Barbara, A.N. CLELAND, University of Chicago — In previous work we have shown that optomechanical resonators fabricated out of piezoelectric materials may provide a means for coherent transduction between microwave and optical frequency photons. Electrical microwave signals are efficiently converted to microwave photons, and these photons in turn modulate the optical response of an optomechanical crystal. In this talk, we will describe new designs we are pursuing in this same direction, with simplified fabrication and a predicted much greater electrical-to-optical coupling strength. We will outline the current device design, simulations, fabrication, and preliminary measurements.

3 This work is funded through DARPA/DSO.

Thursday, March 5, 2015 8:00AM - 11:00AM –
Session S39 GQI: Focus Session: Superconducting Qubits: Materials and Characterization
213AB - Kevin Osborn, Laboratory for Physical Sciences

8:00AM S39.00001 The Roles of Materials, Processing, and Design in Quantum Information Circuits

8:36AM S39.00002 High Quality Factor MBE-grown Aluminum on Silicon Planar Resonators

8:48AM S39.00003 Developing TiN resonators with high kinetic inductance

9:00AM S39.00004 Enhancing the coherence of 3D qubits suitable for multi-qubit experiments

We acknowledge support from IARPA under contract W911NF-10-1-0324
9:12AM S39.00005 Integrating superconducting qubit systems for improved quantum operations\(^1\). STEFAN FILIPP, SARAH SHELDON, EASWAR MAGESAN, LEV S. BISHOP, MATTHIAS STEFFEN, JERRY M. CHOW, JAY M. GAMBITTA, IBM TJ Watson Research Center, Yorktown Heights NY, USA — Recent progress in the field of superconducting circuits has led to qubit coherence times exceeding by far typical single and two-qubit gate times. In this regime, in which relaxation (T_1) and dephasing (T_2) times are above 40 and 50 microseconds, respectively, quantum gates are not limited by intrinsic noise sources. We enter this regime by optimizing the design of coplanar transmon qubits to reduce the influence of surface loss. Furthermore, we have eliminated spurious microwave resonances which we can detect by monitoring the qubit coherence while sweeping the frequency of an external microwave drive applied to the system. To improve T_2 times, we minimize dephasing caused by thermal photons in coupled resonator modes by increasing the attenuation of the readout drive lines. To maintain the ability to drive fast gates with strong microwave signals while preserving coherence, we employ weakly capacitively coupled control lines providing independent control of the qubits and allowing for improved two-qubit entangling gate operations.

\(^1\)We acknowledge support from ARO under contract W911NF-14-1-0124.

9:24AM S39.00006 Improving Superconducting Qubit Lifetimes with Broadband Filters\(^1\). NICHOLAS BRONN, ANTONIO CORCOLES, JARED HERTZBERG, SRIKANTH SRINIVASAN, JERRY CHOW, JAY GAMBITTA, MATTHIAS STEFFEN, IBM TJ Watson Research Center, YANBING LIU, ANDREW HOUCK, Princeton University — In circuit quantum electrodynamics, the state of the qubit is read out via a resonator at a different frequency than that of the qubit. Spontaneous qubit decay via the resonator may be suppressed by engineering an impedance mismatch at the qubit frequency, while still allowing a large coupling between the resonator and external environment necessary for fast, high fidelity readout. We present a stepped-impedance filter with a large stop-band in the qubit frequency range and demonstrate its effect on qubit lifetime. This filter is also effective when used in an off-chip geometry.

\(^1\)We acknowledge support from IARPA under contract W911NF-10-1-0324.

9:36AM S39.00007 Strong interaction of a transmon qubit with 1D band-gap medium\(^1\). YANBING LIU, DARIUS SADRI, ANDREW HOUCK, Princeton University, NICHOLAS BRONN, JERRY CHOW, JAY GAMBITTA, IBM — The spontaneous emission of an atom will be enhanced or suppressed in a structured vacuum, commonly known as Purcell effect. Moreover, in a frequency gap medium, an atom-photon bound state is predicted to exist in the band gap, causing the localization of light. Here using the technology of circuit quantum electrodynamics, we experimentally explore this mechanism by fabricating a microwave step-impedance filter strongly coupled to a transmon qubit. Standard transmission and spectroscopy measurements support the existence of atom-photon bound states in the system. Correlation measurement shows that the atom-photon interaction induces strong correlation of the transmitted light through the system.

\(^1\)Thanks support from IARPA

9:48AM S39.00008 Parallel Loss Channels in Superconducting Epitaxial Aluminum Resonators , CHRISTOPHER RICHARDSON, NATHAN SIWAK, LEI HE, Laboratory for Physical Sciences — Superconducting epitaxial aluminum (epi-Al) on silicon and sapphire has demonstrated low-loss performance that is desirable for linear circuit elements in quantum computing. Most often, it is process artifacts that limit the performance of devices fabricated from epi-Al. Two common artifacts are photoresist residue that is impossible to observe with optical microscopy and line edge defects on the aluminum sidewalls. Superconducting quarter-wave resonators exhibit both saturable power dependence akin to conventional two-level-systems, and power independent loss that strongly impacts yield and is fabrication process dependent. Correlations between detailed electron microscopy, and resonator quality factor measurements with values above and below 10^16 will be discussed.

10:00AM S39.00009 Characterization of Fabrication Defects in Superconducting Epitaxial Aluminum Resonators , NATHAN SIWAK, LEI HE, JUSTIN HACKLEY\(^1\), CHRISTOPHER RICHARDSON, Laboratory for Physical Sciences — A continuing challenge in superconducting quantum computing is the creation of low-loss superconducting aluminum resonators. Significant processing difficulties lie in the removal of residues resulting from conventional Cl-based plasma etching without damaging the aluminum patterns. Correlations of resist residues and corrosion pit defect densities with cleaning process variations are completed using charge contrast-enhanced imaging in a scanning electron microscope. These quantified defects provide insight into the effectiveness of specific device processing steps in reducing these artifacts which can introduce additional loss mechanisms and limit potentially high performance devices.

\(^1\)Currently at Northrop Grumman Corp.

10:12AM S39.00010 Effects of 780 nm Optical Illumination on Loss in Superconducting Microwave Resonator\(^1\). R.P. BUDOYO, J.B. HERTZBERG, C.J. BALLARD, K.D. VOIGT, JQI and CNAM, Dept. of Physics, University of Maryland, College Park, J.R. ANDERSON, C.J. LOBB, F.C. WELLSTOOD, JQI and CNAM, Dept. of Physics, University of Maryland, College Park — Understanding the effects of light incident on a superconducting circuit is an important step toward building a hybrid quantum system where a superconducting qubit or resonator is coupled to atoms trapped on a tapered optical fiber. We fabricated a microscale thin-film Al superconducting LC resonator (frequency 6.72GHz) on sapphire substrate and mounted it inside an Al 3d cavity (TE101 mode frequency 7.50GHz). Using an optical fiber, we illuminated the resonator with 780 nm light, and measured the change in internal quality factor and resonant frequency of the resonator as a function of applied optical power. The results suggest that the illumination causes an increase in rf drive-dependent dissipation. While optical illumination is expected to enhance dissipation due to quasiparticles, rf drive dependence is more typically seen in two-level-system dissipation. We compare the results with the change in loss from increased resonator temperature, and discuss various mechanisms of loss from optical illumination.

\(^1\)Work supported by NSF through the Physics Frontier Center at the Joint Quantum Institute (JQI), and by the Center of Nanophysics and Advanced Materials (CNAM).
The resonator has a resonance frequency of 6.14 GHz, a quality factor Q of \(2.59 \times 10^3\) and is mounted inside a superconducting aluminum 3D cavity. A tapered optical fiber enters and exits the 3D cavity through two small holes in opposite sides of the cavity, placed so that the fiber can pass close to the resonator. The 3D cavity is mounted on an x-z piezo-translation stage that allows us to change the relative position of the lumped-element resonator and fiber. When the resonator is brought near to the fiber, we observe a shift in resonance frequency due to the presence of the fiber dielectric. When light is sent through the fiber, Rayleigh scattering causes a position-dependent illumination of the resonator, generating quasiparticles and thereby affecting its resonance frequency and Q. Our model of the resonator response includes the generation, diffusion, and recombination of quasiparticles in the resonator and shows that the frequency response allows us to track the position of the fiber in situ.

**Work supported by NSF through the Physics Frontier Center, Dept. of Physics, Univ. of Maryland.**

10:36AM S39.00012 Robustness of superconducting high-Q resonators against direct quasiparticle injection, U. PATEL, Department of Physics, University of Wisconsin, Madison, Wisconsin 53706, I. NSANZINEZA, B. L. T. PLOURDE, Department of Physics, Syracuse University, Syracuse, New York 13244, R. MCDERMOTT, Department of Physics, University of Wisconsin, Madison, Wisconsin 53706 — A longstanding goal of the superconducting qubit community is to integrate a superconducting quantum circuit with classical cryogenic digital logic based on the Single Flux Quantum (SFQ) logic family. Since the SFQ circuit transitions to the finite voltage state, care must be taken to protect the quantum circuit against quasiparticle-induced decoherence. Here we describe experiments to characterize the robustness of high-Q superconducting linear resonators against direct quasiparticle injection. We use NIS junctions to controllably inject quasiparticles into the groundplane of a superconducting resonator chip. We monitor resonator Q and frequency shift versus injection current for different device geometries. Finally, we discuss strategies to protect the resonator circuit from quasiparticle poisoning.

10:48AM S39.00013 Energy relaxation in transmons coupled to superconducting lumped-element resonators, B. SURI, S. NOVIKOV, Dept. of Physics, Univ. of MD, F.C. WELLSTOOD, JQI, CNAM, Dept. of Physics, Univ. of MD, B.S. PALMER, Lab. for Physical Sciences, Dept. of Physics, Univ. of MD, College Park, MD. — We report on the energy relaxation of a series of Al/AIOx/Al transmon qubits coupled to superconducting Al lumped-element resonators on a sapphire substrate measured at 20 mK. For some of our transmon devices, which have transition frequencies between 4 and 8 GHz, we find that the coupling of the transmon to the 50 \(\Omega\) transmission line through the lumped-element resonator is the dominant mechanism of relaxation limiting the lifetimes to 1 \(\mu\)s or smaller. By increasing the resonator’s resonant frequency from 5.4 to 7.2 GHz, increasing the loaded quality factor of the resonator, and lowering the transmon-resonator coupling, we were able to decouple the transmon from the dissipative environment by an order of magnitude. We observe an improvement in the lifetimes of the transmons, with new limits possibly set by material losses. Microwave simulations, analytical results and experimental measurements on multiple devices will be presented.

**Thursday, May 3, 2015 8:00AM - 10:48AM**

Session S41 DPOLY: New Directions in Polymer Physics 214A - Julie Albert, Tulane University

8:00AM S41.00001 Selective-Assemblies of Frank-Kasper A15 and Other Superlattices via Precisely Controlled Positional Interactions in Nano-Sized Giant Tetrahedra, MINGJUN HUANG, CHIH-HAO HSU, JING WANG, KAN YUE, STEPHEN Z.D. CHENG, University of Akron — Diverse self-assembled hierarchical structures in soft materials including small molecules, polymers, and biomacromolecules have been intensely studied. Herein, we report a class of precisely defined, rigid, nano-sized giant tetrahedra molecules, which are constructed by positioning polyhedral oligomeric silsesquioxane (POSS) molecular nanoparticles with different functional groups at the apices of a tetrahedron framework. Designed symmetry breaking of these giant tetrahedra accurately controlled the positional interactions, leading to diverse selectively assembled, highly ordered supramolecular structures. In particular, a Frank-Kasper A15 superlattice was obtained from a series of giant tetrahedra with three hydrophobic and one hydrophilic POSS cages, which resembled the essential structure of certain metal alloys, but with tunable feature sizes at much larger length scales. Formation of the A15 phase is due primarily to the deformability of the self-assembled spherical building blocks that allows size polydispersity from monodisperse giant tetrahedra.

8:12AM S41.00002 Relaxation suppression in stretched block-copolymer matrix above \(T_g\), DMITRIY ALHAZOV, MICHAEL BURMAN, ARKADII ARINSTEIN, EYAL ZUSSMAN, Technion - Israel Institute of Technology — As was shown in our recent paper [1], electrosyn polymer thermoplastic polyurethane (TPU) block-copolymer nanofiber mats start massively to contract upon heating up to \(\sim 90^\circ C\), whereas cast TPU films expand as expected. Further studies have shown that such temperature threshold is an artifact caused by process kinetics. It also turned out that cast TPU films can also massively contract upon heating, but only after the following thermo-mechanical programming: stretching the films (\(~100\%) at high temperature (\(~90^\circ C\), cooling to room temperature under constant strain, and finally, unloading the stretched films. Such behavior in films demonstrates that the contraction in electrosyn fibers cannot be attributed only to confinement. Rather, the phenomenon in question should be attributed to relaxation suppression in non-equilibrium (stretched) states of TPU polymer matrix. This conclusion is unpredicated since the temperatures of the tested samples (before heating) were much higher than the glass transition temperature of the soft phase, and the concentration of hard segments in TPU macromolecules is too low in order to form a percolated “solid” structure. In such a situation the relaxation of the non-equilibrium is expected. A possible physical explanation of the observed phenomenon, based on the blob concept, is proposed.


8:24AM S41.00003 The Influence of Interfacial Block Copolymer on the buckling and drainage of an emulsion droplet approaching a flat surface, DAMITH ROZAIRO, ANDREW B. CROLL, North Dakota State Univ — When a liquid droplet surrounded by a homogeneous fluid approaches a flat wall it can buckle and trap a thin layer of the surrounding fluid. The thin layer of trapped fluid slowly drains out, driven by the capillary forces which will eventually flatten the buckled droplet. The dynamics of these interactions are a critical stage of many industrial and biomedical applications. There is now a body of research surrounding the process and the effects of small surfactant molecules on thin film drainage. Long chain surfactants (block copolymers) are seen increasing used in emulsion stabilization, however, the unique effects of long polymer surfactants on surfactant dynamics in simple hydrodynamic processes are often ignored. In this work we experimentally study how a self-assembled diblock copolymer interface on an emulsion droplet influences the entrainment and subsequently drainage of surrounding fluid. Specifically, we investigate several different polystyrene-b-poly(ethylene oxide) (PS-PEO) molecules on toluene droplets in water as they approach an atomically flat silica surface. The film drainage rate is found to vary with the molecular weight of the PS-PEO molecules. Remarkably, we observe slower drainage rate for longer PEO chains, which can be understood with a simple hydrodynamic model.
8:36AM S41.00004 Electrostatically driven selective deposition of nanoparticles on chemically modified block copolymer patterns

1. TOM WAGNER, Institute of Physical Chemistry RWTH Aachen, LARISA TSARKOVA, DIW - Leibniz Institute for Interactive Materials, ALEXANDER BOEKER, Institute of Physical Chemistry RWTH Aachen — Targeting applications in catalysis, circuitry, molecule-recognition and optoelectronics, we selectively assembled negatively charged gold nanoparticles (AuNPs) on microphase separated poly(styrene-block-2-vinylpyridine) (PS-b-P2VP) thin films by electrostatic interactions. Chemical crosslinking of PS-b-P2VP films results in positively charged P2VP domains (qP2VP). Control of charge density of the P2VP blocks is governed by varying the degree of crosslinking. To quantify the contribution of coulombic interactions we performed combinatorial studies including micro contact printing of negatively charged AuNPs onto qP2VP-homopolymer films as well as selective AuNP deposition on PS-b-qP2VP films by immersion. During manufacture, the chemical composition of precursors and final composites has been monitored by ATR-IR and XPS-measurements whereas AFM- and FESEM-measurements revealed topographical features. XRR- and GISAXS-measurements provided information on the inner structure of the film. AuNP adsorption kinetics was followed by in-situ electrochemical impedance spectroscopy (EIS). Finally, the complementary analyses allowed for better understanding the fundamentals of electrostatically driven NP-adsorption on soft polymer surfaces.

2National Research Fund of Luxembourg (AFR)

8:48AM S41.00005 The effect of added block copolymer on oil in oil emulsions

ITAURU ASANO, TIMOTHY LODGE, Univ of Minn - Minneapolis — Oil-in-oil emulsions, formed by polymer A and polymer B in the presence of an organic solvent (A/solvent-in-B/solvent), are a unique class of emulsion, because both phases are composed of organic components. Here, the effects of PS-b-PEGs (PS: polystyrene and PEG: polyethylene glycol) on the stability of the oil-in-oil emulsions composed of PS/CHCl<sub>3</sub>-in-PEG/CHCl<sub>3</sub> were studied by varying the molecular weight (20 < M<sub>n</sub> < 200 kg/mol) and the volume fraction (0.40 < f<sub>PEG </sub> < 0.82) of the PS-b-PEG. We found that higher M<sub>n</sub> of PS-b-PEGs with low f<sub>PEG</sub> were able to stabilize the emulsions with reduced droplet size. In particular, using a large PS-b-PEG (200 kg/mol, f<sub>PEG </sub> = 0.52), the emulsion was stable for more than 2 weeks, and the droplet size decreased to the nanoscale, around 300 nm in diameter, whereas the emulsion was unstable with large droplets (>50 μm) without the PS-b-PEG. In order to reveal the mechanism of stabilization, dye-labeled PS-b-PEGs in the emulsions were directly monitored by fluorescence microscopy.

9:00AM S41.00006 Assembly of polymeric nanoparticles: Molecular dynamics study

SABINA MASKEY, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — The assembly of polymeric nanoparticles or polydots has been studied using molecular dynamics simulations. These polydots are highly fluorescent and have potential applications in intracellular imaging, bio-sensors and other optoelectronic devices. Therefore their assembly is the key to their utilization. Here we probe the assembly of polydots made by para dialkyl phenyleneethynylene (PPEs) whose conformation determines their degree of conjugation and enhance their electro-optical response. As in our previous study, PPE polydots were prepared by collapsing polymer by the procedure developed. The polydots were brought together two ways. Allowing the particles to approach each other at a constant velocity of 50m/s resulted in the particles bouncing off each other which is consistent with the dense object which we have previously reported. Then polydots were brought together at constant force and interface between them has been followed. Our results show that polydots under high velocity and forces remain stable. Closer look at the interface reveals that backbones of the polymer do not inter-penetrate and side chains dominate the interface. This interfacial structure suggests that one could retain the structure of polydots upon assembly.

1 NSF CHE-1308298

9:12AM S41.00007 Assembly of Magnetite Nanoparticles Grafted with Ion-Containing Diblock Copolymers

1. YANG JIAO, PINAR AKCORA, Stevens Inst of Tech — Polystyrene (PS)-grafted iron oxide nanoparticles are shown to organize into highly ordered anisotropic nanostructures in bulk forms as of microphase separated morphologies of block copolymers. Ordered strings that are of one particle in width are created in composite films. In this work, we design a novel system of ion-containing block copolymer-grafted magnetic nanoparticles and study the effect of phase separation in grafted block copolymer on the aggregation of magnetic nanoparticles in the presence of ionic liquid, [HMIM][TFSI]. Styrene sulfonates neutralized with trietylammmonium are clicked to the thiolated ends of grafted PS through a thiol-ene click reaction. We show that the phase separated copolymer brush lead to stacking of strings of nanoparticles into planar structures. Miscibility of block-grafted nanoparticles is being enhanced by the solvation of sulfonated groups with ionic liquid. Further, we demonstrate that the copolymer-grafted particles can be easily directed under magnetic fields in liquid organic compared to their uncharged forms. The conductivity results indicate that the good miscibility between sulfonated particles and ionic liquid significantly enhances conductivity.

3We acknowledge financial support from NSF-DMR CAREER grant (#1048865).

9:24AM S41.00008 Engineer concentration gradient drug particles using microfluidic systems

JIANBIN WANG, PAVITHRA SUNDARARAJAN, ADAM PROCOPIO, LARRY ROSEN, JERRY KLINZING, PATRICK MARSAC, Merck, MERCK RESEARCH LABORATORIES TEAM — Particles designed with spatial composition gradients have attracted increasing attention in the pharmaceutical industry. The designed distributions of drug, polymer or surfactants in the concentration gradient drug particles could enable control of the drug release kinetics or targeted drug delivery. Here, we present a technique for generating concentration gradient particles from concentration gradient droplets using a microfluidic device. The concentration gradients in the liquid stream and the droplets were monitored with fluorescence microscopy and the concentration gradients were largely maintained. X-ray computed tomography was used to characterize the internal structure and concentration gradient profile in the solid particles. We successfully generated the concentration gradient particles in the coupled evaporative diffusive system by keeping the non-dimensional relative time scale for evaporation to diffusion to be 0.1 or less. Our experiments were instrumental to gaining fundamental insights into the processes controlling the concentration gradients in the particle and the droplet.

9:36AM S41.00009 Steered molecular dynamics of epoxy-amine reactions in EPON862-DETDA

YAE JI KIM, SAMUEL REEVE, ALEJANDRO STRACHAN, Purdue Univ — The combination of steered molecular dynamics (SMD) and Jarzynski’s equality has made free energy calculations for simulations of non-equilibrium pulling processes possible. This has been widely studied in protein folding and is now applied for epoxy-amine reactions for the first time using the reactive interatomic potential ReaxFF. This reaction in epoxy EPON862 and curing agent DETDA, commonly used in aerospace composite materials, is investigated in both the gas and condensed phases. The potential of mean force (PMF) is calculated during the simultaneous breaking of the epoxy ring and approach of the amine nitrogen to the terminal carbon. Minimization of the PMF is carried out by varying the timing of the reaction (e.g. delayed approach of C-N), as well as a variation of adaptive SMD via a parallel replica method. This adaptive SMD breaks the reaction into a series of time stages, reducing the necessary number of independent simulations and resulting in more rapid convergence of the PMF. Reaction completion is predicted using various initial geometric and molecular features.
10:00AM S41.00011 Chirality Transfer in Chiral Homopolymers and Chiral Block Copolymers

UMASS AMHERST, BUMJOON KIM, KAIST, RYAN HAYWARD, UMASS AMHERST — Conjugated polymer nanofibrils produced by solution assembly represent efficiently charge transporting nanostructures with promise for improving the performance of organic electronics. Despite their advantages, they have limitations that hinder their application, such as low electrical conductivity and device-to-device variations in the IETS spectra, which are possibly originated from defects in the molecular junctions and insulating wall. We also observed discrepancies and device-to-device variations in the IETS spectra, which are possibly originated from defects in the molecular junctions and insulating wall.

10:12AM S41.00012 Polydot at the interface with DPPC membrane: A Molecular Dynamics Simulation Study†, SADITH WIJESINGHE, DVORA PERAHIA, Clemson University, GARY GREST, Sandia National laboratories, CHRISTOPH JUNGHANS. Alamos National laboratories — Luminescent polymers confined into long lived polydots are of potential interest because of their tunable properties and biocompatibility. These desired properties of polydots make them potential candidates for target drug delivering agents and bio markers. The first and foremost step in such applications is introducing these polydots to biological membranes which consist of different lipids whose collective dynamics mediate the cell membrane functions. Experimental studies suggest that their ability to penetrate cells depend on the polydot morphology, charge and the environmental characteristics including the type of the cell membrane. Here we report the results of an all atom molecular dynamics simulation of a carboxylate substituted dinonyl poly para phenylene ethynylene (PPE) polydot in one-component bilayer composed 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC). Introduction of a polydot into the DPPC membrane initially results in deformation of the membrane however after equilibrated, the membrane relaxes and the polydot is stable within the membrane.

10:24AM S41.00013 Investigation of a new approach for high-yield molecular electronic junctions with direct metal transfer method†, HYUNHAK JEONG, Seoul Natl Univ, HEEJUN JEONG, Hanyang Univ, TAKHEE LEE², Seoul Natl Univ — To investigate the charge transport characteristics through molecular junctions which utilize molecules as an active channel, several approaches to form molecular junctions have been demonstrated [1]. Specifically, solid state device structure-based methods have been considered, however, one of the major obstacles of this method is generation of filamentary path which results in low device yield. To overcome this, several other methods that utilize a protective interlayer have been reported [2,3]. But, it is still difficult to investigate the genuine transport characteristics through molecular junctions because of the adoption of the interlayers. Here, we propose a new approach for high-yield molecular junctions with a direct metal transfer method. With this method, we measured inelastic electron tunneling spectroscopy (IETS) characteristics of molecular junctions made with alkanethiolate. We also observed discrepancies and device-to-device variations in the IETS spectra, which are possibly originated from defects in the molecular junctions and insulating wall.

1 The National Creative Research Laboratory program (Grant No. 2012026372) through the National Research Foundation of Korea (NRF) funded by the Korea Ministry of Science, ICT & Future Planning.

2 corresponding author

10:36AM S41.00014 Photo-crosslinking and Post-Functionalization of Solution Assembled Conjugated Polymer Nanofibers, HYEONG JUN KIM, KAIST, MATTHEW SKINNER, ALEJANDRO BRISENO, TODD EMRICK, UMASS AMHERST, RONG-MING HO, Department of Chemical Engineering, National Tsing Hua University — Herein, we deals with the chirality transfer of chiral polymers on different length scales. Helical conformation could be formed due to the stereoregularity of chiral entities in the chiral polymers and the BCPs*. Helical superstructures and phases can be fabricated by self-assembling polymer chains with helical conformation through intramolecular and intermolecular interactions. The transfer of chiral information from molecules to macroscopic level and the control of the handedness of the helical architectures are discussed. The examples of chirality transfer in the self-assembled chiral polymers and BCPs* are introduced. As found, the molecular chirality of constituted chiral entities in the chiral polymers and the BCPs* and corresponding conformational chirality plays an important role in the formation of helical architectures with exclusive handedness. Also, we deal with the chirality transfer in specific model systems, chiral polylactides and polylactide-containing BCPs*, at which homochiral evolution from chiral entity to helical phase is demonstrated. A methodology for systematic studies of the chirality transfer from molecular level to phase scale is suggested. Through the design and synthesis of macromolecules and the operation of self-assembly, the mechanisms of chirality transfer on different length scales can be understood, giving supplementary information to disclose the mysteries of morphological evolution from the molecular level.

9:48AM S41.00010 Phase Transition in a Model of Y-shaped Molecules†, DONOVAN RUTH, Lehigh University, RAUL TORAL, IFISC (CSIC-UIB), DANIELLE HOLZ, Drew University, JEFFREY RICKMAN, JAMES GUNTON, Lehigh University — Increasing attention in statistical mechanics is being given to non-spherical molecules, such as polypeptide chains and protein molecules. One example is provided by immunoglobinulin, which has a ‘Y’ shape. In this work, we determine the phase diagram of ‘Y’-shaped molecules on a triangular lattice through Monte Carlo Grand Canonical ensemble simulation, using histogram reweighting, multicanonical sampling and finite size scaling. We show that (as expected) this model is a member of the Ising universality class. For low temperatures, we implemented multicanonical sampling to induce faster phase transitions in the simulation. By studying several system sizes, we use finite size scaling to determine the two phase coexistence curve, including the bulk critical temperature, critical chemical potential and critical density.

1 G. Harold and Leila Y. Mathers Foundation, National Science Foundation PHY-0849416 and PHY-1359195

Thursday, March 5, 2015 8:00AM - 11:00AM – Session S42 DPOLY: Electrically and Optically Active Polymers 214B - Chelsea Chen, Lawrence Berkeley National Laboratory

8:00AM S42.00001 ABSTRACT WITHDRAWN –
8:12AM S42.00002 Orthogonal Photolithography as transformative patterning technique for Organic Electronics and Photonics, ALEX ZAKHIDOV, Texas State University — Orthogonal photolithography (OP) takes advantage of the fact that the vast majority of organic semiconducting materials are either oleophilic or hydrophilic and are hence orthogonal to highly fluorinated chemicals. Therefore, appropriate fluorinated photoresists can be used to pattern organic layers without compromising performance of organic device. The availability of such orthogonal photoresists promises to enable the fabrication of complex device structures, expanding the range of possibilities for organic electronics. Particular, OP technique enables sub-pixel high-resolution patterning for OLED displays [1]. Once RGB sub-pixel structuring is realized it is expected to improve (up to 10 times) the efficiency of a display. Moreover, processing solvents used for OP can be used as encapsulation media to improve heat management of high brightness OLED devices [2]. Other applications of OP include ultra-small channel OTFTs [3]. OTFT based circuits and high voltage failure/proof organic solar cells.


8:24AM S42.00003 Self-assembled peptide nanostructure-based polymeric electronic materials1, SOMA KHANRA, SUCHI GUHA, University of Missouri, Columbia, WENDEL ALVES, THIAGO CIPRIANO, Universidade Federal do ABC, Santo Andre- Sao Paulo, Brazil — Peptide-based nanostructures derived from natural amino acids are superior building blocks for organic semiconductor-based and biocompatible devices as they can be used in a bottom-up process without the need for expensive lithography. Based on self-assembly and mimicking the strategies occurring in nature, peptide materials play a unique role in a new generation of hybrid materials for the electronics of the 21st century. In this work we functionalize diphenylalanine (FF)-containing peptides with conducting polymers, such as Poly (3-hexylthiophene) (P3HT) and polyfluorene (PF). The FF-polymer composites were synthesized by two methods: liquid-vapor and solid vapor phase. Electron microscopy images show micrometer size tubes with approximately 200 nm in diameter with homogeneous morphology. Photodiodes and light-emitting diode structures have been fabricated from FF-P3HT and FF-PF, respectively. We compare the electrical and optical properties of the FF-polymer composite devices with pristine polymer devices. Our results show that FF nanostructures with organic semiconductors could open up a new generation of bio-compatible materials in organic electronics.

1This work was supported by National Science Foundation, Award No-1339011.

8:36AM S42.00004 Investigation of Different Organic Solar Cell Active Region Structures Deposited by Resonant Infrared Matrix-Assisted Pulsed Laser Evaporation (RIR-MAPLE)1, ADRIENNE STIFF-ROBERTS, RYAN MCCORMICK, AYOMIDE ATEWOLOGUN, Department of Electrical and Computer Engineering, Duke University, STIFF-ROBERTS RESEARCH GROUP TEAM — In this work, we use RIR-MAPLE to investigate organic solar cells (OSCs) featuring different P3HT:PCBM active region structures: bulk heterojunction (BHJ), bilayer, and gradient composition. Two deposition capabilities of RIR-MAPLE, nanoscale domains in blended polymeric films and multi-layer polymeric films regardless of constituent solubility, enable the deposition of these structures. While the BHJ yields better exciton dissociation due to large donor/acceptor interfaced area, the bilayer provides better charge transport due to reduced interfacial recombination. In contrast, the gradient structure could optimize both exciton dissociation and charge transport. P3HT materials characterization includes UV-Vis absorbance for Spano analysis and grazing-incidence, wide angle X-ray scattering (GIWAXS) for structural information. The OSC device characterization includes external quantum efficiency (EQE) and current-density voltage measurements. In addition, a dynamic Monte Carlo model is used to simulate the different structures in order to generate EQE spectra for comparison to the measured device performance. This work was supported, in part, by the Office of Naval Research under Grant N00014-10-1-0481 and the National Science Foundation Triangle MRSEC on Soft Matter.

1This work supported in part by ONR and NSF.

8:48AM S42.00005 Intrinsic series resistance of organic photovoltaic devices , NON THONGPRONG, PHILLIP DUXBURY , Michigan State Univ — Bilayer organic photovoltaics (OPV) are theoretically and computationally studied in order to find intrinsic physical origins of series and parallel resistances; $R_s$ and $R_p$. New current density-voltage (J-V) characteristic equations were derived in a similar manner to the work by Giebink et al., using reasoning based on hole and quasi-Fermi energies. We also developed a computational model combining previous developments by Koster et al. and Barker et al. with the interface model of Giebink et al. The computational model reveals that there are space charge regions around the donor-acceptor interface. These regions are the cause of an intrinsic $R_s$ due to their low carrier density which induces a shift of the quasi-Fermi levels from the electrode work functions. Recombination of charge transfer excitons (polaron pairs) across the interface can be viewed as a leakage path. An intrinsic origin of $R_p$ in this model is then polaron pair recombination. Both resistances are dependent on the applied voltage and these dependences are calculated using our computational model. The analysis is extended to include the presence of traps, yielding expressions for $R_s$ and $R_p$ and for the ideality factors as a function of applied voltage.

9:00AM S42.00006 Photovoltaic Cells Involving Nonconjugated Conductive Polymer, Iodine-doped Styrene-Butadiene-Rubber (SBR) , JUSTIN VAN CLEAVE, MRINAL THAKUR, Photonic Materials Research Laboratory, Auburn University, AL — Photovoltaic cells have been fabricated using titanium dioxide/ iodine-doped Styrene-Butadiene-Rubber/ carbon on indium-tin-oxide coated PET substrates. Photo-currents and photo-voltages were measured for varying intensities of light from a white light bulb, with emission from 300 to 700 nm. Iodine-doped SBR has absorption in the range of ~250 to 750 nm. The cells as fabricated were characterized and were found to show significantly higher conversion efficiencies than previously reported. For an incident light intensity of about 5 mW/cm$^2$ a maximum photo-current density of about 0.2 mA/cm$^2$ and photo-voltage of about 0.8 V were recorded. The low cost of nonconjugated conductive polymers including SBR may provide a cheaper alternative to other materials for photovoltaic applications.

9:12AM S42.00007 Polymer/solvent bicontinuous microemulsions for use as organic solar cell active layers , DYLAN KIPP, University of Texas at Austin, OLGA WODO, University at Buffalo SUNY, BASKAR GANAPATHYSUBRAMANIAN, Iowa State University, VENKAT GANESAN, University of Texas at Austin — The paradigm for the optimal morphology of an organic solar cell is characterized by cocontinuous, interpenetrating donor and acceptor domains with nanoscale dimensions and high interfacial areas. One well known equilibrium morphology that fits these characteristics is the bicontinuous microemulsion noted in the context of flexible polymeric blends. Currently, design rules are not available for producing bicontinuous microemulsion morphologies from blends of conjugated polymer + block copolymer + solvent and locate the channels of morphologies with characteristics like that of the bicontinuous microemulsion. Our theoretical analysis results in empirical design rules for producing bicontinuous microemulsion morphologies from blends of conjugated polymer + block copolymer + fullerene.

9:24AM S42.00008 Block Copolymer nanocomposite thin films for high energy-density capacitors , SAUNIL SAMANT, University of Akron, SHIMELIS HAILU, Howard University, CHRISTOPHER GRABOWSKI, MICHAEL DURSTOCK, Air Force Research Lab, DHARMARAJ RAGHAVAN, Howard University, ALAMGIR KARIM, University of Akron, UNIVERSITY OF AKRON COLLABORATION — The energy storage capacity of solid-state capacitors is governed by product of relative permittivity (ε) and square of breakdown strength (Vbd) of dielectric medium. Polymer films are widely used as the dielectric medium in capacitors due to their high Vbd and low loss but they suffer from poor permittivities. Composite dielectrics combine the high ε ceramic fillers with high Vbd polymer matrix but usually result in loss of Vbd due to aggregation induced field enhancements. For optimum enhancement of dielectric properties, it is essential to improve matrix-filler interaction and control the dispersion of fillers. To that effect we graft a BCP onto the nanofiller and disperse it within a host BCP with similar composition. Using Directed Self-assembly we fabricate BCP nanostructured films with highly dispersed functionalized nano-fillers that are not only expected to enhance the overall ε, but the well-ordered BCP nanostructures also improve Vbd by providing sharp interfacial barriers acting as charge traps. The impact of filler functionalization, BCP morphology and nanofiller loading on dispersion and capacitor performance will be reported.

9:36AM S42.00009 Theoretical Prediction of Room Temperature Thermal Superconductivity in Single Polythiophene Chains , WEI LV, ASEGUN HENRY, Georgia Inst of Tech — We used molecular dynamics simulations and a new formalism for calculating the nodal contributions to thermal conductivity to study individual polythiophene chains. The simulations suggest that it is possible to achieve divergent/infinite thermal conductivity (e.g., thermal superconductivity) in individual polythiophene chains. The new modal analysis method allowed for exact pinpointing of modes responsible for the anomalous behavior, which turned out to be transverse vibrations in the plane of the aromatic rings at frequencies ~ 0.05 THz. Within the 5 ns of integration time, one mode in particular exhibits a thermal conductivity contribution greater than 100 W m-1 K-1, which is larger than many 3D bulk materials that consist of a large multitude of modes. Further investigation showed that the divergence arises from persistent correlation between the three lowest frequency modes on chains that have exact multiples of 30 unit cells in length. Sonification of the superconducting mode heat fluxes indicated distinct patterned differences between the convergent and divergent simulations, which suggests the phenomena may differ from previous models and a new explanation of the anomalous behavior may be required for polymers.

9:48AM S42.00010 Nonvolatile 1D Photonic Films Composed of Lamellar Forming Block Copolymer/Ionic Liquid , ATSUSHI NORO, YUSUKE TOMITA, YUSHU MATSUSHITA, Nagoya University, JOSEPH WALISH, Massachusetts Institute of Technology, EDWIN THOMAS, Rice University, NAGOYA UNIVERSITY/RICE UNIVERSITY COLLABORATION — Block copolymer photonic films were prepared by infiltrating an ionic liquid (IL) into lamellar-forming polystyrene-b-poly(2-vinylpyridine) (PS-P2VP) block copolymer thin films with approximately 50/50 composition. The nonvolatile nature of IL enabled direct nanostructural observation of the films under the vacuum at room temperature by transmission electron microscopy, which revealed selective swelling of P2VP layers by the IL. Ultra-small-angle X-ray scattering also provided the quantitative nanostructure information of the photonic films, revealing the domain periodicity distance was over 100 nm. In addition to these nanostructural observations, reflectivity spectra of the photonic films were also investigated by a fiber optic spectrophotometer. The wavelength at the peak top of reflected light from the photonic films was found to increase with increasing the molecular weight of block copolymers used for film preparation. Furthermore, tunability of the wavelength was attained by infiltrating the IL into blend thin films of lamellar-forming PS-P2VP block copolymer.

10:00AM S42.00011 DNA in Nanoscale Electronics , JASON SLINKER, MARC MCMILLAN, CHRIS WOHLGAMUTH, The University of Texas at Dallas, ALON GORODETSKY, The University of California-Irvine — Functional nanoelectronics are sought for next generation integrated circuits, but several challenges limit the use of most nanoscale devices on large scales. DNA has great potential for use as a molecular wire due to high yield synthesis, near-unity purification, and nanoscale self-organization. Nonetheless, a thorough understanding of ground state DNA charge transport (CT) under biologically relevant conditions, where the double-helical structure is preserved, is lacking. We measured DNA CT through double-stranded DNA monolayers on gold by assessing 17 base pair bridges at discrete points with redox active probes. This was performed under temperature-controlled and biologically relevant conditions with cyclic and square wave voltammetry, with redox peaks analyzed to assess transfer rate and yield. We demonstrated that the yield of transport is strongly tied to the stability of the duplex, linearly correlating with the melting temperature. Transfer rate was found to be temperature-activated and to follow inverse distance dependence, consistent with a hopping mechanism of transport. These results establish the governing factors of CT speed and yield through DNA for device configurations, guiding subsequent application in nanoscale electronics.

10:12AM S42.00012 DNA-guided nickel ion chain memristive system development and characterization , CHA-CHING CHANG, HSUEH-LIANG CHU, Department of Biological Science and Technology, National Chiao Tung University, WEN-BIN JIAN, YU-CHANG CHEN, Department of Electrophysics, National Chiao Tung University — DNA is a nanowire in nature with multiple high Vbd polymer matrix but usually result in loss of Vbd due to aggregation induced field enhancements. For optimum enhancement of dielectric properties, it is essential to improve matrix-filler interaction and control the dispersion of fillers. To that effect we graft a BCP onto the nanofiller and disperse it within a host BCP with similar composition. Using Directed Self-assembly we fabricate BCP nanostructured films with highly dispersed functionalized nano-fillers that are not only expected to enhance the overall ε, but the well-ordered BCP nanostructures also improve Vbd by providing sharp interfacial barriers acting as charge traps. The impact of filler functionalization, BCP morphology and nanofiller loading on dispersion and capacitor performance will be reported.

10:24AM S42.00013 Bio-inspired peptide nanostructures for organic field-effect transistors , GRANT KNOTTS, Univ of Missouri - Columbia, THIAGO CIPRIANO, Universidade Federal do ABC, AMRIT LAUDARI, Univ of Missouri - Columbia, ROBERTA BIANCHI, WENDEL ALVES, Universidade Federal do ABC, SUCHI GUHA, Univ of Missouri - Columbia — Polymer-based nanoelectronics are used from natural amino acids. However, superior blocking blocks for biocompatible devices as they can be used in a bottom-up process without the need for expensive lithography. A dense nanostructured network of 1,1−diphenylalanine (FF) was synthesized using the solid-vapor phase technique. The formation of the nanostructures and structure-phase relationships were investigated by electron microscopy and Raman scattering. Thin films of 1,1−diphenylalanine micro/nanostructures (FF-MNs) were used as the dielectric layer in pentacene-based field-effect transistors (FETs) and metal-insulator-semiconductor diodes both in bottom-gate and top-gate structures. Bias-stress studies show that FF-MN based pentacene FETs are more resistant to degradation than pentacene FETs using FF thin film (without any nanostructures) as the dielectric layer when both are subjected to sustained electric fields. Furthermore, it is demonstrated that the FF-MNs can be functionalized for detection of enzyme-analyte interactions. This work opens up a novel and facile route towards scalable organic electronics using peptide nanostructures as scaffolding and as a platform for biosensing.

3This work was supported in part by the MOST project (NSC 103-2112-M-009-011-MY3).

4This work was supported through the US National Science Foundation under Grant Nos. IIA-1339011 and ECCS-1305642 as well as CNPq (Brazil) grant no. 400239/2014-0.
10:36AM S42.00014 Residual Stresses and Photoluminescence of Conjugated Polymer Thin Films, YA-WEI YANG, YI CHIEN, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu 300, Taiwan, TSANG-LANG LIN, Department of Engineering Science and Systems, National Tsing Hua University, Hsinchu 300, Taiwan, GUNTER REITER, Institute of Physics and Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, Freiburg, Germany, ARNOLD CHANG-MOU YANG, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu 300, Taiwan — Molecular recoiling forces (residual stress) in ultrathin polymer films (< 100 nm) were engendered by non-equilibrium chain conformations and intermolecular packing frozen from rapid solvent evaporation during film preparation. These forces when acting on conjugated macromolecules were found to contribute to large photoluminescence (PL) enhancements. The packing of the rigid-rod macromolecules into thin solid films, however, was somewhat different from that of flexible chains. As revealed by x-ray reflectivity, although the thicknesses of the solvent-trap layer (~2nm) next to substrate were almost identical, the local density was ~10 times less in MEH-PPV films than in polystyrene (PS) films (20 nm). It indicates that molecular strains induced by solvent evaporation were much smaller of conjugated polymers, hinting smaller residual stresses in the films. Concomitantly, local deformations of rubber substrate under a dewetting polymer film, a good measure of the molecular recoiling forces, were considerably smaller for MEH-PPV films than for PS. The PL dependence on residual stresses of pristine MEH-PPV films hence clearly elucidates the strong molecular stress effect on optoelectronic efficiencies.

10:48AM S42.00015 Polymeric Carbon Dioxide Capture Membranes for Artificial Photosynthesis, DANIEL MILLER, NATHANIEL LYND, Lawrence Berkeley Natl Lab — Production of carbon-rich fuels via artificial photosynthetic processes depends on the continuous availability of a carbon source. In a proposed artificial photosynthetic system, hydrogen and oxygen from solar water splitting are combined with CO$_2$ captured from the atmosphere to produce a liquid fuel such as methanol. Membrane-based processes provide advantages over other gas separation technologies, including mechanical simplicity, a relatively small footprint, and energy efficiency. We describe the synthesis and characterization of polymeric anion exchange materials for CO$_2$ concentration from gas mixtures such as the atmosphere. Transport of CO$_2$ through the membrane is promoted by an opposing flux of water, which reacts with CO$_2$ through equilibrium reactions to form charged species (bicarbonate, carbonate, and hydroxide) within the membrane. CO$_2$ transport will be discussed as a function of membrane material characteristics, including charge density, and process characteristics, including feed stream relative humidity and CO$_2$ concentration on each side of the membrane. The development of several membrane materials will be discussed. Results of experimental gas transport studies will be presented.

Thursday, March 5, 2015 8:00AM - 11:00AM
Session S43 DPOLY: Focus Session: Dynamics of Glassy Polymers Under Confinement I

8:00AM S43.00001 Structural Recovery for a Single Polystyrene Ultrathin Film Using Flash DSC, YUNG P. KOH, SIYANG GAO, SINDEE L. SIMON, Texas Tech University — The kinetic features of the glass transition under nanoconfinement of ultrathin films are studied using nanocalorimetry, with a particular focus on the cooling rate dependence of the glass transition temperature (Tg) and on the time-dependent structural recovery behavior of a 20 nm-thick polystyrene film. Measurements are performed using a commercial rapid-scanning chip calorimeter, the Mettler Toledo Flash differential scanning calorimeter (DSC). The Tg depression of the 20 nm-thick film is found to be a function of cooling rate, decreasing with increasing cooling rate, at high enough cooling rates (e.g., 1000 K/s), Tg is the same as the bulk within the error of the measurements. Structural recovery is performed as a function of aging time and temperature, and the evolution of the fictive temperature is followed. The advantages of the Flash DSC include sufficient sensitivity to measure enthalpy recovery for a single 20 nm-thick film, as well as extension of the measurements to aging temperatures as high as 15 K above nominal Tg and to aging times as short as 0.01 s. The aging behavior will be compared to that for bulk-like single thin films measured by Flash DSC, as well as to the results for stacked ultrathin films measured using conventional DSC.

8:12AM S43.00002 Dynamics of Poly(2-vinylpyridine)/Silica Nanocomposites from Brillouin and Raman Light Scattering, SHIWANG CHENG, ALEXANDER KISLIUK, Chemical Sciences Division, Oak Ridge National Lab, VLADIMIR NOVIKOV, Chemical Sciences Division, Oak Ridge National Lab; Department of Chemistry, University of Tennessee, ADAM P. HOLT, Department of Physics, University of Tennessee, ALEXEI P. SOKOLOV, Chemical Sciences Division, Oak Ridge National Lab; Department of Physics and Astronomy, Department of Chemistry, University of Tennessee — Recent studies show an interfacial layer exists between polymer matrix and nanoparticle surface in polymer nanocomposites (PNCs)[1], which could potentially explain the drastic mechanical enhancement in such materials [2]. Dynamics of this interfacial layer were captured by various techniques, where the typical dynamic range was limited to be below 1 GHz. However, the fast dynamics (above 1 GHz) of the interfacial layer is also important to the application of PNCs under severe conditions. Unfortunately, little work has been done to explore the structure and the dynamics of this layer at high frequencies. In this study, we demonstrated that Brillouin Light Scattering (BLS) can be used to estimate the thickness of the interfacial layer and its mechanical properties. By combining BLS and Raman Scattering, we probed the dynamics in the range from 1 GHz to 5 THz of the Poly(2-vinylpyridine)/Silica nanocomposites with loadings from 5% wt to 52% wt. The various features observed can also be explained in the spirit of the existence of an interfacial layer between the polymer matrix and nanoparticles. [1] Holt, A. P., et al; Macromolecules 2014, 47, 1837-1843. [2] Papon, A. et al; Soft Matter 2012, 8, 4090-4096.

8:24AM S43.00003 Improving Dielectric Breakdown Strength: Physically Aging Amorphous Polymers and Nanocomposites, RICHARD A. VAIA, CHRISTOPHER A. GRABOWSKI, HILMAR KOERNER, United States Air Force Research Laboratory — Processing conditions play a significant role in maximizing the available energy storage density of polymer dielectrics. Trapped solvents and voids act as defect sites that prematurely trigger breakdown and reduce dielectric strength. To address these issues, solvent-cast films are conventionally annealed above the glass transition and under vacuum; however these procedures can yield materials far from thermodynamic equilibrium with substantial free-volume. Here in, we demonstrate improvement in dielectric performance via controlled post-deposition annealing based on their structural relaxation characteristics. Using enthalpy relaxation studies, we quantify how local chain packing evolves in the glass during controlled cooling or physical aging, and how this impacts dielectric breakdown, complex permittivity, and energy storage density for polystyrene, poly(methyl methacrylate), and their related blended and single-component nanocomposites. These process-performance correlations, and their dependence on nanocomposite topology, provide a basis for the rational design of dielectrics for high performance capacitors.
we have recently begun investigating polymer-polymer interfaces where the magnitude of the Tg perturbation at the interface can be readily determined. Such
in systems that exhibit kinetic arrest, i.e. a glass transition. It has been applied to investigate the behavior of sample mobility at and near this transition in
which polymer chains physically adsorb to the substrate when annealed at sufficient temperature. This process, dubbed “irreversible adsorption” has been connected with changes in Tg under confinement.
model system consisting of polystyrene (PS) irreversibly adsorbed on silica. Incorporating fluorescently-labeled PS in a series of single and multi-layer films, we
selectively measure the Tg of adsorbed layers, with and without a free surface, as a function of annealing time. We then further anneal the bilayer films and
measure changes in the Tg of the irreversibly adsorbed layers to investigate chain interpenetration and its implications for the influence of irreversible adsorption on the Tg distribution throughout the film.

8:48AM S43.00005 Influence of the Free Interface on the Glass Transition Temperature of Irreversibly Adsorbed Polystyrene Thin Films. MARY BURROUGHGS, RODNEY PRIESTLEY, Department of Chemical and Biological Engineering, Princeton University — Polymers confined to the nanometer length scale have been shown to exhibit deviations in the glass transition temperature (Tg) from that of the bulk. Confinement effects on Tg have largely been attributed to the combined influences of the free surface and substrate interface. Recent work with polymer thin films has investigated a phenomenon at the substrate interface in which polymer chains physically adsorb to the surface. These studies also show that the deviations from bulk dynamics begin at a particular temperature (T*), providing an explanation for why some studies observe no interfacial effects in ultra-thin polymer films. A puzzling aspect of this work is that computational studies and studies on molecular
structures have largely been attributed to the combined influences of the free surface and substrate interface. Using our Limited Mobility (LM) model, we implement a new kinetic constraint such that the presence of mobility is required to facilitate local density equilibration. The LM model was developed to study dynamic heterogeneity in systems that exhibit kinetic arrest, i.e. a glass transition. It has been applied to investigate the behavior of sample mobility at and near this transition in bulk, buried slab, and supported film systems. Here we aim to probe the competition between kinetic and thermodynamic driving forces in the vicinity of the glass transition in polymer thin films. Here we use fluorescence, a technique capable of probing local dynamics, to study the Tg of a model system consisting of polystyrene (PS) irreversibly adsorbed on silica. Incorporating fluorescently-labeled PS in a series of single and multi-layer films, we selectively measure the Tg of adsorbed layers, with and without a free surface, as a function of annealing time. We then further anneal the bilayer films and measure changes in the Tg of the irreversibly adsorbed layers to investigate chain interpenetration and its implications for the influence of irreversible adsorption on the Tg distribution throughout the film.

9:00AM S43.00006 Modeling Mobility in Glassy Thin Films. JEFFREY DEFELICE, JANE LIPSON, Dartmouth College, NICHOLAS TITTO, Cambridge University, SCOTT MILNER, Pennsylvania State University — In this talk we explore the role of mobility in glassy systems and examine the effect of coupling sample mobility to system equilibration. Using our Limited Mobility (LM) model, we implement a new kinetic constraint such that the presence of mobility is required to facilitate local density equilibration. The LM model was developed to study dynamic heterogeneity in systems that exhibit kinetic arrest, i.e. a glass transition. It has been applied to investigate the behavior of sample mobility at and near this transition in bulk, buried slab, and supported film systems. Here we aim to probe the competition between kinetic and thermodynamic driving forces in the vicinity of the glass transition in polymer thin films. Here we use fluorescence, a technique capable of probing local dynamics, to study the Tg of a model system consisting of polystyrene (PS) irreversibly adsorbed on silica. Incorporating fluorescently-labeled PS in a series of single and multi-layer films, we selectively measure the Tg of adsorbed layers, with and without a free surface, as a function of annealing time. We then further anneal the bilayer films and measure changes in the Tg of the irreversibly adsorbed layers to investigate chain interpenetration and its implications for the influence of irreversible adsorption on the Tg distribution throughout the film.

9:12AM S43.00007 Perturbation of Glassy Dynamics in Thin Polymer Films due to Interfaces. CONNIE B. ROTH, Dept. of Physics, Emory University — Many confinement studies have focused on free-standing polymer films, having been historically billed as the simplest system, containing only two symmetric air-polymer interfaces with no substrate interactions. However, free-standing films have instead exhibited some of the most complex molecular weight (MW)-dependent average film glass transition temperature Tg(h) behavior with decreasing film thickness. We have previously demonstrated that high MW free-standing polystyrene (PS) films can exhibit two distinct transitions in thermal expansion on cooling, with qualitatively different MW dependencies suggesting that two separate mechanisms are acting simultaneously to propagate enhanced mobility from the free surface deeper into the material. To investigate the nature of these transitions, we present physical aging measurements below and in-between these two transitions. How the presence of a free surface alters the Tg in confined systems is complicated by the ill-defined magnitude of the perturbation in local mobility. Thus, we have recently begun investigating polymer-polymer interfaces where the magnitude of the Tg perturbation at the interface can be readily determined. Such studies provide a more well-defined system for investigating the length scales over which such perturbations are propagated, which we believe are associated with the glass transition.

9:48AM S43.00008 A Comparison of Particle Embedment and Nanoindentation: Probing the Surface Properties of Polymeric Materials. MEIYU ZHAI, HEEDONG YOON, GREGORY MCKENNA, Texas Tech Univ — In this work, we report the results from a comparison of viscoelastic surface properties of polymer obtained from two different techniques: the spontaneous particle embedment technique and nanoindentation technique. The surface compliance for polystyrene(PS) and poly(isobutyl methacrylate) (PiBMA) were determined using multi curve fitting method to extract the viscoelastic response from the experimental results. The surface layer rheological properties obtained from particle embedment experiment and indentation are compared both with each other and with the bulk properties. For both materials we observed surface softening when the test temperature is below the macroscopic glass transition temperature. This is followed by a crossover to a surface stiffening region when the test temperature is higher than the macroscopic glass transition temperature. KEYWORDS: nanoindentation, particle embedment, multi curve fitting method, viscoelastic properties

1 National Science Foundation grant No. CHE 1112416 John R. Bradford Endowment at Texas Tech University.

10:00AM S43.00009 Investigating the effect of chain architecture on the dynamics of thin entangled polymer films. ETHAN GLOR, ZAHRA FAKHRRAAI, Univ of Pennsylvania — Recent work in polymer physics shows that the structural relaxation time near a free surface of a thin polystyrene film is significantly different from that of the bulk polymer. This can have a large influence on their properties. For instance, studies have shown that polystyrene thin films exhibit a decreased glass transition temperature as the thickness decreases below 60 nm. A wide range of experimental techniques show that the dynamics at the free surface of polystyrene have a weaker temperature dependence than that of the bulk. Here we use cooling rate dependent Tg measurements (CR-Tg) to show that the dynamics in thin, entangled polystyrene films are directly influenced by the free surface. These studies also show that the deviations from bulk dynamics begin at a particular temperature (T*), providing an explanation for why some studies observe no interfacial effects in ultra-thin polymer films. A puzzling aspect of this work is that computational studies and studies on molecular glasses, which also exhibit enhanced surface dynamics, do not observe T*. We use CR-Tg to study thin films of various polymers to determine 1. If T* is a phenomenon common to all polymer glasses, and 2. If the value of T* is dependent on the chemistry or Tg of the polymer.
10:12AM S43.00010 Dynamic glass transition measurements on nm-thin films of low molecular mass substances using AC chip-nanocalorimetry, MATHIAS AHRENBERG, CHRISTOPH SCHICK, HEIKO HUTH, Institute of Physics, University of Rostock, Germany — We are using AC chip nano-calorimetry for the in-situ investigation of the dynamic glass transition of vapor-deposited thin films of toluene and indomethacin of thicknesses between several hundred nm down to ten nm. With these experiments on low molecular mass substances we complement our data on similar thin polymer films. Firstly, the deposition-related thermodynamic state (stable glass) of each film is erased by transforming them into ordinary glasses. Secondly, upon reheating the thin ordinary glass films a direct comparison of the subsequently measured frequency-dependent dynamic glass transition temperatures becomes possible. The frequency of temperature modulation can be varied from 1 Hz up to about 1000 Hz. Film thicknesses for indomethacin are measured ex-situ with an atomic force microscope directly on the membrane of the chip-sensors. Similar to the thin polymer films no thickness dependence of the dynamic glass transition temperature (main relaxation) is seen. The results are in agreement with the explanation given by Cangialosi et al. 1, 2. M. Ahrenberg et al., The Journal of Chemical Physics, 2013, 138, 024501-024511. 2. H. Huth et al., Eur. Phys. J. Special Topics, 2007, 141, 153-160. 3. S. Napolitano and D. Cangialosi, Macromolecules, 2013, 46, 8051-8053.

10:24AM S43.00011 Why do some diluents alter the magnitude of nanoconfinement effects on the glass transition?1, JAYACHANDRA HARI MANGALARA, NICHOLAS WEINER, MICHAEL MARVIN, DAVID SIMMONS, University of Akron — Polymers subject to nanoconfinement can exhibit large alterations in their glass transition and associated dynamic and mechanical properties. Several studies have indicated that introduction of small-molecule additives can attenuate the magnitude of nanoconfinement effects, offering a potential method of tuning the properties of nanostructured polymers in applications from microelectronics to structural nanocomposites. However, the relationship between additive molecular properties and their effects on nanoconfined glass formation remains poorly understood. A number of studies have implicated changes in the fragility of glass formation in mediating these effects; however, this remains a matter of considerable debate. Here, we report on two sets of simulations of nanoconfined polymer films: one in which we introduce several oligomeric additives with effects ranging from suppression to enhancement of bulk Tg and fragility; one in which we introduce several oligomeric additives with effects ranging from suppression to enhancement of bulk Tg and fragility; one in which we reduce the polymer’s bulk fragility via a simple, additive-free, structural modification. Results provide new insight into the impact of additives on nanoconfined glass formation as well as into the role of fragility in determining nanoconfinement effects.

1This material is based upon work supported by the National Science Foundation under Grant No. DMR1310433.

10:36AM S43.00012 Tuning the Tg-Confinement Effect by Controlling the Amount of Residual Surfactant Present in Emulsion Polymerized Polystyrene Thin Films, LAWRENCE CHEN, JOHN TORKELSON, Northwestern University — The nanoconfinement effect of polystyrene (PS) ultra-thin films supported on silica has been well studied over the past two decades. In order to systematically study the influence surfactants have on the Tg-confinement effect in thin films, PS was synthesized using conventional emulsion polymerization (E-PS) using sodium dodecyl sulfate (SDS) as the surfactant. After rigorous purification, the amount of SDS remaining in the bulk E-PS sample was quantified by using a modified Epton’s Method to be 0.023 wt%. This technique not only allows us to quantitate the amount of surfactant present in bulk polymer but also allows for the fine-tuning of surfactants present in the polymer. We find that a minute amount of surfactant is capable of significantly suppressing the Tg-confinement effect as well as narrowing the Tg breadth in sufficiently thin E-PS films; the magnitude of the Tg-confinement effect is strongly dependent on the amount of residual SDS present. Interestingly, when E-PS films undergo XPS depth profiling we demonstrate that the anionic surfactant preferentially resides at the free surface layer of the film thus eliminating the free surface effect.

10:48AM S43.00013 Homogeneous nucleation of polymers under confinement and its relation to the liquid-to-glass “transition”1, YASUHITO SUZUKI, Max-Planck Institute for Polymer Research, HATICE DURAN, TOBB University of Economics and Technology, MARTIN STEINHART, Universität Osnabrück, HANS-JÜRGEN BUTT, Max-Planck Institute for Polymer Research, GEORGE FLOUDAS, University of Ioannina — The crystallization and local dynamics of model semi-crystalline polymers confined to self-ordered nanoporous alumina (AAO) were studied as a function of pore size, molecular weight and cooling/heating rate by differential scanning calorimetry, wide-angle X-ray diffraction and dielectric spectroscopy. In contrast to the bulk, polymers located inside nanoporous alumina crystallize via distinct nucleation mechanisms. Under confinement, the usual heterogeneous nucleation of bulk polymers is suppressed. Instead, within the smaller pores polymer crystallization is initiated via homogeneous nucleation. We provide the phase diagram of crystallizable polymers under confinement. We find that homogeneous nucleation is strongly coupled to the local viscosity and hence to the liquid-to-glass “transition.” Dielectric spectroscopy revealed that confinement affects both the distribution of relaxation times (much broader under confinement) and the rate of segmental motion (faster dynamics under confinement).

Thursday, March 5, 2015 8:00AM - 11:00AM – Session S44 GSNP GSOFT: Focus Session: Granular Materials and Continuum Descriptions of Discrete Media I

8:00AM S44.00001 Giant drag reduction due to interstitial air in sand, DEVARAJ VAN DER MEER, University of Twente, TESS HOMAN, Laboratoire de Physique, ENS Lyon, France — When an object impacts onto a bed of very loose, fine sand, the drag it experiences depends on the ambient pressure in a surprising way: Drag is found to increase significantly with decreasing pressure. We use a modified penetrometer experiment to investigate this effect and directly measure the drag on a sphere as a function of both velocity and pressure. We observe a drag reduction of over 90% and trace this effect back to the presence of air in the pores between the sand grains. Finally, we construct a model based on the modification of grain-grain interactions that is in full quantitative agreement with the experiments.

8:12AM S44.00002 Scattering of a legged robot in a heterogeneous granular terrain1, FEIFEI QIAN, DANIEL GOLDMAN, Georgia Institute of Technology — Many granular substrates are composed of particulates of varying size, from fine sand to pebbles and boulders. Ambulatory locomotion on such heterogeneous substrates is complicated in part due to fluctuations introduced by heterogeneities. To discover principles of movement in such substrates, we developed an automated system, the “Systematic Creation of Arbitrary Terrain and Testing of Exploratory Robots” (SCATTER), to create heterogeneous granular substrates of varying properties such as compaction, inclination, obstacle shape/size/distribution and obstacle mobility within the substrate. We investigate how the presence of a single “boulder” affects the locomotion of a 6-legged robot (15cm, 150g). The robot’s trajectory is straight before boulder interaction, and is scattered to an angle after the interaction. Surprisingly, the interactions with the boulder can lead to both negative and positive scattering angles—an effective attraction and repulsion between the robot and the boulder. The scattering pattern depends sensitively on the leg-boulder contact position and the boulder mobility within the fine sand. However, the scattering pattern dependence upon contact position on the boulder is insensitive to boulder shape (created using 3D printing), orientation and roughness.

1This work is funded by DARPA Young Faculty Award and Army Research Laboratory (ARL)
8:24AM S44.00003 Stability of an isolated granular band in a rotating tumbler, PAUL B. UMBANHOWAR, DARIUS WHEELER, JULIO M. OTTINO, RICHARD M. LUEPTOW, Northwestern University — Granular mixtures tend to segregate into axial bands when tumbling in long, horizontal cylinders. To better understand this phenomenon we experimented and computationally studied the stability of a single band of large spherical particles initially located between two regions of small spherical particles. Unlike previous work with bidisperse particles, where the band spread axially in a diffusive-like fashion, we found that a single band can stabilize to a constant width much smaller than the cylinder length depending on the size ratio of large to small particles, R_c, and the fill fraction of the tumbler, f. Stable bands were observed for $f < 0.3$ and $1.3 < R_c < 2.5$; for $R_c$ outside this interval and $f > 0.3$, bands were unstable and grew diffusively. For $R_c < 1.3$ large particles diffuse axially in the flowing layer, while for $R_c > 2.3$ axial motion of large particles occurs mainly at the intersection of the downstream terminus of the flowing layer and the cylinder wall. Lastly, band stability was independent of initial band width for the range we tested (4-40 mm). We discuss possible band stabilization mechanisms in light of these observations.

8:36AM S44.00004 The cause of coarsening, MATTHIAS SCHROETER, MPIDS Goettingen, TILO FINGER, RALF STANARIUS, Universitaet Magdeburg — The coarsening process of bands of smaller grains in a horizontally rotated cylindrical drum is a counterintuitive process. Our X-ray tomography results point to an effective surface tension as the driving mechanism. Additionally, we report on a novel microsegregation phenomenon.

8:48AM S44.00005 Analysis of inter-event times for avalanches on a conical bead pile with cohesion, SUSAN LEHMAN, NATHAN JOHNSON, CATHERINE TIEMAN, ELLIOT WAINWRIGHT, Department of Physics, College of Wooster, Wooster, OH — We investigate the critical behavior of a 3D conical bead pile built from uniform 3 mm steel spheres. Beads are added to the pile by dropping them onto the apex one at a time; avalanches are measured through changes in pile mass. We investigate the dynamic response of the pile by recording avalanches from the pile over tens of thousands of bead drops. We have previously shown that the avalanche size distribution follows a power law for beads dropped onto the pile apex from a low drop height. We are now tuning the critical behavior of the system by adding cohesion from a uniform magnetic field and find an increase in both size and number for very large avalanches and decreases in the mid-size avalanches. The resulting bump in the avalanche distribution moves to larger avalanche size as the cohesion in the system is increased. We compare the experimental inter-event time distribution to both the Brownian passage-time and Weibull distributions, and observe a shift from the Weibull to Brownian passage-time as we raise the threshold from measuring time between events of all sizes to time between only the largest system-spanning events. These results are both consistent with those from a mean-field model of slip avalanches in a shear system [Dahmen, Nat Phys 7, 554 (2011)].

9:00AM S44.00006 Ultra-fast parallel magnetic resonance imaging of granular systems, ALEXANDER PENN, Laboratory for Energy Science and Engineering, ETH Zurich and Institute for Biomedical Engineering, University and ETH Zurich, KLAAS P. PRUESSMANN, Institute for Biomedical Engineering, University and ETH Zurich, CHRISTOPH MULLER, Laboratory for Energy Science and Engineering, ETH Zurich — Several non-intrusive techniques have been applied to probe the dynamics of two-phase granular systems, with the most prominent examples being X-ray tomography, positron emission particle tracking (PEPT), electrical capacitance tomography and magnetic resonance imaging (MRI). MRI comes with the particular advantage that by implementing suitable pulse sequences not only spin densities (i.e. voidage), but also velocity, acceleration, diffusion and chemical reactions can be measured. However, so far the investigation of two-phase granular systems has been performed on relatively small-bore systems (max. diameter 60 mm). Such systems are, however, heavily influenced by wall effects. Furthermore, largely only single-coil detection has been employed, limiting severely the temporal resolution of the data acquisition. Here, we report the acquisition of ultra-fast MRI measurements in large volume vessels using medical MRI scanners. Specifically, parallel MRI, i.e. the simultaneous use of multiple receiver coils, has been exploited to speed up the data acquisition. In combination with advanced pulse sequences, we were able to probe the rapid dynamics (voidage and velocity measurements) of gas-solid systems.

9:12AM S44.00007 3D imaging of particle-scale rotational motion in granular flows, MATT HARINGTON, MICHAEL LIN, WOLFGANG LOSERT, University of Maryland — In current granular research, many strides have been made in the characterization of three-dimensional motion and structure through the use of novel imaging techniques. In the context of measuring individual motion of spherical grains, these techniques tend to be limited to translational motion. While this is often sufficient, it neglects the rotational motion that can arise from torques that grains exert on each other, and that potentially propagate across mesososcopic structures. This has left a gap that prevents researchers from fully characterizing the behavior of real granular flows. In particular, the role of individual rotational motion has not been fully explored in the context of bulk processes such as shear-banding, segregation, and irreversibility. In our current work, the Refractive Index Matched Scanning technique is expanded to extract the orientation of near-spherical grains in a quasistatic shear flow. Particle tracking is then applied to directly measure the rotational motion of individual grains. In an initial study, the presence of rolling modes in the shear band of a circular shear cell has been confirmed. From here, we are extending the method further to determine the role of collective rotations within and across neighborhoods.

9:24AM S44.00008 Simulation of granular flows through their many phases, SACHITH DUNATUNGA, Massachusetts Inst of Tech-MIT — The material point method (MPM) is combined with a constitutive model which allows material to traverse through its many common phases during the flow process. When dense, the material is treated as a pressure sensitive elasto-viscoplastic solid obeying a yield criterion and a plastic flow rule given by the $\mu(t)$ inertial rheology of granular materials. When the free volume exceeds a critical level, the material is deemed to separate and is treated as disconnected, stress-free media. By using the MPM framework, extremely large strains and nonlinear deformations such as those common to granular flows can be represented. The method has been shown to replicate results such as Beveloo scaling in silo discharge, as well as the Bagnold profile on an inclined plane.

9:36AM S44.00009 Modeling granular inclined plane flow phenomena with Nonlocal Granular Fluidity, KEN KAMRIN, MIT, DAVID HENANN, Brown University — The continuum theory of Nonlocal Granular Fluidity (NGF) has previously been shown to predict steady granular flow fields in many different geometries, including those such as split-bottom cells, which have been historically resistant to continuum modeling. Central to NGF is a direct inclusion of a particle length-scale, which renders the rheology nonlocal, capturing the cooperatively of granular motion. In this talk we describe how the model also captures the behaviors observed in granular inclined plane flows. We show that the model predicts a quantitatively accurate “stopping curve” which indicates the conditions that determine when a flowing layer comes to a stop, which depends explicitly on the thickness of the layer. We also explore other known phenomena in this geometry, such as the dependence of the flow profile on layer thickness, the collapse of the Froude number as a function of thickness vs the stopping height, and the possibility of modeling both starting and stopping curves within the same model.

9:48AM S44.00010 Flow Profiles and Fluctuations Measured for Granular Flow in a Vertical Channel, DONALD CANDELA, KEVIN FACTO, Univ of Mass - Amherst — The average velocity profiles and the velocity fluctuations were measured for flows of a dense granular medium (corn poppy seeds) through a long vertical channel, using NMR. The flow profiles seem to be in good agreement with non-local constitutive laws that have been proposed. In particular, there is a shear band near the channel wall with width that is independent of the flow rate. However, the measured velocity fluctuations do not agree with expectations from a simple interpretation of the underpinnings of the non-local rheology. For example, there are large fluctuations in the velocity of the central portion of the flow, away from the walls. This apparent discrepancy may be due to the absence of constant-pressure boundary conditions in granular flow through a fixed-size channel.

1Supported by NSF Grant CBET-0651397
10:00AM S44.00011 High speed impacts on a granular material\(^1\) — YUE ZHANG, Duke University, ABRAHAM CLARK, Yale University, LOU KONDIC, NJIT, BOB BEHRINGER, Duke University — When an object strikes a granular material, its momentum and energy are transferred to the grains and dissipated. When the ratio of the intruder speed, \(v_0\), to a typical granular sound speed, \(c\), is small, this energy transfer is intermittent along force-chain-like structures, leading to an inertial drag term proportional to the square of the intruder speed. However, many natural and industrial examples of granular impact occur much closer to \(M' \equiv v_0/c \sim 1\), a regime which is difficult to reach in a lab setting using many common granular materials. To address this, we perform experiments (and matching simulations) with granular materials comprised of photoelastic disks of varying stiffness (and thus, varying \(c\)), in order to probe regimes closer to \(M' \sim 1\). As \(M'\) increases, the inertial drag law fails and the material begins to behave more elastically, with a shock-like front propagating away at impact. This causes the penetration depth to be greatly reduced, and in extreme cases, the intruder can rebound temporarily. We understand this transition to damped, elastic-like behavior by comparing the grain-grain collision time to the time for the intruder to move one grain diameter.

\(^1\)Supported by DTRA grant HDTRA1-10-1-0021, NASA grant NNX10AU01G, and NSF grant DMR1206351

10:12AM S44.00012 Avalanches, and evolution of stress and fabric for a cyclically sheared granular material\(^1\) — DENGMING WANG, Lanzhou University, JONATHAN BARES, DONG WANG, BOB BEHRINGER, Duke University — Granular materials yield for large enough shear stress, leading to avalanches. We seek to understand the relation between macroscopic avalanches and the microscopic granular structure. We present an experimental study of a 2D granular material subjected to cyclic pure shear, which we visualized by a photo-elastic technique. We start from a stress-free sample of frictional particles in the shear-jamming regime \((\phi_s \leq \phi < \phi_j)\). We apply multiple cycles of pure shear: shear in one direction, followed by a reversal to the original boundary configuration. The strain is made in small quasi-static steps: after each small step, we obtain polarized and unpolarized images yielding particle-scale samples and locations. Statistical measures of the avalanches are in reasonable agreement with recent mean-field avalanche models by Dahmen et al. (Nature Physics 7, 554 (2011)) The system structure evolves slowly to reduce the stress at the extremum of strain, similar to the relaxation observed by Ren et al. (Phys. Rev. Lett. 110, 018302 (2013)) in a simple shear experiment. To understand how this relaxation occurs, we track the stress and fabric tensors and measures of the strain field over many cycles of shear.

\(^1\)Supported by NASA grant NNX10AU01G, and NSF grants DMR1206351 and DMS1248071

10:24AM S44.00013 Statistics from granular stick-slip experiment\(^1\) — AGHIL ABED ZADEH, JONATHAN BARENT, ROBERT BEHRINGER, Duke Univ — We carry out experiments to characterize stick-slip for granular materials. In our experiment, a constant speed stage pulls a slider which rests on a vertical bed of circular photoelastic particles in a 2D system. The stage is connected to the slider by a spring. We measure the force on the spring as well as the slider’s acceleration by a force sensor attached to the spring and accelerometers on the slider. The distributions of energy release and time duration of avalanches during slip obey power laws. We apply a novel event recognition approach using wavelets to extract the avalanche properties. We compare statistics from the wavelet approach with those obtained by typical methods, to show how noise can change the distribution of events. We analyze the power spectrum of various quantities to understand the effect of the loading speed and of the spring stiffness on the statistical behavior of the system. Finally, from a more local point of view and by using a high speed camera and the photoelastic properties of our particles, we characterize the internal granular structure during avalanches.

\(^1\)This work is supported by NSF Grant DMR1206351 and NASA grant NNX10AU01G

10:36AM S44.00014 Force network in a three-dimensional sheared material , NICOLAS BRODU, INRIA Bordeaux, JONATHAN BARES, Duke University, JOSHUA DIJKSMAN, Wageningen UR, ROBERT BEHRINGER, Duke University — Force chains in 2D granular material have been widely studied over the past decade. However the force network evolution when a 3D granular medium is sheared remains poorly understood due to the complexity of experimental observations. We present an experimental set-up to measure interparticle forces in the case of the quasi-static deformation of a 3D sphere packing subjected to shear and compression. We perform these experiments on slightly polydispersed and los-friction soft hydrogel spheres. We measure the microscopic force network in a this three dimensional packing through imaging the entire packing at each loading steps. By resolving particle deformations via custom image analysis software, we extract all particle contacts and contact forces with a very good accuracy. We address the rising up of the Reynolds pressure from the microscopic force network and a statistical ensemble analogous to equilibrium counterpart for 3D frictionless particles.

10:48AM S44.00015 Granular dynamics under shear with deformable boundaries , DREW GELLER, SCOTT BACKHAUS, ROBERT ECKE, Los Alamos National Laboratory — Granular materials under shear develop complex patterns of stress as the result of granular positional rearrangements under an applied load. We consider the simple planar shear of a quasi-two-dimensional granular material consisting of bi-dispersed nylon cylinders confined between deformable boundaries. The aspect ratio of the gap width to total system length is 50, and the ratio of particle diameter to gap width is about 10. This system, designed to model a long earthquake fault with long range elastic coupling through the plates, is an interesting model system for understanding effective granular friction because it essentially self tunes to the jamming condition owing to the hardness of the grains relative to that of the boundary material, a ratio of more than 1000 in elastic moduli. We measure the differential strain displacements of the plates, the inhomogeneous stress distribution in the plates, the positions and angular orientations of the individual grains, and the shear force, all as functions of the applied normal stress. There is significant stick-slip motion in this system that we quantify through our quantitative measurements of both the boundary and the grain motion, resulting in a good characterization of this sheared 2D hard sphere system.

Thursday, March 5, 2015 8:00AM - 10:48AM –
Session S45 DPOLY: Focus Session: Polymer Nanocomposites: Dynamics 216AB - Laura Clarke, North Carolina State University

8:00AM S45.00001 Dynamics in Polymer Nanocomposites\(^1\) — NIGEL CLARKE, University of Sheffield — Since nanoparticles are increasingly being added to polymers to impart mechanical and functional properties, we are exploring how nanoparticles impact polymer dynamics with a focus on the diffusion coefficients. In high molecular weight polymer melts, chain diffusion is well described by the reptation model. Motion proceeds as a snake-like diffusion of the chain as a whole, along the contour of a tube that mimics the role of physical entanglements, or topological constraints, with other chains. In polymer nanocomposites there are additional constraints due to the dispersed nanoparticles in the polymer matrix. Chain motion can be altered by nanoparticle size, shape, aspect ratio, surface area, loading and the nature of the interactions between the nanoparticles and the polymer matrix. We have observed a minimum in the diffusion coefficient as a function of nanoparticle concentration when the nanoparticles are rod-like and a collapse of the diffusion coefficient onto a master curve when the nanoparticles are spherical. We are simulating the dynamics using molecular and dissipative particle simulations in order to provide physical insight into the local structure and dynamics, and have also carried out highly coarse grained Monte Carlo simulations of entangled polymers to explore how reptation is affected by the presence of larger scale obstacles.

\(^1\)We acknowledge support from the NSF/EPSRC Materials World Network Program
8:36AM S45.00002 Determination of the Tracer Diffusion Coefficient of Soft Polystyrene Nanoparticles using Neutron Reflectivity. ADAM IMEL, BRAD MILLER, University of Tennessee-Knoxville, WADE HOLLEY, Oak Ridge National Laboratory, DURAIJAI BASKARAN, JIMMY MAYS, MARK DADMUN, University of Tennessee-Knoxville — The diffusion properties of nanoparticles in polymer nanocomposites are largely unknown and depend intimately on the dispersion of the nanoparticles. We examine the diffusion of soft, organic nanoparticles, which disperse in a polymer matrix due to the interpenetration of polymer chains and particles and the reduction in the depletion entropy in the system. The impact of the presence of soft nanoparticles on the diffusion coefficient of polystyrene chains has recently been determined with neutron reflectivity. This was completed by monitoring the interdiffusion of deuterated and protonated polystyrene nanocomposite bilayers with and without the soft nanoparticles dispersed throughout both layers and extracting the diffusion coefficient from the one-dimensional solution to Fick’s second law of diffusion. In this work, we extend this method to bilayer systems with only the soft nanoparticles as one of the layers and a linear deuterated polystyrene as an adjacent layer. The development of this method allows us to determine the tracer diffusion coefficient of the soft polystyrene nanoparticles for the first time by analyzing the mutual diffusion coefficient from Fick’s second law and the fast and slow modes theories for diffusion.

8:48AM S45.00003 Viscosity of Polymer Nanocomposite with Athermal Hairy Nanoparticles. FEI CHEN, OPHELIA TSUI, Boston Univ — We studied the zero shear viscosity of polymer nanocomposites (PNC) containing silica nanoparticles grafted with polystyrene ligands blended with polystyrene homopolymer. As the ratio of the molecular weight of the homopolymer, P, to that of the ligands, N, was increased from about 0.01, we observed a transition from viscosity enforcement to viscosity reduction near P/N = 1. Interestingly, many of the samples exhibiting viscosity reduction have the dry diameter of the particles exceeding the radius of gyration of the homopolymer (i.e., 2r > Rg), making them exceptional cases according to the viscosity phase diagram published by Kalathi et al. (Phys. Rev. Lett. 109, 198301 (2012)). We discuss whether hydrodynamic effect and plasticizer effect might have caused our observations.

9:00AM S45.00004 Probing the interfacial region in polymer-graphene oxide nanocomposites. MICHAEL WEIR, Department of Physics and Astronomy, University of Sheffield, STEPHEN BOOTHROYD, DAVID JOHNSON, RICHARD THOMPSON, Durham University, NIGEL CLARKE, University of Sheffield, KARL COLEMAN, Durham University — Graphene and related two-dimensional materials are excellent candidates as filler materials in nanocomposites due to their extraordinary physical properties and high aspect ratio. We are studying graphene oxide (GO), a highly functionalized form of graphene, due to its relative ease of dispersion within polymer matrices. Interruptions to the pristine two-dimensional carbon network by oxygen-containing groups, which provide functionality, also make GO rather flexible. In this paper we show that GO is wrinkled and rough over a hierarchy of length scales from a few nanometers to a few microns, when it is incorporated in composites with poly(methyl methacrylate) (PMMA) and polystyrene (PS). Small-angle neutron scattering measurements, highlighting individual polymer chains, show a decrease in polymer radius of gyration with increasing GO concentration in PMMA/GO nanocomposites. The decrease is consistent with models of a solid interface in a polymer melt. The interface influences the polymer matrix within an interface volume stretching on the order of one polymer radius of gyration from the surface. This work is a direct measurement of the effect of the nanofiller upon the polymer matrix and progresses our understanding of interfacial interactions within nanocomposites.

9:12AM S45.00005 Polymer dynamics in PMMA-carbon nanocomposites. RANA ASHKAR, University of Maryland-College Park/NIST, MANSOUR ABDULBAKI, University of Houston, CHRISTOPHER BERTRAND, MADHUSUDAN TYAGI, ANTONIO FARAONE, PAUL BUTLER, National Institute of Standards and Technology, RAMANAN KRISHNAMOORTI, University of Houston — Particle-polymer interactions in nanocomposites can lead to significant heterogeneities in the polymer dynamics and remarkably impact the material properties. While dynamical perturbations are expected to be limited to interfacial polymer segments, for nanoparticle concentrations above percolation, however, the interfacial regions overlap. The impact of interfacial-polymer network results in a complex relaxation behavior of the polymer, that is unanticipated from dilute nanoparticle dispersions in polymer matrices. Neutron spectroscopy on C60 and SWNT composites reveals that dynamical perturbations can extend to non-interfacial polymer segments and significantly influence their local mobility and their meso-scale cooperative relaxations. In this case of attractive particle-particle interactions, a gradual decrease in the polymer mean-square displacement is observed with increasing nanoparticle loadings below the percolation threshold. However, once the nanoparticles are percolated – be it C60 or SWNT – the mean-square displacement seizes to change with increasing loading, indicating kinetic arrest of the polymer. Interestingly, upon percolation, the composites experience an order of magnitude slowdown in the structural relaxations relative to the pure matrix.

9:24AM S45.00006 Macromolecular Diffusion in Dynamic Polymer Nanocomposite1. CHIA-CHUN LIN, MATTEO CARNELLO, University of Pennsylvania, NIGEL CLARKE, University of Sheffield, KAREN WINNEY, RUSSELL COMPSTO, University of Pennsylvania — We consider diffusion of tracer particles in the presence of mobile nanoparticles in polymer nanocomposites (PNCs). These nanoparticles are mobile on the time scale of polymer dynamics and have dimensions less than the entanglement mesh size (i.e., tube diameter). The PNC consists of titanium dioxide nanorods (NR, diameter=4.5nm; length=30.1nm) grafted with phenyl groups uniformly dispersed in a polystyrene (P=650kg/mol; tube diameter=8nm) matrix up to 10 volume percent. Three deuterated polystyrenes (dPS; M=800, 1800 and 3200 kg/mol) are chosen because their diffusion relative to NR allows for investigating fixed and mobile NR by simply changing M. For all M, the reduced tracer diffusivities are observed to decrease monotonically as NR loading increases. However, the reduced diffusion of dPS (3200 kg/mol) is faster than expected compared to the fixed NR case. These findings suggest that mobile NR do not effectively slow down tracer diffusion relative to fixed particles. To test this hypothesis, dPS diffusion is investigated in a high molecular weight matrix PS (2000 kg/mol) in order to slow down NR diffusion relative to dPS (3200 kg/mol). New models are needed to incorporate these mobility dependent entanglements into a comprehensive understanding of dynamics in PNCs.

1Primary fundings: NSF/EPSRC Materials World Network DMR-1210379 (KIW, RJC) and EP/5065373/1 (NC). Support also by the NSF/MRSEC-DMR-11-20001, and Polymer Programs DMR 09-07493

9:36AM S45.00007 Dynamics of Brush-grafted Nanoparticles in Polymer Melts1. RUSSELL COMPSTO, CHIA-CHUN LIN, Univ of Pennsylvania, KOHJI OHNO, Kyoto University, MICHAEL HORE, Case Western Reserve University, JEFFREY METH, Central Research & Development, DuPont Co., NIGEL CLARKE, Univ of Sheffield, KAREN WINNEY, Univ of Pennsylvania — Grafting a polymer brush to organic nanoparticles, which dispers in a polymer matrix due to the interpenetration of polymer chains and particles and the reduction in the depletion entropy in the system. The impact of the presence of soft nanoparticles on the diffusion coefficient of polystyrene chains has recently been determined with neutron reflectivity. This was completed by monitoring the interdiffusion of deuterated and protonated polystyrene nanocomposite bilayers with and without the soft nanoparticles dispersed throughout both layers and extracting the diffusion coefficient from the one-dimensional solution to Fick’s second law of diffusion. In this work, we extend this method to bilayer systems with only the soft nanoparticles as one of the layers and a linear deuterated polystyrene as an adjacent layer. The development of this method allows us to determine the tracer diffusion coefficient of the soft polystyrene nanoparticles for the first time by analyzing the mutual diffusion coefficient from Fick’s second law and the fast and slow modes theories for diffusion.

1Primary supports from NSF/EPSRC Materials World Network DMR 1210379 (KIW, RJC) and EP/5065373/1 (NC)
of Pennsylvania — The tracer diffusion of deuterated polystyrene (dPS; DuPont Nanocomposite Technologies, Central Research & Development, RUSSELL COMPOSTO, Department of Materials Science and Engineering, University of Pennsylvania, ADAM HOLT, Department of Physics and Astronomy, University of Tennessee, Knoxville, SHIWANG CHENG, Department of Materials Science and Engineering, Chungnam National University, NIGEL CLARKE, Department of Physics and Engineering, The University of Sheffield, KAREN WINEY, Department of Materials Science and Engineering, University of Pennsylvania, JEFFREY METH, DuPont Nanocomposite Technologies, Central Research & Development, RUSSELL COMPOSTO, Department of Materials Science and Engineering, University of Pennsylvania — The tracer diffusion of deuterated polystyrene (dPS; $M_n = 23 - 1866$ kg/mol) with a thickness (l) is measured diffusing away from hydroxyl-terminated, phenyl-terminated, and PS-grafted silicon substrates. For a hydroxyl-functionalized substrate, short polymer chains ($M_n < 23$ and 49 kg/mol; $l > >> R_g$) exhibit a diffusion coefficient that is comparable to bulk PS, whereas long polymer chains ($M_n = 532$ and 1866 kg/mol; $l < R_g$) are significantly slower than the bulk case. This slowing down is consistent with the observation by Zheng et al. [1]. In particular, bimodal diffusion coefficient was observed for intermediate molecular weight ($M_n = 168$ kg/mol; $l \sim R_g$). For phenyl-functionalized and PS-grafted substrates, no significant differences in the diffusion coefficients are observed although long polymer chains showed a moderate slowing down. These experiments demonstrate that the polymer diffusion of thin, confined films ($\sim R_g$) away from the substrate is determined by the friction due to surface-monomer contacts, and is sensitive to the chemical state of the substrate, providing a new insight into the role of the interfacial interactions on polymer dynamics.


10:00AM S45.00009 Role of the Interfacial Interactions from an Adjacent Wall on Polymer Diffusion . JIHOON CHOI, Department of Materials Science and Engineering, Chungnam National University, NIGEL CLARKE, Department of Physics and Astronomy, The University of Sheffield, KAREN WINEY, Department of Materials Science and Engineering, University of Pennsylvania, JEFFREY METH, DuPont Nanocomposite Technologies, Central Research & Development, RUSSELL COMPOSTO, Department of Materials Science and Engineering, University of Pennsylvania — The tracer diffusion of deuterated polystyrene (dPS; $M_n = 23 - 1866$ kg/mol) with a thickness (l) is measured diffusing away from hydroxyl-terminated, phenyl-terminated, and PS-grafted silicon substrates. For a hydroxyl-functionalized substrate, short polymer chains ($M_n = 23$ and 49 kg/mol; $l > >> R_g$) exhibit a diffusion coefficient that is comparable to bulk PS, whereas long polymer chains ($M_n = 532$ and 1866 kg/mol; $l < R_g$) are significantly slower than the bulk case. This slowing down is consistent with the observation by Zheng et al. [1]. In particular, bimodal diffusion coefficient was observed for intermediate molecular weight ($M_n = 168$ kg/mol; $l \sim R_g$). For phenyl-functionalized and PS-grafted substrates, no significant differences in the diffusion coefficients are observed although long polymer chains showed a moderate slowing down. These experiments demonstrate that the polymer diffusion of thin, confined films ($\sim R_g$) away from the substrate is determined by the friction due to surface-monomer contacts, and is sensitive to the chemical state of the substrate, providing a new insight into the role of the interfacial interactions on polymer dynamics.

10:12AM S45.00010 Length-Scale Dependent Viscosity in Semidilute Polyelectrolyte Solutions . RYAN POLING-SKUTVIK, RAMANAN KRISHNAMOORTI, JACINTA CONRAD, Univ of Houston — Using optical microscopy and particle tracking algorithms, we measured the mean-squared displacements (MSDs) of fluorescent polystyrene particles with diameters ranging from 300 nm to 2 μm suspended in semidilute solutions of high molecular weight partially hydrolyzed polyacrylamide. The solutions had polymer concentrations ranging from 0.67 to 67%, where $c^*$ is the overlap concentration, and estimated correlation lengths of $\sim 100$ to 900 nm. At short times, the particles exhibited subdiffusive behavior characterized by MSD $\sim t^\alpha$ with $\alpha < 1$. On long time scales, the particles transitioned to Fickian diffusion ($\alpha = 1$) and their diffusivity was calculated from the slope of the MSD. Whereas the large particles agreed with predictions using the Stokes-Einstein equation and bulk zero-shear viscosity, the smaller particles diffused much faster than predicted. The relative diffusivities do not collapse onto a single curve, but rather form a continuum that varies with particle size. This indicates that the particles experience a size-dependent effective viscosity mediated by the ratio of particle diameter to characteristic length scales in the polymer solution.

10:24AM S45.00011 Temperature Dependence of Rheology and Polymer Diffusion in Silica/Poly styrene Nanocomposites1, WEI-SHAO TUNG, University of Pennsylvania, NIGEL CLARKE, University of Sheffield, RUSSELL COMPOSTO, University of Pennsylvania, JEFFREY METH, DuPont Nanocomposite Technologies and DuPont Central Corporate Analytical Services, KAREN WINEY, University of Pennsylvania — Temperature-time superposition using the WLF equation is well-established for both the zero shear viscosity and the polymer diffusion coefficient in homopolymer melts. This talk will present the temperature-dependence of polymer dynamics in polymer nanocomposites comprised of polystyrene and phenyl-capped silica nanoparticles (0 – 50 vol%). The WLF equation fits the temperature dependence of the tracer polymer diffusion coefficient and the fitting parameter (B/fo) decreases smoothly with nanoparticle concentration suggesting an increase in the thermal expansion coefficient for the free volume. The WLF equation also fits the temperature dependence of the zero shear viscosity from oscillatory shear experiments, although the fitting parameter (B/fo) increases substantially with nanoparticle concentration. This discrepancy between the diffusion and rheology will be discussed with respect to the reptation model, which predicts that the temperature dependence of polymer diffusion depends predominately on the temperature dependence of local viscosity, and the elastic response in nanocomposites.

1National Science Foundation DMR-12-10379

10:36AM S45.00012 Anomalous Drag Reduction and Hydrodynamic Interactions of Nanoparticles in Polymer Nanocomposite Thin Films . JAYDEEP BASU, NAIFASA BEGAM, Department of Physics, Indian Institute of Science, Bangalore, India, SIVASURENDER CHANDRAN, Department of Physics, Albert Ludwigs University of Freiburg, Germany, MICHAEL SPRUNG, PETRA-III, DESY, Germany — One of the central dogma of fluid physics is the no-slip boundary condition whose validity has come under intense scrutiny, especially in the fields of micro and nanofluidics. Although various studies show the violation of the no-slip condition its effect on flow of colloidal particles in viscous media has been rarely explored. Here we report unusually large reduction of effective drag experienced by polymer grafted nanoparticles moving through a highly viscous film of polymer, well above its glass transition temperature. The extent of drag reduction increases with decreasing temperature and polymer film thickness. We also observe apparent divergence of the wave vector dependent hydrodynamic interaction function of these nanoparticles with an anomalous power law exponent of $\sim 2$ at the lowest temperatures and film thickness. Such strong hydrodynamic interactions are not expected in polymer melts where these interactions are known to grow with increasing polymer molecular weight (MW). Our measurements reveal an opposite trend: the magnitude of the effect on segmental dynamics decreases with increasing MW. Based on detailed analysis of dielectric spectroscopy and small angle x-ray scattering measurements we provide a qualitative explanation of the unexpected observation.

Thursday, March 5, 2015 8:00AM - 11:00AM — Session S46 GMAG GQI: Invited Session: Hybrid Spin-Strained Systems in Diamond 217A - Sunil Bhave, Cornell University
8:00AM S46.00001 Coherent control over diamond nitrogen-vacancy center spins with a mechanical resonator\(^1\), GREGORY FUCHS, Cornell University — We demonstrate coherent Rabi oscillations of diamond nitrogen-vacancy (NV) center spins driven directly by a mechanical resonator without mediation by a magnetic driving field. Using a bulk-mode acoustic resonator fabricated from single crystal diamond, we exert non-axial ac stress on NV centers positioned at an antinode of a gigahertz frequency mechanical mode. When the \( \Delta m_j \approx -1 \) to +1 spin state splitting energy is tuned into resonance with a driven mechanical mode, we observe \( \Delta m_j = \pm 2 \) spin transitions, which are forbidden by the magnetic dipole selection rule. To rule out stray electric and magnetic fields as the origin of these spin transitions, we study the spin signal as a function depth within the diamond resonator. We find that the spin signal reproduces the periodicity of the acoustic standing wave, confirming the mechanical origin of the observed spin resonance \(^1\). Using single-crystal diamond mechanical resonators with \( fQ \) products of \( 2 \times 10^{12} \), we observe coherent mechanically driven Rabi oscillations up to 4 MHz. \(^2\) For ensembles of NV centers coupled to the resonator, we analyze Rabi oscillations and their dephasing with a combination of spatially inhomogeneous mechanical driving and fluctuating magnetic fields from a noisy spin environment. Additionally, we examine the coherence of mechanically controlled NV center qubits and compare it to the coherence of magnetically controlled spin qubits in the NV center ground state spin manifold. This work demonstrates direct and coherent coupling between NV center spins and resonator phonons, which has potential for NV-based metrology using hybrid spin-mechanical sensors, fundamental research into spin-phonon interactions at the nanoscale, and as a platform for hybrid spin-mechanical quantum systems. \(^1\) E. R. MacQuarrie et al., Phys. Rev. Lett. 111, 227602 (2013). \(^2\) E. R. MacQuarrie et al., arXiv:1411.5325 (2014). 

\(^1\) Funding from ONR is gratefully acknowledged. In collaboration with E. R. MacQuarrie, T. A. Gosavi, A. M. Moehele, N. R. Jungwirth, and S. A. Bhave.

8:36AM S46.00002 Strain-mediated mechanical coupling to diamond spins\(^1\), ANIA BLESZYNJSKI JAYICH, UC Santa Barbara — Nitrogen-vacancy (NV) centers in diamond are atomic-scale spin systems with remarkable quantum properties that persist to room temperature. The recent demonstration of high-quality single-crystal diamond resonators has led to significant interest in a hybrid system consisting of NV spins that interact with the resonant phonon modes of a macroscopic mechanical resonator through crystal strain. We demonstrate dynamic, strain-mediated coupling of the mechanical motion of a diamond cantilever to the spin of an embedded NV. Via quantum control of the spin, we quantitatively characterize the axial and transverse strain sensitivities of the nitrogen-vacancy ground-state spin. The nitrogen–vacancy center is an atomic scale sensor and we demonstrate spin-based strain imaging with a strain sensitivity of \( 3 \times 10^{-6} \) strain Hz\(^{-1/2} \). We discuss prospects for reaching the regime of quantum coupling between phonons and spins, and we present our results in this direction. This hybrid system has exciting prospects for a phonon-based approach to integrating NVs into quantum networks.

\(^1\) Funding from the AFOSR MURI and NSF CAREER programs are gratefully acknowledged.

9:12AM S46.00003 Dynamics of a strain-coupled, hybrid spin-oscillator system, JEAN TEISSIER, University of Basel — A single spin coupled to a mechanical oscillator forms a prototypical hybrid quantum system. With a strong and robust coupling mechanism, such devices could yield high-performance nanoscale sensors, be applied for quantum information processing tasks or ultimately be used to study macroscopic objects in the quantum regime. In this talk, I will present our recent experiments where we established a novel type of such a hybrid spin-oscillator system. Specifically, we implemented for the first time diamond nanomechanical resonators, which are coupled to embedded Nitrogen-Vacancy (NV) centre electronic spins through crystalline strain. This strain coupling mechanism is highly robust, potentially strong and leads to interesting dynamics due to the nontrivial strain coupling Hamiltonian. I will illustrate these aspects though our recent experimental results, which include the first quantitative determination of the relevant strain coupling constants and the demonstration of resolved sideband operation in our devices. I will also discuss recent experiments in which we demonstrated coherent driving of NV spins through time-varying strain fields and studied the resulting intriguing dynamics of the strain-driven NV spin system. Our results constitute first essential steps towards future experiments of our hybrid system in the quantum regime. Examples for these include spin-based oscillator sideband cooling or the recently proposed generation of spin-squeezing in nanomechanical oscillators.

9:48AM S46.00004 Phonon cooling and lasing with nitrogen-vacancy centers in diamond, PETER RABL, Institute of Atomic and Subatomic Physics, Vienna University of Technology — Diamond has emerged as a promising material for quantum applications, due in part to its optical and mechanical properties and in part to its addressable quantum defects. In this talk I will discuss the deformation potential interaction between nitrogen-vacancy (NV) centers and isolated mechanical modes in diamond nanostructures. Even on a single phonon level, this coupling can lead to significant shifts of the electronic and spin levels of the defect center and could provide a new tool to access and manipulate the quantum state of macroscopic mechanical systems. I will describe applications of this coupling mechanism for actuation (lasing) and ground state cooling of diamond nanoresonators and show how the combination of these schemes leads to PT-symmetry breaking phase transitions in coupled resonator arrays with engineered loss and gain.


Thursday, March 5, 2015 8:00AM - 10:48AM — Session S47 DBIO: Focus Session: Mechanical Structure-Function Relations in Biological Matter I 217B - Moumita Das, Rochester Institute of Technology

8:00AM S47.00001 Time evolution of cell size distributions in dense cell cultures, EVGENIY KHAIN, Oakland University — Living cells in a dense system are all in contact with each other. The common assumption is that such cells stop dividing due to a lack of space. Recent experimental observations have shown, however, that cells continue dividing for a while, but other cells in the system must shrink, to allow the newborn cells to grow to a normal size. Due to these “pressure” effects, the average cell size dramatically decreases with time, and the dispersion in cell sizes decreases, too. The collective cell behavior becomes even more complex when the system is expanding: cells near the edges are larger and migrate faster, while cells deep inside the colony are smaller and move slower. This exciting experimental data still needs to be described theoretically, incorporating the distribution of cell sizes in the system. We propose a mathematical model for time evolution of cell size distribution both in a closed and open system. The model incorporates cell proliferation, cell growth after division, cell shrinking due to “pressure” from other cells, and possible cell detachment from the interface of a growing colony. This research sheds light on physical and biological mechanisms of cell response to a dense environment and on the role of mechanical stresses in determining the distribution of cell sizes in the system.
8:12AM S47.00002 Sorting of colors in the retina . EREZ RIBAK, AMICHAI LABIN, SHADI SAFURI, IDO PERLMAN, Technion - Israel Institute of Technology — Our image of the world is detected by photoreceptors, lying at the bottom of the nearly-transparent retina. Lateral neural layers for processing the image temporally, spectrally, and spatially come in front the photoreceptors, not behind them. This reverse order is a long-standing puzzle, which we wish to explain. We found out that cone photoreceptors are attached to metabolic Muller cells which span the retina. Cones provide colour vision at day time, and are surrounded by sensitive rods which function at night. We showed by an analytical and a computational method that the Muller cells also serve as fibre optics, concentrating green-red light into the cones, while the excessive blue is scattered to the nearby rods. Spatial and spectral laboratory measurements validate that indeed the shapes and refractive index values of the Muller cells and the surrounding retina separate the colours according to the spectral sensitivities of both cones and rods. These results also explain other effects of vision acuity and colour sensitivity. References A M Labin and E N Ribak, Phys Rev Lett 104, 158102 (2010). A M Labin, S K Safari, E N Ribak and I Perlman, Nature Comm 5, 4319 (2014). A M Labin and E N Ribak, “Color sorting by retinal waveguides”. Submitted.

8:24AM S47.00003 Role of the transverse arch in stiffness of the human foot1 MARCELO A. DIAS, Aalto University, DHIRAJ K. SINGH, MAHESH M. BANDI, Okinawa Institute of Science and Technology, MOHSHUSUDHAN VENKADESAN, Yale University, SHREYAS MANDRE, Brown University — Human ancestors evolved from walking, around 6 million years (Ma) ago, to regular endurance running, around 2 Ma ago. Simultaneously, the feet evolved from a relatively flat structure like that of current day Chimpanzees (or our hands), to the modern human foot with two arches, a longitudinal and a transversal arch. The feet play a crucial role in locomotion by providing sufficient stiffness for propulsion, and being soft and pliable to absorb impacts and store energy elastically. Here we show that the transverse arch could play a central role in stiffness modulation. We first treat the foot as an elastic shell that is with intrinsically elastic. Calculations, numeric and physical experiments all show that for a foot-like shell, the stiffness has a power-law dependence on transverse curvature beyond a critical value. On the other hand, for purely longitudinally curved feet, or transverse curvature below the critical value, lead to low stiffness like a flat plate. Discrete realizations of a continuum shell, more closely resembling the human foot, also exhibit curvature induced stiffening. These results shed light on the role of the quintessentially human feature of a doubly arched foot, and suggest mechanical consequences of disorders such as a collapsed arch.

HFSR RGY0091/2013

8:36AM S47.00004 Correlating Viscoelasticity with Metabolism in Single Cells using Atomic Force Microscopy1, MATTHEW CAPORIZZO, CHARLES ROCO, CARME COLL-FERRER, Materials Science Engineering, DAVID ECKMANN, Anesthesiology and Critical Care, RUSSEL COMPOSTO, Materials Science Engineering — Variable indentation-rate rheometric analysis by Laplace transform (VIRRAL), is developed to evaluate Des-Gel drug carriers as biocompatible delivery agents. VIRRAL provides a general platform for the rapid characterization of the health of single cells by viscoelasticity to promote the self-consistent comparison between cells paramount to the development of early diagnosis and treatment of disease. By modelling the frequency dependence of elastic modulus, VIRRAL provides three metrics of cytoplasmic viscoelasticity: low frequency stiffness, high frequency stiffness, and a relaxation time. THP-1 cells are found to exhibit a frequency dependent elastic modulus consistent with the standard linear solid model of viscoelasticity. VIRRAL indicates that dextran-lysozyme drug carriers are biocompatible and deliver concentrated toxic material (rhodamine or silver nanoparticles) to the cytoplasm of THP-1 cells. The signature of cytotoxicity by rhodamine or silver exposure is a frequency independent 2-fold increase in elastic modulus and cytoplasmic viscosity while the cytoskeletal relaxation time remains unchanged independent of cytoplasmic stiffness. This is consistent with the known toxic mechanism of silver nanoparticles, where mitochondrial injury leads to ATP depletion and metabolic stress causes a decrease of mobility within cytoplasm.

1 NSF DMR08-32802, NIH T32-HL007954, and ONR N000141410538

8:48AM S47.00005 Linking Mechanics and Statistics in Epidermal Tissues, SANGWOO KIM, SASCHA HILGENFELDT, Univ of Illinois - Urbana — Disordered cellular structures, such as foams, polycrystals, or living tissues, can be characterized by quantitative measurements of domain size and topology. In recent work, we showed that correlations between size and topology in 2D systems are sensitive to the shape (eccentricity) of the individual domains: From a local model of neighbor relations, we derived an analytical justification for the famous empirical Lewis law, confirming the theory with experimental data from cucumber epidermal tissue. Here, we go beyond this purely geometrical model and identify mechanical properties of the tissue as the root cause for the domain eccentricity and thus the statistics of tissue structure. The simple model approach is based on the minimization of an interfacial energy functional. Simulations with Surface Evolver show that the domain statistics depend on a single mechanical parameter, properties of the tissue as the root cause for the domain eccentricity and thus the statistics of tissue structure. The model is relevant to diagnostic applications in a variety of animal and plant tissues.

9:00AM S47.00006 Cell mechanics and immune system link up to fight infections . ANDREW EKPENYONG, Dept. of Physics, Creighton University, SI MING MAN, PANAGIOTIS TOURLOMOUSIS, SARRA ACHOURI, EUGENIA CAMMAROTA, KATHERINE HUGHES, ALESSANDRO RIZZO, GILBERT NG, Univ of Cambridge, UK, JOCHEN GUCK, Technical Univ. Dresden, Germany, CLARE BRYANT, Univ of Cambridge, UK — Infectious diseases, in which pathogens invade and colonize host cells, are responsible for one third of all mortality worldwide. Host cells use special proteins (immunoproteins) and other molecules to fight viral and bacterial invaders. The mechanisms by which immunoproteins enable cells to reduce bacterial loads and survive infections remain unclear. Moreover, during infections, some immunoproteins are known to alter the cytoskeleton, the structure that largely determines cellular mechanical properties. We therefore used an optical stretcher to measure the mechanical properties of primary immune cells (bone marrow derived macrophages) during bacterial infection. We found that macrophages become stiffer upon infection. Remarkably, macrophages lacking the immunoprotein, NLR-C4, lost the stiffening response to infection. This in vitro result correlates with our in vivo data whereby mice lacking NLR-C4 have more lesions and hence increased bacterial distribution and spread. Thus, the immune-protein-dependent increase in cell stiffness in response to bacterial infection (in vitro result) seems to have a functional role in the system level fight against pathogens (in vivo result). We will discuss how this functional link between cell mechanical properties and innate immunity, effected by actin polymerization, reduces the spread of infection.

9:12AM S47.00007 Topology optimization of trabecular bone in the human spine , AHMED ELBANNA, University of Illinois Urbana Champaign — It is widely believed in the realm of biology that the trabecular structure of long bones self-optimizes in response to mechanical loads, in accordance with Wolff’s law. Here, we examine this idea by applying techniques from topology optimization the human spine. We consider different domain geometries as well as different load cases to account for the various loading conditions and changes in shape that take place within the spine during day-to-day activities and over the years. We show that the classical approach of minimizing compliance subject to a volume constraint does not yield a sponge-like architecture but results in only vertical trabeculae. Additional constraints/objective functions have to be considered simultaneously. We show that more realistic trabecular geometries may be produced by taking into consideration the function of trabecular bone as a reservoir for minerals and bone marrow production. By maximizing the surface area of the generated voids while minimizing the total volume of the trabeculae subject to a constraint on their buckling strength, we recover the sponge-like structure. Our results shed light on the optimizing conditions for bone structure beyond Wolff’s law and provide guidelines for biomimetic material design.
9:24AM S47.00008 Structure and Sequence Search on Aptamer-Protein Docking . JIAJIE XIAO, KEITH BONIN, MARTIN GUTHOLD, FREDDIE SALSBURY, Wake Forest University — Interactions between proteins and deoxyribonucleic acid (DNA) play a significant role in the living systems, especially through gene regulation. However, short nucleic acids sequences (aptamers) with specific binding affinity to specific proteins exhibit clinical potential as therapeutics. Our capillary and gel electrophoresis selection experiments show that specific sequences of aptamers can be selected that bind specific proteins. Computationally, given the experimentally-determined structure and sequence of a thrombin-binding aptamer, we can successfully dock the aptamer onto thrombin in agreement with experimental structures of the complex. In order to further study the conformational flexibility of this thrombin-binding aptamer and to potentially develop a predictive computational model of aptamer-binding, we use GPU-enabled molecular dynamics simulations to both examine the conformational flexibility of the aptamer in the absence of binding to thrombin, and to determine our ability to fold an aptamer. This study should help further de-novo predictions of aptamer sequences by enabling the study of structural and sequence-dependent effects on aptamer-protein docking specificity.

9:36AM S47.00009 Non-thermal fluctuations in living cells reveal nonlinear mechanical properties of the cytoskeleton1, H. DANIEL OU-YANG, MING-TZO WEI2, DIMITRIS VAVYLONIS, SABRINA JEDLICKA, Lehigh University — Living cells are a non-equilibrium mechanical system, largely because intracellular molecular motors consume chemical energy to generate forces that reorganize and maintain cytoskeletal functions. Persistently under tension, the network of cytoskeletal proteins exhibits a nonlinear mechanical behavior where the network stiffness increases with intracellular tension. We examined the nonlinear mechanical properties of living cells by characterizing the differential stiffness of the cytoskeletal network for HeLa cells under different intracellular tensions. Combining active and passive microrheology methods, we measured non-thermal fluctuating forces and found them to be much larger than the thermal fluctuating force. From the variations of differential stiffness caused by the fluctuating non-thermal force for cells under different tension, we obtained a master curve describing the differential stiffness as a function of the intracellular tension. Varying the intracellular tension by treating cells with drugs that alter motor protein activities we found the differential stiffness follows the same master curve that describes intracellular stiffness as a function of intracellular tension. This observation suggests that cells can regulate their mechanical properties by adjusting intracellular tension.

1 NSF DMR 0923299
2 currently at Princeton University

9:48AM S47.00010 Geometry, Mechanics, and Microstructure: Relating Structure to Function in Articular Cartilage . JESSE SILVERBERG, Wyss Institute for Biologically Inspired Engineering — Climbing cucumbers, popping pollen grains, wrinkled fingers, and curly hair. At heart, the modern revival of mechanics covers a diverse range of biological materials living at the intersection of function and form. It’s at this point, where geometry, mechanics and microstructure meet, that we find buckling instabilities, mechanical phase transitions, exotic stress responses, and fracture. While these phenomena are widely observed in many inert materials, we also find them being actively employed in biological tissues, where they have evolved as essential tools for survival. In this talk, I’ll specifically address articular cartilage, a biological material that enables smooth and painless joint motion. Using a combination of experimental techniques, an unusual structure-function relationship for this material is empirically determined, and a model based on percolating fiber networks is offered as a solution. In the end, a central theme will emerge placing this tissue in the wider context of “elastic network materials,” and a wider need for advanced imaging methods will be called for.

10:24AM S47.00011 Effect of Isotropic Assumption on Material Property Reconstructions of the Human Brain using Magnetic Resonance Elastography . AARON ANDERSON, CURTIS JOHNSON, JOSEPH HOLTROP, Univ of Illinois - Urbana, MATHEW MCGARRY, KEITH PAULSEN, Dartmouth College, BRADLEY SUTTON, Univ of Illinois - Urbana, ELIJAH VAN HOUTEN, Universite de Sherbrooke, JOHN GEORGIADES, Univ of Illinois - Urbana — Neurodegenerative diseases affect the microstructure of the brain and thus have a significant effect on the tissue mechanical properties. In vivo techniques, like magnetic resonance elastography (MRE), have shown promise as a contrast technique for disease detection. MRE is a non-invasive technique for measuring the viscoelastic mechanical properties of biological tissue by applying a low-amplitude shear wave, capturing the wave patterns with specialized magnetic resonance imaging techniques, and employing an isotropic nonlinear inversion ( NLI) material property reconstruction. When distinctly different shear wave patterns are applied, NLI reconstructs differences in the real component of the shear modulus of ~ 2 [kPa] within well ordered white matter (WM). The difference is significant due to the human brain only having a range of real shear modulus from 0 [kPa] (cerebral spinal fluid) to ~ 5 [kPa] (white matter). The focus of this investigation is to quantify the effect of propagation direction on the reconstructed material properties and examine their relationship to the underlying microstructure in a well ordered, WM regions of the brain (corpus callosum).
8:12AM S48.00002 Mixed Strategies in cyclic competition\textsuperscript{1}, BEN INTOY, MICHEL PLEIMLING, Virginia Tech — Physicists have been using evolutionary game theory to model and simulate cyclically competing species, with applications to lizard mating strategies and competing bacterial strains. However, these models assume that each agent plays the same strategy, which is called a pure strategy in game theory, until they are beaten by a better strategy which they immediately adopt. We relax this constraint of an agent playing a single strategy by instead letting the agent pick its strategy randomly from a probability distribution, which is called a mixed strategy in game theory. This scheme is very similar to multiple occupancy models seen in the literature, the major difference being that interactions happen between sites rather than within them. Choosing strategies out of a distribution also has applications to economic/social systems such as the public goods game. We simulate a model of mixed strategy and cyclic competition on a one-dimensional lattice with three and four strategies and find interesting spatial and stability properties depending on how discretized the choice of strategy is for the agents.

\textsuperscript{1}This work is supported by the US National Science Foundation through grant DMR-1205309.

8:24AM S48.00003 Spatial games with cyclic interactions: the response of empty sites\textsuperscript{1}, BART BROWN, MICHEL PLEIMLING, Virginia Tech — Predator-prey models of the May-Leonard family employ empty sites in a spatial setting as an intermediate step in the reproduction process. This requirement makes the number and arrangement of empty sites important to the formation of space-time patterns. We study the density of empty sites in a stochastic predator-prey model in which the species compete in a cyclic way in two dimensions. In some cases systems of this type quickly form domains of neutral species after which all predation, and therefore, reproduction occur near the interface of competing domains. Using Monte Carlo simulations we investigate the relationship of this density of empty sites to the time-dependent domain length. We further explore the dynamics by introducing perturbations to the interaction rates of the system after which we measure the perturbed density, i.e. the response of empty sites, as the system relaxes. A dynamical scaling behavior is observed in the response of empty sites.

\textsuperscript{1}This work is supported by the US National Science Foundation through grant DMR-1205309.

8:36AM S48.00004 Critical fluctuations near the pitchfork bifurcations of period-doubling maps\textsuperscript{1}, ANDREW NOBLE, University of California, Davis, SABA KARIMEDDINY, University of Massachusetts, Amherst, ALAN HASTINGS, University of California, Davis, JONATHAN MACHTA, University of Massachusetts, Amherst — Period-doubling maps, such as the logistic map, have been a subject of intense study in both physics and biology. The period-doubling route to chaos proceeds through a sequence of supercritical pitchfork bifurcations. Here, motivated by applications to population ecology, we investigate the asymptotic behavior of period-doubling bifurcations subject to environmental or demographic noise. We demonstrate, analytically, that fluctuations in the vicinity of each noisy pitchfork bifurcation are described by finite-size mean-field theory. Our results establish an exact correspondence between the bifurcations of far-from-equilibrium systems and the mean-field critical phenomena of equilibrium systems.

\textsuperscript{1}This material is based upon work supported by the National Science Foundation under INSPIRE Grant No. 1344187.

8:48AM S48.00005 Population dynamics of microbial communities in the zebrafish gut, MATTHEW JEMIELITA, MICHAEL TAORMINA, Department of Physics, University of Oregon, ADAM BURNS, Institute of Ecology and Evolution, University of Oregon, JENNIFFER HAMPTON, ANNAH ROLIG, TRAVIS WILES, KAREN GUILLEMIN, Institute of Molecular Biology, University of Oregon, RAGHUVEER PARTHASARATHY, Department of Physics, University of Oregon — The vertebrate intestine is home to a diverse microbial community, which plays a crucial role in the development and health of its host. Little is known about the population dynamics and spatial structure of this ecosystem, including mechanisms of growth and interactions between species. We have constructed an experimental model system with which to explore these issues, using initially germ-free larval zebrafish inoculated with defined communities of fluorescently tagged bacteria. Using light sheet fluorescence microscopy combined with computational image analysis we observe and quantify the entire bacterial community of the intestine during the first 24 hours of colonization, during which time the bacterial population grows from tens to thousands of bacteria. We identify both individual bacteria and clusters of bacteria, and quantify the growth rate and spatial distribution of these distinct subpopulations. We find that clusters of bacteria grow considerably faster than individuals and are located in specific regions of the intestine. Imaging colonization by two species reveals spatial segregation and competition. These data and their analysis highlight the importance of spatial organization in the establishment of gut microbial communities, and can provide inputs to physical models of real-world ecological dynamics.

9:00AM S48.00006 Responses of many-species predator-prey systems to perturbations\textsuperscript{1}, SHADI ESMAILY, MICHEL PLEIMLING, Virginia Tech — We study the responses of many-species predator-prey systems, both in the well-mixed case as well as on a two-dimensional lattice, to permanent and transient perturbations. In the case of a weak transient perturbation the system returns to the original steady state, whereas a permanent perturbation pushes the system into a new steady state. Using Monte Carlo simulations, we monitor the approach to stationarity after a perturbation through a variety of quantities, as for example time-dependent particle densities and correlation functions. Different types of perturbations are studied, ranging from a change in reaction rates to the injection of additional individuals into the system, the latter perturbation mimicking immigration.

\textsuperscript{1}This work is supported by the US National Science Foundation through grant DMR-1205309.

9:12AM S48.00007 Anticipating Changing in Environments: Adaptation in Fluctuating Environments in A Heterogeneous Microbial Communities, MERZU BELETE, University of Houston, GÁBOR BÁLÁZSI, Stony Brook University — The environments in which micro-organisms grow often fluctuate. To survive in temporally changing environments, cells have evolved mechanisms to survive environmental changes. One survival mechanism is generating phenotypic differences among identical cells in a given environment, with cells randomly switching between phenotypes. Such cells form subpopulations that proliferate at different rates. Optimal population fitness was attributed before to matching cellular and environmental switching rates. However, the conditions for this optimum are not well understood. In particular, it is unknown how the growth rates of the phenotypes affect the optimum. We use mathematical models to address this question. We find that the existence of the predicted optimum depends on cell growth rates in each phenotype. The predicted optimum exists for wider parameter regimes if the environmental durations are long. In addition, we study how mutants arising among such phenotypically heterogeneous cells spread in the population.

9:24AM S48.00008 The Statistical Mechanics of Zombies, ALEXANDER A. ALEMI, MATTHEW BIERBAUM, CHRISTOPHER R. MYERS, JAMES P. SETHNA, Cornell University — We present results and analysis from a large scale exact stochastic dynamical simulation of a zombie outbreak. Zombies have attracted some attention lately as a novel and interesting twist on classic disease models. While most of the initial investigations have focused on the continuous, fully mixed dynamics of a differential equation model, we have explored stochastic, discrete simulations on lattices. We explore some of the basic statistical mechanical properties of the zombie model, including its phase diagram and critical exponents. We report on several variant models, including both homogeneous and inhomogeneous lattices, as well as allowing diffusive motion of infected hosts. We build up to a full scale simulation of an outbreak in the United States, and discover that for ‘realistic’ parameters, we are largely doomed.

This work is supported by the US National Science Foundation through grant DMR-1205309.
9:36 AM S48.00009 Mutation Accumulation and Fitness Collapse at Population Frontiers, MAXIM LAVRENTOVICH, University of Pennsylvania, DAVID NELSON, Harvard University — Rapid, deleterious mutations occurring in, e.g., viral populations and cancerous tissue, may accumulate and lead to fitness loss. Previous studies show that sufficiently rapid accumulation in one-dimensional populations leads to a fitness collapse, governed by the directed percolation (DP) universality class. We compare this situation to the collapse in effectively two-dimensional populations, such as the frontiers of three-dimensional range expansions. A phase diagram is computed as a function of the mutation rate $\mu$ and strength $s$. Relative to one-dimensional populations, we find that the collapse occurs in a smaller region of phase space. The scaling combination governing the phase diagram shape is $|\mu|/s$ for one-dimensional populations. We argue that the evolutionary dynamics is described by a set of coupled DP Langevin equations near the transition, and that the coupling terms lead to deviations from expected DP scaling.

9:48 AM S48.00010 Spiraling patterns in evolutionary models inspired by bacterial games with cyclic dominance¹, MAURO MOBILIA, University of Leeds — Understanding the mechanisms allowing the maintenance of biodiversity is a central issue in biology. Evolutionary game theory, where the success of one species depends on what the others are doing, provides a promising framework to investigate this complex problem. Experiments on microbial populations have shown that cyclic local interactions promote species coexistence. In this context, rock-paper-scissors games - in which rock crushes scissors, scissors cut paper, and paper wraps rock - are often used to model the dynamics of populations in cyclic competition. After a brief survey of some inspiring experiments, I will discuss the subtle interplay between individuals' mobility and their local interactions in two-dimensional rock-paper-scissors systems. This leads to the loss of biodiversity above a certain mobility threshold [1], and to the formation of spiraling patterns below the critical mobility rate [1-4]. I will then study a generic rock-paper-scissors metapopulation model formulated on a two-dimensional grid of patches. When these have a large carrying capacity, the model's dynamics is faithfully described in terms of the system's complex Ginzburg-Landau equation properly derived from a multiscale expansion. The properties of the ensuing complex Ginzburg-Landau equation are exploited to derive the system's phase diagram and to characterize the spatio-temporal properties of the spiraling patterns in each phase. This enables us to analyze the spiral waves stability, how these are influenced by linear and nonlinear diffusion, and to discuss phenomena such as far-field breakup [5-7].

¹Presentation mainly based on joint work with B. Szczesny and A. M. Rucklidge. Fruitful earlier collaborations with E. Frey, Q. He, T. Reichenbach, and U. C. Täuber are also acknowledged. Work supported by the UK EPSRC (grant No. EP/P505593/1).

10:24 AM S48.00011 Phase transition in predator-prey ecosystems and a connection to transitional turbulence¹, HONG-YAN SHIH, NIGEL GOLDENFELD, Department of Physics, University of Illinois at Urbana-Champaign — We suggest how the transition from laminar fluid flow to turbulence can be connected to the extinction phase transition in spatially-extended predator-prey systems. By measuring the statistics of spontaneous relaminarization, spatiotemporal intermittency and expanding turbulent puffs in hydrodynamics equations and mapping them to the corresponding states in the predator-prey model, the extinction event and the formation and propagation of spatial patterns in ecology can be interpreted as the instabilities in fluid systems. We also summarize the general phenomena of such predator-prey dynamics in a wide class of transitional turbulence systems such as magnetohydrodynamics.

¹This work was partially supported by the National Science Foundation through grant NSF-DMR-1044901.

10:36 AM S48.00012 Evolutionary games of condensates in coupled birth-death processes, MARKUS F. WEBER, JOHANNES KNEBEL, TORBEN KRÜGER, ERWIN FREY, Ludwig-Maximilians-Universität München — Condensation phenomena occur in many systems, both in a classical and a quantum mechanical context. Typically, the entities that constitute a system collectively concentrate in one distinct state during condensation. For example, cooling of an equilibrated bosonic gas may lead to condensation into the quantum ground state. Notably, the mathematical theory of this Bose-Einstein condensation is not limited to quantum theory but was also successfully applied to condensation in random networks. In our work, we follow the opposite path. We apply the theory of evolutionary dynamics to describe condensation in a bosonic system that is driven and dissipative. It was shown that the system may condense into multiple quantum states, but into which states has remained elusive. We find that vanishing of relative entropy production determines these states. We illuminate the physical principles underlying the condensation and show that the condensates do not need to be static but may engage in “evolutionary games” with exchange of particles. On the mathematical level, the condensation is described by coupled birth-death processes. The generic structure of these processes implies that our results also apply to condensation in other systems, ranging from population biology to chemical kinetics.

10:48 AM S48.00013 A Second Law for Markov Processes, BLAKE POLLARD, University of California, Riverside — In this talk we describe the notion of an open Markov process. An open Markov process is a generalization of an ordinary Markov process in which populations are allowed to flow in and out of the system at certain boundary states. We show that the rate of change of relative entropy in an open Markov process is less than or equal to the flow of relative entropy through its boundary states. This can be viewed as a generalization of the Second Law for open Markov processes.
8:00AM S49.00001 Collisions of deformable cells lead to collective migration1, IGOR ARANSON, Argonne National Laboratory, JAKOB LÖBER, Technical University of Berlin, Germany, FALKO ZIEBERT, Albert-Ludwig-University, Freiburg, Germany — Collective migration of eukaryotic cells plays a fundamental role in tissue growth, wound healing and immune response. The motion, arising spontaneously or in response to chemical and mechanical stimuli, is also important for understanding life-threatening pathologies, such as cancer and metastasis formation. We present a phase-field model to describe the movement of many self-organized, interacting cells. The model takes into account the main mechanisms of cell motility - actomyosin dynamics, as well as substrate-mediated and cell-cell adhesion. It predicts that collective cell migration emerges spontaneously as a result of inelastic collisions between neighboring cells. Collisions lead to a mutual alignment of the cell velocities and to the formation of coherently-moving multi-cellular clusters. Small cell-to-cell adhesion, in turn, reduces the propensity for large-scale collective migration, while higher adhesion leads to the formation of moving bands. Our study provides valuable insight into biological processes associated with collective cell motility.

1J. L. acknowledges funding from the German Science Foundation (DFG) within the GRK 1558. F. Z. acknowledges funding from the German Science Foundation (DFG) via project ZI 1232/2-1. I. S. A. was supported by the US Department of Energy (DOE), Office of...

8:12AM S49.00002 A self-propelled particle model with experimentally quantified cell polarization, GIUSEPPE PASSUCCI, MEGAN E. BRASCH, Syracuse University, NICHOLAS O. DEAKIN, CHRISTOPHER E. TURNER, SUNY Upstate Medical, JAMES H. HENDERSON, M. LISA MANNING, Syracuse University — Self-propelled particle (SPP) models have been used extensively to study collective cell motion, but they do not always accurately capture the long-time behavior observed in experiments. Furthermore, the equation for polarization in these models is not experimentally well-constrained. Therefore we developed a novel method for quantifying polarization in 3D breast carcinoma cells in a wound healing geometry. During cell movement, the nuclei orient toward the anterior of a cell while the Golgi body orients towards the posterior; we simultaneously imaged and tracked the Golgi and nuclei and constructed a polarization vector defined by the Golgi-nuclei axis. We find that cells in the bulk are not highly polarized, while those on the edge are highly polarized outward perpendicular to the wound edge. We also study the temporal correlations between a cell’s internal polarization determined by the Golgi-nuclei axis and the polarization of its motion determined from nuclei displacements. We incorporate these polarization dynamics into a SPP model, and compare wound healing and long-time diffusion in the model to the experiments. These SPP equations can also be coarse-grained to generate a continuum model.

8:24AM S49.00003 Modeling traction forces in collective cell migration, JULIANE ZIMMERMANN, Center for Theoretical Biological Physics, Rice University, MARKUS BASAN, Department of Physics, University of California at San Diego, RYAN L. HAYES, Center for Theoretical Biological Physics, Rice University, WOUTER-JAN RAPPEL, Department of Physics, University of California at San Diego, HERBERT LEVINE, Center for Theoretical Biological Physics, Rice University — Collective cell migration is an important process in embryonic development, wound healing, and cancer metastasis. We have developed a particle-based simulation for collective cell migration that describes flow patterns and finger formation at the tissue edge observed in wound healing experiments [1]. We can apply methods for calculating intercellular stress to our simulation model, and have thereby provided evidence for the validity of a stress reconstitution method from traction forces used in experiments [2]. To accurately capture experimentally measured traction forces and stresses in the tissue, which are mostly tensile, we have to include intracellular acto-myosin contraction into our simulation. We can then reproduce the experimentally observed behavior of cells moving around a circular obstacle [3], and suggest underlying mechanisms for cell-cell alignment and generation of traction force patterns. [1] Basan, M., J. Elgeti, E. Hannezo, W.-J. Rappel, H. Levine. Proc. Natl. Acad. Sci. USA. 2013. [2] Zimmermann, J., R. L. Hayes, M. Basan, J. N. Onuchic, W.-J. Rappel, H. Levine. Proc. Natl. Acad. Sci. USA. 2013. [3] Kim, J. H., X. Serra-Picamal, D. T. Tambe, ..., J. J. Fredberg. Nature Mater. 2013.

8:36AM S49.00004 Mimicking the Interfacial Dynamics of Flowing White Blood Cells, MARIA SANTORE, University of Massachusetts — The rolling of particles on surfaces, facilitated by hydrodynamic forces combined with localized surface interactions of the appropriate strengths, spatial arrangements, and ranges, is a technologically useful means of transporting and manipulating particles. One's intuition for the rolling of a marble or a car tire cannot be extrapolated down to microparticle length scales because the microparticle interactions are dominated by electrostatic, van der Waals, and hydrogen bonding interactions rather than a friction that depends on an imposed normal force. Indeed, our microparticle rolling systems are inspired by the rolling of white blood cells on the inner walls of blood vessels and the innate immune response: Selectin molecules engage with their counterparts on the opposing surfaces to slow cell motion relative to that for freely flowing cells. In the resulting rolling signature, ligand-receptor binding and crack closing on the front of the cell are balanced with molecular dis-bonding and crack opening at the rear. The contact region is relatively static, allowing other interactions that may be present (for instance signaling) to occur for a finite duration. Thus, achieving particle rolling in synthetic systems is important because it facilitates particle-surface interactions in a continuous nonfouling fashion where the contact surface is continually renewed. In developing a synthetic model for this system, we employ polymers to modify flowing particles and/or planar collectors, producing heterogeneous interfaces which can support rolling or produce other motion signatures such as skipping, arrest, or free flow. We identify, in the synthetic system, combinations of variables that produce rolling and demonstrate how the distinction between rolling and arrest is not a simple matter of the adhesion strength between the particles and the collector. Rolling is a cooperative process and the coordination of binding in one location with dis-bonding in another requires appropriate length scales in the design of the interface and in the processing parameters as well.

9:12AM S49.00005 ABSTRACT WITHDRAWN

9:24AM S49.00006 Long Range Order of Motile Defects in Active Nematic Liquid Crystals, STEPHEN DECAMP, GABRIEL REDNER, MICHAEL HAGAN, ZVONIMIR DOGIC, Brandeis University — Active 2D nematic liquid crystals exist in a dynamical steady state in which -1/2 and +1/2 defects are spontaneously generated and annihilated at a constant rate. Active stresses in the material are thought to destroy nematic order through the generation of these defects. We present an active nematic mesophase in which motile defects of charge +1/2 spontaneously acquire long range order. The system is composed of microtubule filaments and kinesin motor protein clusters which are confined to a flat, 2D oil-water interface. The addition of ATP results in microtubule bundles which exhibit kinesin-driven extensile motion. By tuning the density of the nematic material at the 2D interface, we can tune the order parameter of the +1/2 defect ordered mesophase. Additionally, the defect alignment persists over samples at the centimeter scale.

9:36AM S49.00007 Defect-Stabilized Phases in Extensile Active Nematics, GABRIEL REDNER, STEPHEN DECAMP, ZVONIMIR DOGIC, MICHAEL HAGAN, Brandeis University — Active nematics are liquid crystals which are driven out of equilibrium by energy-dissipating active stresses. The equilibrium nematic state is unstable in these materials, leading to beautiful and surprising behaviors including the spontaneous generation of topological defect pairs which stream through the system and later annihilate, yielding a complex, seemingly chaotic dynamical steady-state. In this talk, I will describe the emergence of order from this chaos in the form of previously unknown broken-symmetry phases in which the topological defects themselves undergo orientational ordering. We have identified these defect-ordered phases in two realizations of an active nematic: first, a suspension of extensile bundles of microtubules and molecular motor proteins, and second, a computational model of extending hard rods. I will describe the defect-stabilized phases that manifest in these systems, our current understanding of their origins, and discuss whether such phases may be a general feature of extensile active nematics.
9:48AM S49.00008 Worms on a plane: simulation studies of an active nematic phase of flexible chains. MICHAEL VARGA, MOHAMMAD NAJAFI, ROBIN SELINGER, Kent State Univ - Kent — We present simulation studies of flexible nematogen “worms” composed of soft spheres assembled into flexible polymer-like chains. These elongated, flexible chains are confined to a planar substrate with periodic boundary conditions or else confined within bounding walls. We consider a variety of driving mechanisms including unidirectional gliding and gliding with random reversals. We also model actuation via kinesin motor clusters which attach and travel along a pair of neighboring chains of opposite polarity, producing inter-chain sliding forces and driving the chains in opposite directions. We examine resulting nematic order, defect nucleation, motion, and annihilation, and density fluctuations as a function of chain length, flexibility, density, and driving mechanism. In a geometry where the chains are constrained to move in tandem with tight spacing, we observe spontaneous formation of organized beating. We compare our results to experimental and theoretical studies of gliding bacteria [1] and kinesin-driven microtubules [2]. [1] Perumal et al. PRL 108, 098102 (2012), [2] Sanchez et al. Nature 491,431 (2012).

1Supported by NSF DMR-1409658 and NSF DMR-1106014.

10:00AM S49.00009 Instabilities and patterns in an active nematic film. PRAGYA SRIVASTAVA, CRISTINA MARCHETTI, Physics Department, Syracuse University, NY-13244 — Experiments on microtubule bundles confined to an oil-water interface have motivated extensive theoretical studies of two-dimensional active nematics. Theoretical models taking into account the interplay between activity, flow and order have remarkably reproduced several experimentally observed features of the defect-dynamics in these “living” nematics. Here, we derive minimal description of a two-dimensional active nematic film confined between walls. At high friction, we eliminate the flow to obtain closed equations for the nematic order parameter, with renormalized Frank elastic constants. Active processes can render the “Frank” constants negative, resulting in the instability of the uniformly ordered nematic state. The minimal model yields emergent patterns of growing complexity with increasing activity, including bands and turbulent dynamics with a steady density of topological defects, as obtained with the full hydrodynamic equations. We report on the scaling of the length scales of these patterns and of the steady state number of defects with activity and system size.

1National Science Foundation grant DMR-1305184 and Syracuse Soft Matter Program.

10:12AM S49.00010 Dynamics of an overdamped active nematic liquid crystal. ELIAS PUTZIG, APARNA BASKARAN, Brandeis University — A continuum model for the dynamics of an overdamped (often termed “dry”) active nematic liquid crystal will be presented here. This talk will focus on how such a model can be used to describe the formation and self-propulsion of defects which has been seen in active liquid crystals in experiments and simulations. We will start with a general model which shows phase-separations and structure formation near the critical density (for the isotropic-nematic phase transition), and show how this model can be extended to describe extensile active nematics which are deeper within the ordered phase. The spontaneous formation of defects occurs when the contribution of the extensile stresses, to the dynamics of the order parameter, gives rise to a bend instability. This leads to a steady state of defect formation and annihilation, and the self-propulsion of defects, as is seen in experiments and simulation.

1This work was supported through the NSF (NSF-DMR-1149266), Brandeis-MRSEC through the NSF (DMR-0820492), and the HPC cluster at Brandeis which provided computing time. EFP also acknowledges support through (NIH-5T32EB009419) and IGERT (DGE-1068620).

10:24AM S49.00011 The geometry and topology of turbulence in active nematics. LUCA GIOMI, Univ of Leiden — The problem of low Reynolds number turbulence in active nematic fluids is theoretically addressed. Using numerical simulations I demonstrate that an incompressible turbulent flow, in two-dimensional active nematics, consists of an ensemble of vortices whose areas are exponentially distributed within a range of scales. Building on this evidence, I construct a mean-field theory of active turbulence by which several measurable quantities, including the spectral densities and the correlation functions, can be analytically calculated. Due to the profound connection between the flow geometry and the topological properties of the nematic director, the theory sheds light on the mechanisms leading to the proliferation of topological defects in active nematics and provides a number of testable predictions. A hypothesis, inspired by Onsager’s statistical hydrodynamics, is finally introduced to account for the equilibrium probability distribution of the vortex sizes.

10:36AM S49.00012 Instabilities and boundary effects in a droplet of active polar liquid crystal. CARL WHITFIELD, RHODA HAWKINS, University of Sheffield — Using the active gel theoretical framework, we have performed analytical calculations and numerical simulations of a droplet of active polar liquid crystal at low Reynolds number. This system is a simplified model of a cytoskeletal network that generates internal stresses by converting chemical energy (in the form of ATP) into mechanical work via molecular motors. A physical understanding of these systems can give an insight into the complex and varied dynamics of eukaryotic cell migration and division. We perform a linear stability analysis on the system by separating the behaviour into two limits. One where the internal polarisation is dominated by the shape of the boundary and one where it is deformed by density fluctuations and the correlation functions, can be analytically calculated. Due to the profound connection between the flow geometry and the topological properties of the nematic director, the theory sheds light on the mechanisms leading to the proliferation of topological defects in active nematics and provides a number of testable predictions. A hypothesis, inspired by Onsager’s statistical hydrodynamics, is finally introduced to account for the equilibrium probability distribution of the vortex sizes.

10:48AM S49.00013 Interacting active elastic dimers: Two cells moving on a rigid track. MOUMITA DAS, Rochester Institute of Technology; DAVID MAYETT, J. M. SCHWARZ, Syracuse University — Cell migration in morphogenesis and cancer metastasis typically involves an interplay between different cell types. The rules governing such interplay remain largely unknown, however, a recent experiment studying the interaction between neural crest (NC) cells and placodal cells reveals an example of such rules. The study found that NC cells chase the placodal cells by chemotaxis, while placodal cells run away from NC cells when contacted by them. Motivated by this observation, we construct and study a minimal one-dimensional cell-cell model comprised of two cells with each cell represented by two-beads-connected-by-an-active spring. The active spring for each moving cell models the stress fibers with their myosin-driven contractility (and alpha-actinin extendability), while the friction coefficients of the beads describe the inter-chain sliding forces and driving the chains in opposite directions. We examine resulting nematic order, defect nucleation, motion, and annihilation, and density fluctuations as a function of chain length, flexibility, density, and driving mechanism. In a geometry where the chains are constrained to move in tandem with tight spacing, we observe spontaneous formation of organized beating. We compare our results to experimental and theoretical studies of gliding bacteria [1] and kinesin-driven microtubules [2]. [1] Perumal et al. PRL 108, 098102 (2012), [2] Sanchez et al. Nature 491,431 (2012).

1Supported by NSF DMR-1409658 and NSF DMR-1106014.
8:00AM S50.00001 Self-assembly of novel molecules, VECAR1

1This research is supported by the Louisiana Board of Regents-RCS grant (LEQSF(2012-15)-RD-A-19).

8:12AM S50.00002 Self-assembly of Colloids in a Suspended Droplet: In-situ small-angle X-ray scattering

JITENDRA BAHADUR, Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA; DEBASHIS SEN, S. MAZUMDER, Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, India; G. SANTORO, S. YU, S.V. ROTH, Photon Science, Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85 D-22607, Hamburg, Germany; Y.B. MELNICHENKO, Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA — An in-situ scanning SAXS experiments have been performed to probe the drying of a single suspended colloidal droplet. It has been demonstrated that shell formation can be predicted just by measuring the temporal evolution of the spatial transmission profile. The shrinkage of the droplet stops after formation of a shell. The shell thickness and droplet radius have been estimated by fitting the transmission profiles using analytical expressions. It is revealed that the evolution of volume fraction of colloids is linear during the initial stage of drying and follows a sigmoidal growth behavior at later stages. Further, the interaction between colloidal particles at different drying stages has been investigated. We provide experimental proofs of a transition from repulsive interaction between colloids into a capillary driven short range attraction for shell formation during drying. The present work demonstrates that in-situ SAXS is a very valuable technique for monitoring the dynamic processes of colloidal self-assembly and provides the opportunity to probe the drying of complex fluids without the interference from a substrate.

8:24AM S50.00003 Self-assembly of graded refractive index in squids: a patchy colloid explanation

JING CAI, PAUL HEINEY, ALISON SWEENEY, Univ of Pennsylvania — Squids have a spherical eye lens that achieves both acute and highly sensitive vision under water. The spherical shape necessitates a graded refractive index (GRIN) to form sharp images. This index variation comes from a gradient in protein packing fraction ranging from approximately 0.05 to 1.0. This presents a materials conundrum: optical transparency requires that the protein density fluctuation at length scales > 100 nm is minimized throughout the lens, something that is difficult to achieve with simple spherical particles. Here we show that squids have accomplished this by evolving a suite of proteins that can act as patchy colloids with specific low valence (M=2 or M=3). We conducted small angle X-ray scattering (SAXS) at different radial positions of the lens, and performed a Monte Carlo simulation to estimate structures consistent with the SAXS result. This analysis suggests that lens proteins may form a density gradient gel structure, with density mediated by a tightly controlled protein coordination number in each region. Patchy colloid theory may therefore explain both the GRIN and the transparency evolved in the lens.

8:36AM S50.00004 Self-assembly of tetrahedral plasmonic nanoclusters for optical metafluids

NICHOLAS SCHADE, Department of Physics, Harvard University; VINOTHAN MANOHARAN, School of Engineering and Applied Sciences and Department of Physics, Harvard University — We direct the assembly of clusters of gold nanoparticles that behave as nanoscale electromagnetic resonators. We use spherical gold nanoparticles that are exceptionally smooth, monocrystalline, and monodisperse. These particles exhibit highly reproducible scattering spectra compared with gold colloids that are available commercially. We pack these positively charged particles with negatively charged dielectric particles. The gold particles stick to the dielectric particles permanently and randomly in a process that can be modeled mathematically as “random parking,” a type of non-equilibrium self-assembly. By controlling the particles’ sizes, stoichiometry, and interactions, we maximize the yield of tetrahedral clusters, the ideal structures for isotropic metamaterials. We measure the optical properties of these structures with dark-field spectroscopy to characterize their suitability as building blocks for a bulk, isotropic, optical metafluid.

8:48AM S50.00005 Drying of Discotic Suspensions

ADITYARAM NARAYAN, ZHENGDONG CHENG, TAMU, Artie McFerrin Department of Chemical Engineering, Mary Kay O’Connor Process Safety Center — We study the evaporation driven self-assembly of exfoliated 7-Zirconium Phosphate nanoplatelets that formed continuous films at various low concentrations. These self-assembly mechanism is different from the well-known coffee-ring effect for low aspect ratio particles. The film formation can be tuned by solvent properties, temperature and concentration of the nanoparticles. By the virtue of very large surface area, these platelets can be used as flame retardant coatings after proper functionalization. These work point to a simple procedure to create uniform films by high aspect ratio nanoplates with potentially diverse applications.

9:00AM S50.00006 Self-assembly mechanism for limit-periodic structure1

CATHERINE MARCOURX, JOSHUA SOCOLAR, Duke University — Limit-periodic (LP) structures, which are the union of an infinite set of periodic lattices with ever increasing lattice constants, present a challenge for self-assembly protocols. We consider the possibility of forming a LP phase in a slow quench of a collection of colloidal particles designed to mimic the Taylor-Socolar monolite system2. A toy model with discrete tile orientations and mismatch energies yields the LP state through an infinite sequence of phase transitions. Here we present the results of Monte Carlo simulations of slow quenches of identical hard disks with embedded magnetic dipoles, allowing for continuous rotations of the close-packed disks. Surprisingly, an extremely slow quench still results in the spontaneous emergence of the LP state even when the system has a periodic ground state. The series of phase transitions preempts the formation of the periodic phase, leading to low energy states separated from the ground state by insurmountable free energy barriers.

1Supported by the NSF Research Triangle MRSEC (DMR-1121107)
9:12AM S50.00007 Non-additive simple potentials for pre-programmed self-assembly. CARLOS MENDOZA, IIM-UNAM — A major goal in nanoscience and nanotechnology is the self-assembly of any desired complex structure with a system of particles interacting through simple potentials. To achieve this objective, intense experimental and theoretical efforts are currently concentrated in the development of the so-called ‘patchy’ particles. Here we follow a completely different approach and introduce a very accessible model to produce a large variety of pre-programmed two-dimensional (2D) complex structures. Our model consists of a binary mixture of particles that interact through isotropic interactions that is able to self-assemble into targeted lattices by the appropriate choice of a small number of geometrical parameters and interaction strengths. We study the system using Monte Carlo computer simulations and, despite its simplicity, we are able to self assemble potentially useful structures such as chains, stripes, Kagomé, twisted Kagomé, honeycomb, square, Archimedean and quasi-crystalline tilings. Our model is designed such that it may be implemented using discotic particles or, alternatively, using exclusively spherical particles interacting isotropically. Thus, it represents a promising strategy for bottom-up nano-fabrication. Reference: Daniel Salgado-Blanco and Carlos I. Mendoza, “Non-additive simple potentials for pre-programmed self-assembly”, arXiv:1409.2916 [cond-mat.soft]

9:24AM S50.00008 Heterogeneous crystal nucleation on curved surfaces observed by real-space imaging. URS GASSER, ANDREA SCOTTI, Paul Scherrer Institut, FLORIAN ZIESE, GEORG MARET, University of Konstanz — Crystal nucleation in a supercooled liquid, i.e. the formation of critical crystal nuclei, is not well understood for both homogenous and heterogeneous nucleation. The structural transformation from the liquid to crystal precursors and finally to the structure of bulk crystal and its connection with the free energy barrier for nucleation are not well understood. The large differences between measured and calculated nucleation density rates obtained for many materials reflect this lack of understanding. We use confocal microscopy with single-particle resolution to observe heterogeneous nucleation of colloidal crystals on curved seed surfaces. The radius of curvature ranges from 4 to 40 particle diameters, allowing to observe the transition from the strong suppression of heterogeneous nucleation at small radii of curvature - an effect not captured by classical nucleation theory - to fast heterogeneous nucleation as expected from classical nucleation theory. We determine the critical nucleus size, estimate the surface tension of crystal precursors and critical nuclei, characterize their structure, and compare with expectations from classical nucleation theory. While the smallest crystal precursors are found to be almost unaffected by the curvature, the effect is significant for nuclei

9:36AM S50.00009 Computer Simulation Study of the Nucleation of Rotator Phases in Hard Polyhedral Particles. VIKRAM THAPAR, FERNANDO ESCOBEDO, Cornell University — The nucleation kinetics of the rotator phase in hard cuboctahedra, truncated octahedra, and rhombic dodecahedra is simulated via a combination of forward flux sampling and umbrella sampling. We compute the degrees of supersaturation at their corresponding pressures by improving upon the interfacial method used to estimate the liquid-rotator coexistence pressure. The nucleation rates are obtained by calculating the mean first passage time from liquid to rotator phase using forward flux sampling, and the free-energy barriers are estimated using umbrella sampling. For comparable degrees of supersaturation, the polyhedra are found to have significantly lower free-energy barriers and faster nucleation rates than hard spheres. This difference primarily stems from localized orientational ordering, which steers polyhedral particles to pack more efficiently. Orientational order hence fosters here the growth of orientationally disordered nuclei. The results are compared to preliminary data for the disorder-to-order transition for other polyhedral systems including systems pinned on a 2D interface.

9:48AM S50.00010 Interplay of isotropic and directional interactions and its role in phase behavior. DEBRA AUDUS, National Institute of Standards and Technology, FRANCIS STARR, Wesleyan University, JACK DOUGLAS, National Institute of Standards and Technology — Patchy particles, which interact through non-isotropic interactions have been studied extensively both computationally and theoretically in part because they are minimal models of protein solutions. Although proteins are inherently complicated molecules with complex shapes and interactions, when in solution, they associate and phase separate like patchy particles. However, patchy particles considered computationally are often composed of hard spheres with short-ranged attractive spots decorating the surface. Such a parameterization ignores the isotropic attractive interactions, which can potentially play an important role in phase behavior. To gain insight into this problem, we investigate patchy particles with isotropic interactions that range from purely repulsive to weakly attractive and explore how the interplay between isotropic interactions and directional interactions due to the spots affects both the phase coexistence and association in these systems. We find that for our model that even when the strength of isotropic interactions is weaker than the strength of directional interactions, the isotropic interactions can still dominate.

10:00AM S50.00011 Engineering Crystals Through Shape. GREG VAN ANDERS, University of Michigan, DAPHNE KLOTSA, University of Cambridge, SHARON GLOTZER, University of Michigan — Advances in synthesis techniques have produced colloids and nanoparticles in a diverse array of shapes that can be assembled into bulk crystals. That bulk structure is strongly affected by particle shape in idealized systems is widely established in the literature. However, this literature leaves open three key questions: (i) We know that shape affects structure, but how? (ii) Does shape matter in experimental systems where other interactions are present? (iii) How do we tailor particle shape for a target structure? In this talk we discuss recent work aimed at answering these questions.

10:12AM S50.00012 The size of the boat matters: Scale dependence in macroscopic chains thermalized by the motion of a laboratory-scale ocean. KYLE WELCH, CLAYTON KILMER, ERIC CORWIN, University of Oregon — We use a bath of chaotic surface waves in water to mechanically and macroscopically mimic the thermal behavior of various microscopic systems. The chaotic waves provide isotropic and random agitation to which a temperature can be ascribed. This allows us to passively explore the degrees of freedom of a system, in analogy to thermal motion. We report on a study of 2D macroscopic chains thermalized in this fashion. We show that the behavior of short chains is fundamentally different than the behavior of long chains in both winding angle and end-to-end distance. Furthermore, we find that short chains show anomalous compressional stiffness that rapidly softens as chain length increases. We present simulational work exploring this transition from short to long, treating the chains as self-avoiding polymers. We further apply our techniques to explorations of the evolution of a system of many interacting buoyant particles, focusing on transitions from ordered to disordered states.

10:24AM S50.00013 Directing Translational and Orientational Order of Rectangular Particle Monolayers. MARK FERRARO, THOMAS TRUSKETT, ROGER BONNECAZE, Univ of Texas, Austin — Recent advances have shown that the tunability of nanoparticle interactions can lead to a large number of thermodynamically accessible structures. The role of an external field in the assembly of particulate systems, however, is still incompletely understood. The use of larger scale patterned substrates to drive smaller scale assembly of particle monolayers can potentially expand the set of achievable lattices, and could be used in nanopatterning processes or in the manufacture of functional materials. In this presentation, grand canonical Monte Carlo (GCMC) simulations are used to assess the suitability of graphoepitaxial assembly for particle monolayers. Our prior work has shown that topographically or chemically patterned substrates can sufficiently organize hard-spheres, but many motivating applications can utilize anisotropic particle shapes (e.g. rectangular particles for bit-patterned media). Here, we describe our recent GCMC results for structures formed by rectangular particles in the presence of sparse enthalpic barriers. We examine systems of varying chemical potential, template geometry, and particle aspect ratio. Templates are evaluated by their ability to induce orientational and translational order, while maximizing pattern multiplication effects.
Thursday, March 5, 2015 8:00AM - 11:00AM – Session S51 DCMP: Invited Session: The Valley Hall Effect in van der Waals Materials  Grand Ballroom C1 - Allan MacDonald, University of Texas at Austin

8:00AM S51.00001 Detecting Topological Currents in Gapped Graphene

LEONID LEVITOV, Massachusetts Inst of Tech-MIT — The anomalous Hall effect (AHE), arising due to Berry curvature in materials with broken inversion symmetry, results in topological currents flowing in system bulk transversely to the applied electric field. We will discuss recent work on AHE in materials with several valleys, such as e.g. graphene and transition metal dichalcogenide monolayers, where these currents have been observed [Mak et al., Science 344, 1489 (2014); Gorbachev et al., Science 346, 448 (2014)]. Interestingly, these materials do not fit the paradigm of topological materials with Chern bands and associated topologically protected edge modes dominating (quantized) Hall conductivity. Here, in contrast, gapless edge states may be absent since they are not enforced by topology or symmetry. Further, even when present, these states are not protected against backscattering due to roughness on the atomic scale. Naively, this would lead one to conclude that topological currents cease to exist. If true, this would imply that the key manifestations, such as the valley Hall conductivity and orbital magnetization, vanish in the gapped state. We will argue that the opposite is true: the absence of conducting edge modes does not present an obstacle since once valley currents can be transmitted by the bulk states in the filled Fermi sea beneath the gap. This leads to an interesting behavior: rather than being vanishingly small, valley currents reach maximum value in the gapped state. Such undergap currents can also occur as persistent currents in the thermodynamic ground state and dominate orbital magnetization in valley-polarized gapped systems. We will conclude with discussing requirements for dissipationless valley transport and argue that they can be met under realistic conditions.

9:12AM S51.00003 Valley current generation by electrically induced Berry curvature in double gated bilayer graphene

SEIGO TARUCHA, Department of Applied Physics, The University of Tokyo — Valley degree of freedom is defined for an electronic system having degenerate band structure in a certain crystal configuration and can be used to generate non-dissipative current with accompanying net charge flow by breaking the spatial inversion symmetry. Graphene and transition metal dichalcogenide are two typical valley materials having K and K’ valleys due to the existence of two sub-lattices. The valley current has only recently been studied for monolayer graphene on h-BN where the spatial inversion symmetry is structurally broken by the superlattice potential. We use a double gated bilayer graphene device to electrically break the spatial inversion symmetry and control the Berry curvature. We use valley hall effect to generate a transverse pure valley current and inverse valley hall effect to detect the current. In this device the Fermi energy and the bandgap are independently varied and this allows to prove existence of valley hall effect in the insulating regime where the local resistivity increases with lowering temperature. The insulating regime is particularly interesting because the electric field to valley current conversion is less dissipative in contrast to the case for conventional spin or valley hall systems.

9:48AM S51.00004 Valley and spin currents in 2D transition metal dichalcogenides

WANG YAO, The University of Hong Kong — In two-dimensional (2D) transition metal dichalcogenides (TMDs), carriers are indexed by both the spin and the valley pseudospin (labelling the degenerate band extrema in momentum space). 2D TMDs is therefore an ideal laboratory for exploring these internal quantum degrees of freedom for new electronics, and controlling the flow of spin and pseudospin is at the heart of such applications. We will discuss two mechanisms for generating spin and valley currents of electrons in 2D group-VIB TMDs: (I) the valley and spin Hall effects arising from the Berry curvatures; and (II) the nonlinear valley and spin currents arising from Fermi pocket anisotropy. The two effects have distinct scaling with the electric field, and different dependence of the current direction on the field direction and crystalline axis. We will discuss the possibility to observe and distinguish the two effects as distinct patterns of polarized electroluminescence at p-n junction in 2D TMDs. The nonlinear current response also makes possible the generation of pure spin and valley flows without net charge current, either by an AC bias or by an inhomogeneous temperature distribution. We will also discuss the valley Hall effect of charged excitons in monolayer TMDs, which arises from the effective coupling of the excitonic valley pseudospin to its center of mass motion by the exchange interaction between the electron and hole constituents.

10:24AM S51.00005 Electron dynamics and valley relaxation in 2D semiconductors

KENAN GUNDOGU, North Carolina State University — Single layer transition metal dichalcogenides are 2D semiconducting systems with unique electronic band structure. Two-valley energy bands along with strong spin-orbital coupling lead to valley dependent career spin polarization, which is the basis for recently proposed valleytronic applications. Since the durations of valley population provide the time window in which valley specific processes take place, it is an essential parameter for developing valleytronic devices. These systems also exhibit unusually strong many body affects, such as strong exciton and trion binding, due to reduced dielectric screening of Coulomb interactions. But there is not much known about the impact of strong many particle correlations on spin and valley polarization dynamics. Here we report direct measurements of ultrafast valley specific relaxation dynamics in single layer MoS2 and WS2. We found that excitonic many body interactions significantly contribute to the relaxation process. Brixelcton formation reveals hole valley spin relaxation time. Our results also suggest initial fast intervalley electron scattering and electron spin relaxation leads to loss of electron valley polarization, which then facilitates hole valley relaxation via excitonic spin exchange interaction.
8:00AM S52.00001 Emergent Separation of Valence Bond Regimes in LiZn$_2$Mo$_2$O$_7$\cite{2}. TYREL Mc-QUEEN, Johns Hopkins University — LiZn$_2$Mo$_2$O$_7$ is a S = 1/2 triangular lattice antiferromagnet in which the basic magnetic building block is an Mo$_3$O$_13$ cluster rather than an individual ion. Rather than forming the 120° ordered magnetic state expected for a Heisenberg nearest neighbor triangular antiferromagnet, LiZn$_2$Mo$_2$O$_7$ instead favors a complex valence bond order across different energy and length scales: approximately two thirds of the spins form singlets at T ∼ 100 K, while the remainder form valence bonds at lower temperature, as indicated by inelastic neutron scattering. No static magnetic order is detected by uSR down to T = 0.05 K. What is the origin of this spontaneous separation into different regimes of magnetic fluctuations? Recent experimental data, including the impact of hole doping, will be compared to different theoretical models that have been proposed for this behavior, including an emergent honeycomb lattice by octahedral rotations and partial charge ordering driven by extra intracluster degrees of freedom.

\textsuperscript{1}Supported by U.S. DoE Basic Energy Sciences, Materials Sciences & Engineering DE-FG02-08ER46544

8:36AM S52.00002 Low energy XY spin clusters in a pyrochlore antiferromagnet with weak disorder\textsuperscript{1}. KATE ROSS$^2$, Colorado State University — The spin liquid state of the Heisenberg antiferromagnet (HAFM) on the pyrochlore lattice arises from an extensive degeneracy of correlated yet disordered ground states. How this spin liquid is modified in real materials with imperfect Heisenberg exchange is a rich field of study, with many possible outcomes depending on the relevant perturbations. We have studied a single crystal of a new pyrochlore antiferromagnet, NaCaCo$_2$Fe$_2$. High spin (S = 3/2) Co$^{3+}$ forms a fully ordered pyrochlore sub lattice, while non-magnetic Na$^+$ and Ca$^{2+}$ are intermixed on the A-site. Despite isotropic magnetic properties and large antiferromagnetic coupling (\Theta_{CW} = -140 K), a freezing transition is observed at temperature much lower than the exchange energy (\Gamma \sim 3 K), thus revealing the relatively weak exchange disorder induced by the mixed ion A-site. Unexpectedly, our inelastic neutron scattering measurements reveal that the frozen state is of local XY character and supports low energy XY fluctuations. Yet the system can break free from the XY states at energies above 2.5 meV \sim 3 K; at these energy scales we observe the collinear Ising configurations expected for the weak-disorder HAFM model. The frozen state in NaCaCo$_2$Fe$_2$ provides a new outlook on the role of disorder in selecting spin configurations from the Heisenberg pyrochlore spin liquid state.

\textsuperscript{1}Supported by NSERC of Canada
\textsuperscript{2}Supported from NSERC of Canada

9:12AM S52.00003 Longitudinal and transverse heat transports of quantum spin liquids. MINORU YAMASHITA, ISSP, The University of Tokyo — Study of disordered states of quantum spins in two-dimensions, so-called quantum spin liquids (QSLs), has been attracting attention because 2D QSL can be a new state of matter characterized by unknown quasiparticles. Recent discoveries of materials possessing an ideal 2D triangular or a kagomé lattice have spurred a lot of experimental pursuit to identify the ground state. Especially, identifying the elementary excitation characterizing the ground state has been the central focus of attention. In this presentation, I will present our transport studies of organic insulators with ideal 2D triangular or a kagomé lattice have spurred a lot of experimental pursuit to identify the ground state. Especially, identifying the elementary excitation characterizing the ground state has been the central focus of attention.


9:48AM S52.00004 Doping and disorder in spin liquids. RODERICH MOESSNER, MPI-PKS Dresden — The question of what happens when an unconventional spin state is doped has been a central theme of the field of strongly correlated electrons since Anderson’s proposal of doping the RVB liquid state to obtain a high-temperature superconductor. Recently, there has been much progress in constructing models which exhibit topological spin liquid phases, e.g. in Kitaev’s models or in spin ice. In this talk, we address the properties of defects in such exotic spin states.

10:24AM S52.00005 Unconventional magnetic order stabilized by Kitaev interactions in the three-dimensional honeycomb polytypes of Li$_2$IrO$_3$. RADU COLDEA, University of Oxford — Materials that realize Kitaev spin models with bond-dependent anisotropic interactions have long been searched for, as the resulting frustration effects are predicted to stabilize novel forms of magnetic order or quantum spin liquids. Here we explore the magnetism of the recently-synthesized iridates \beta- and \gamma-Li$_2$IrO$_3$, which have the topology of three-dimensional Kitaev lattices of inter-connected Ir honeycombs. Using single-crystal resonant magnetic x-ray diffraction we find in both cases a surprisingly complex, yet highly symmetric, incommensurate magnetic structure with non-coplanar and counter-rotating Ir moments \cite{1,2}. Our experimental results combined with a theoretical analysis \cite{3} of candidate spin Hamiltonians provide strong evidence that both \beta and \gamma-Li$_2$IrO$_3$ realize a spin Hamiltonian with dominant Kitaev interactions. \cite{1} A. Biffin, R.D. Johnson, I. Kimchi, R. Morris, A. Bombardi, J.G. Analytis, A. Vishwanath, and R. Coldea, Phys. Rev. Lett. 113, 197201 (2014). \cite{2} A. Biffin, R.D. Johnson, Sungkyun Choi, F. Freund, S. Manni, A. Bombardi, P. Manuel, P. Gegenwart, and R. Coldea, Phys. Rev. B. 90, 205116 (2014). \cite{3} I. Kimchi, R. Coldea and A. Vishwanath, arXiv:1408.3640 (2014).

Thursday, March 5, 2015 8:00AM - 11:00AM —
Session S53 DCMP: Invited Session: Symposium on Novel Phenomena in Helium in Reduced Dimensions and Confinement —
Grand Ballroom C3 - Yoonseok Lee, University of Florida

8:00AM S53.00001 Evidence for intertwined superfluid and density wave order in two dimensional $^4$He\textsuperscript{1}. JOHN SAUNDERS, Royal Holloway University of London — We report the identification of a new state of quantum matter with intertwined superfluid and density wave order in a system of two dimensional bosons subject to a triangular lattice potential. Using a torsional oscillator we have measured the response of the second atomic layer of $^4$He adsorbed on the surface of graphite over a wide temperature range down to 2 mK. Superfluidity is observed over a narrow range of film densities, emerging suddenly and collapsing towards a quantum critical point, near to layer completion where a Mott insulating phase is predicted to form. The unusual temperature dependence of the superfluid density in the $T \rightarrow 0$ limit and the absence of a clear superfluid onset temperature are explained, self-consistently, by an ansatz for the excitation spectrum, reflecting density wave order, and a quasi-condensate wavefunction breaking both gauge and translational symmetry.

\textsuperscript{1}Supported by EPSRC (U.K) EP/H048375/1
8:36AM S53.00002 Signatures of Majorana and Weyl Fermions in confined phases of superfluid $^3$He$^1$. JAMES SAULS, Northwestern Univ — The B-phase of superfluid $^3$He exhibits symmetry breaking in which separate invariance under gauge-, spin- and orbital rotations is reduced to the maximal sub-group, $SU(2)_L \otimes SU(2)_T$. Parity is broken, but time-reversal is preserved. Broken relative spin-orbit rotational symmetry implies emergent spin-orbit coupling and non-trivial topology of the ground state, both of which are encoded in the Bogoliubov-Nambu Hamiltonian: $H = (p^3 \tau_3 + c \cdot \tau_i) / \Delta / T$, where $c = \Delta / T$ is several orders of magnitude slower than the Fermi velocity. The topology of the B-phase is expressed in terms of a non-trivial winding number for the mapping between momentum space and Nambu space, $\pi_{3D} = \int \frac{d^3p}{24\pi} \epsilon_{ijk} \text{Tr} \left\{ T C (H^{-1} \partial_{\tau_j} H) \times (H^{-1} \partial_{\tau_k} H) (H^{-1} \partial_{\tau_i} H) \right\} = 2$, where $C$ is the particle-hole transformation. The physical consequence of $\pi_{3D} \neq 0$ is the emergence of a spectrum of Majorana fermions confined on any surface of $^3$He-B whose effective Hamiltonian is described $H = \sum_{p} \sum_{\alpha} \psi^\dagger_{\alpha,p} (\tau_3 + c \cdot \sigma) \psi_{\alpha,p}$. The surface excitations are self-conjugate Majorana fermions with a gapless relativistic dispersion relation $\epsilon(p) = c |p|$, and their spins locked normal to the in-plane momentum and the surface normal, $\mathbf{z}$. In this talk I describe theoretical predictions for experimental signatures based on NMR, mass flow, local ion probes and ultra-sound spectroscopy of these unique quanta that reflect the topological nature of the ground state of superfluid $^3$He.

3Supported by NSF Grant DMR-1106315.

9:12AM S53.00003 Observation of the Polar Phase of $^3$He$^1$. JEEVAK PARPIA, Department of Physics, Cornell University, Ithaca NY 14853 — Exotic pairing of Fermions into a condensed bound state is now well established in many systems. In superfluid $^3$He it is becoming evident that the nature and stability of the emergent order parameter can be altered radically by confinement in regular geometries or by providing anisotropic disorder realized in materials whose nanoscale structure is smaller than the coherence length. The temperature dependent coherence length diverges as the superfluid transition is approached from below and sets the characteristic length scale for confinement. Thus, the degree of confinement can be varied as the temperature is varied below Tc. Additionally, unlike most superconductors, the $^3$He liquid’s properties can be pressure-tuned over a large range. In bulk liquid, (in zero magnetic field) there are two equivalence phases of $^3$He: at high pressure, as the temperature is lowered there is a transition from the chiral A phase to the isotropic B phase. In bulk liquid, the relative stability of the two phases is controlled not by confinement but by strong-coupling interactions. In our highly confined system, both factors (confinement and strong coupling) come into play and depending on pressure we see a succession of two transitions (three phases) within the superfluid as the sample is cooled from the normal state. Drawing on theoretical work we identify the phases as the Polar phase near Tc, followed by a polar distorted A or B phase (depending on pressure) with the low-temperature phase being the B phase at all pressures. These observations are made with a toroidal pendulum that was used to assay the superfluid fraction and the disordered medium is the so-called “Obninsk” alumina aerogel that has highly oriented strands aligned with the torsional axis.

3Research supported by the NSF-DMR1202991.

9:48AM S53.00004 Probing the A-B interface of superfluid helium-3. RICHARD HALEY, Lancaster University — At temperatures around 1 mK helium-3 forms a BCS spin triplet condensate. The order parameter is sufficiently complex that more than one superfluid phase coexists, each exhibiting a different broken symmetry, and there is a model first order transition between the two most stable phases, labeled A and B. The Lancaster Ultra-Low Temperature Group has developed techniques to probe the properties of the A-B interface in the deep sub-mK regime where the superfluid is in the pure condensate phase. Shaped and controllable magnetic fields are used to induce the transition, and to stabilize and move the A-B phase boundary inside the experimental volume. The latent heat of the transition has been measured, and the nucleation behavior shown to be incompatible with conventional thin film droplet nucleation dynamics. In this setup it is the most coherent two-dimensional structure in which we have experimental access. It has been proposed that this 2D surface in the surrounding 3D bulk volume is a good analog of a cosmological brane separating two distinct quantum vacuum states; experiments that simulate brane annihilation and the creation of topological defects have been carried out at Lancaster. Other investigations have included measurements of the surface tension and wetting behavior of the interface. During these studies it was discovered that a large, unpredicted frictional force was acting on the interface even though it is moving through a pure superfluid. Recent breakthrough work on the dynamics of the A-B interface has finally solved this puzzle. Current experiments include a setup where the interface region is probed directly using quartz tuning fork resonators that couple to the local density of broken Cooper pair quasiparticle excitations and thus give insight into the order parameter energy gap structure as A transforms to B.

10:24AM S53.00005 One-dimensional Quantum Fluids. GUILLAUME GERVAIS, McGill University — Fifty year ago, Joachim Mazdak Luttinger generalized the Tomonaga theory of interactions in a one-dimensional metal and show that the prior restrictions imposed by Tomonaga were not necessary. This model is now known as the Tomonaga-Luttinger liquid model (TLL) and most remarkably it does have mathematically exact solutions. In the case of electrons, it predicts that the spin and charge sector should separate, with each of them propagating with their own velocities. While there has been many attempts (some with great success) to observe TLL behavior in clean quantum wires designed on an ultra-clean semiconductor platform, overall the Luttinger physics is experimentally still in its infancy. For instance, little is known regarding the 1D physics in a strongly-interacting neutral system, whether from the point-of-view of TLL theory or even localization physics. Helium-4, the paradigm superfluid, and Helium-3, the paradigm Fermi liquid, should in principle both become Luttinger liquids if taken to the one-dimensional limit. In the bosonic case, this is supported by large-scale Quantum Monte Carlo simulations [1] which found that a lengthscale of ~ 2 nm is sufficient for the system to crossover to the 1D regime and display universal Luttinger scaling [2]. At McGill University, an experiment has been constructed to measure the liquid helium mass flow through a single nanopore. The technique consists of drilling a single nanopore in a SiN membrane using a TEM, and then applying a pressure gradient across the membrane. Previously published data in 45nm diameter hole has determined the superfluid critical velocity to be close to the limit set by the Feynman vortex rings model [3]. More recent work performed on nanopores with radii as small as 3 nm (and a length of 30nm) show that superfluid velocity for superfluid helium-3 to significantly deviate from its bulk value, 2/3. This is an important hint for the crossing over to the one-dimensional state in a strongly-correlated bosonic liquid. References:[1] Del Maestro A, Boninsegni M, Affleck I. [2] Klichkhytzyk B, Gervais G, Del Maestro A. Local superfluidity at the nanoscale. PHYSICAL REVIEW B 88: 064512, 2013. [3] Savard M, Dauphinais G, Gervais G. Hydrodynamics of Superfluid Helium in a Single Nanohole. PHYSICAL REVIEW LETTERS 107: 254501, 2011.

Thursday, March 5, 2015 11:15AM - 2:15PM – Session T1 DMP: Focus Session: Beyond Graphene - Silicene and Germanene 001A - Roland Kawakami, Ohio State University

11:15AM T1.00001 Electron Energy Loss Spectroscopy Studies of Silicene and Graphene. OLEKSIV ROSLYAK, ANTONIOUS BALASSIS, Fordham University, NY, GODFREY GUMBS, Hunter College, CUNY, NY — Silicene is the silicon counterpart of graphene. However, the spin-orbit interaction in silicene opens up a substantial band gap. Consequently, there is an unambiguous low-frequency plasmon excitation originating from intra- and inter-band transitions. Both the plasmon intensity and lifetime depend on the width of the excitation gap separating electron-hole pairs. We present a formalism based on self-consistent field theory to investigates the rate of loss of energy of a beam of charged particles moving parallel and perpendicular to a silicene layer. The energy loss spectrum is presented as a function of the speed of the charged particles. We further study and compare the part of the energy absorbed by collective plasma excitation as well as by single particle excitations. We report clear spectral signatures of semi-metal to either band insulator or topological insulator. Plasmonic features of silicene flakes are also studied and compared to those of pristine graphene.
11:27AM T1.00002 Large Area Transfer and Optoelectronic Properties of Multilayer Epitaxial Germanane. VALID AMAMOU, PATRICK ODENTHAL, University of California Riverside. BETH BUSHONG, The Ohio State University, DANTE O'HARA, University of California Riverside, YUN LIU, The Ohio State University, JEREMIAH VAN BAREN, University of California Riverside, IGOR PINCHUK, The Ohio State University, YU WU, MARC BOCKRATH, HARRY TOM, University of California Riverside, JOSHUA GOLDBERGER, ROLAND KAWAKAMI, The Ohio State University — Germanane (GeH), the germanium-based analog of graphene (CH), is of particular interest due to its direct band gap and surface coherent functionalization. Furthermore, its large spin orbit coupling makes it possible to explore novel physical phenomena such as quantum spin hall effect at room temperature. Currently, large area GeH films are synthesized on Ge(111) wafers using substrate reaction or molecular beam epitaxy combined with chemical processing. This results in a high quality GeH film that is left on top of the germanium substrate. In order to perform the electrical characterization of GeH, it is required to transfer the film to an insulating substrate. Here, we demonstrate a highly efficient, nondestructive electrochemical route for the transfer of molecular beam epitaxy (MBE) GeH film from Ge(111) surfaces. This technique enables us to characterize the optoelectronic properties of epitaxial GeH after transfer such as I-V characteristics and photoconductivity wavelength dependence.

11:39AM T1.00003 Band Parameters of Two-Dimensional Materials: Phosphorene and Silicene. LOK LEW YAN VOON, The Citadel, ALEJANDRO LOPEZ BEZANILLA, Argonne National Lab, JIANWEI WANG, YONG ZHANG, U North Carolina Charlotte, MORTEN WILLATZEN, Technical University Denmark — The method of invariant is used to derive effective Hamiltonians in the presence of strain and external fields for phosphorene and silicene as examples of two-dimensional materials with and without a band gap. The band structure parameters have been obtained by fitting to density-functional theory calculations.

11:51AM T1.00004 Temperature-dependent phase transitions in epitaxial silicene on ZrB2(0001). ANTOINE FLOURENCE, YUKIKO YAMADA-TAKAMURA, Japan Advanced Institute of Science and Technology — Silicene differs from graphene, its carbon counterpart, by a mixed sp2/sp3 hybridization of the Si atoms that gives it particularly interesting mechanical and electronic properties. Silicene can form by the spontaneous and self-terminating segregation of Si atoms on the (0001) surface of zirconium diboride (ZrB2) thin films grown on Si(111) [1]. This stable form of silicene is particularly suitable for the investigation of the temperature dependence of its mechanical properties. Whereas, the amount of Si atoms does not vary, scanning tunneling microscopy and low-energy electron diffraction clearly indicate that two reversible phase transitions occur when the temperature is raised. At room-temperature, the silicene sheet is textured into one-dimensional arrays of interconnected 2.7 nm-wide ribbon-shaped stress domains [1]. Around 870 K, this ordered surface evolves into a surface made of wider domains with no ordering of the domain boundaries. At 930 K, the silicene sheet loses its structure and turns into a two-dimensional gas of Si atoms. While cooling down, silicene crystallizes reversibly. The origin of the phase transitions of epitaxial silicene will be discussed. [1] A. Fluorence et al. Phys. Rev. Lett. 108 245501 (2012).

12:03PM T1.00005 Electron confinement at the Si-MoS2 heterostructure junction. ALESSANDRO MOLLE, DANIELE CHIAPPE, CNR-IMM, Laboratorio MDM, DAVIDE RONDA, CNR-IMM, Laboratorio MDM & Universita degli studi di Milano Bicocca, ALESSIO LAMPERTI, CARLO GRAZIANETTI, EUGENIO CINQUANTA, CNR-IMM, Laboratorio MDM, MARCO FANCIULLI, CNR-IMM, Laboratorio MDM & Universita degli studi di Milano Bicocca — Two dimensional (2D) elementary materials such as silicene, germanene or phosphorene are emerging alternatives to graphene which has the consolidated class of layered metal dichalcogenides. In particular, 2D silicon nanosheets would benefit from the potential integration with the quite ubiquitous Si technology thus opening new scaling perspectives of the conventional electronic devices. In this framework we report here on the 2D epitaxy of a Si monolayer onto a MoS2 template with a locally hexagonal registry [1]. The experimental data are consistent with an ab initio calculated highly stretched silicene lattice [2]. High resolution photoemission spectroscopy investigations evidence a nearly metallic character of the Si nanosheet and a significant band bending on the MoS2 side which claims for a Si-induced electron accommodation. Integration into a bottom gated field effect transistor results in the effective transport at the Si/MoS2 heterostructure interface which is rationalized in terms of an electronic confinement. [1] Chiappe et al, Adv. Mater. 26, 2096 (2014); [2] Scalise et al, 2D Materials 1, 011010 (2014).

12:15PM T1.00006 Poisson's Ratio of Layered Two-dimensional Crystals. SUNGJONG WOO, HEE CHUL PARK, YOUNG-WOO SON, Korea Institute for Advanced Study — We have investigated the elastic properties of multilayered graphene as well as h-BN and MoS2 using a first-principles approach with up-to-date nonlocal exchange-correlation energy functional. Our analysis shows that the Poisson’s ratios of multilayered graphene, h-BN and MoS2 along out-of-plane direction are negative, near zero and positive, respectively, spanning all possibilities for signs of the ratios. While h-BN’s Poisson’s ratios are positive regardless of their disparate electronic and structural properties, the characteristic interlayer interactions as well as atomic stacking structures are shown to determine the sign of their out-of-plane ratios, highlighting their intertwined nature between elastic and electronic properties.

12:27PM T1.00007 Observation of Strong Intermode Coupling in a MoS2 Mechanical Resonator. CHANG-HUA LIU, IN SOO KIM, SPENCER PARK, KUNHO YOON, SARAH HOWELL, LINCOLN LAUHON, Northwestern University — Achieving the strong coupling regime in downscaled oscillators facilitates quantum control of macroscopic mechanics. Many approaches, including the use of dynamical backaction between mechanical resonators and photonic or superconducting cavities, require sophisticated device structures. We will describe strong mode coupling in a simple system: an ultrathin MoS2 mechanical resonator. Thermal fluctuations are exploited to study different vibrational modes of the resonator and observe avoided crossings in the vibrational spectra, indicating the entanglement of mechanical motion. Furthermore, when parametrically pumping the resonator with light, the dynamic optically induced strain leads to Stokes and anti-Stokes sidebands as well as normal-mode splitting. These signatures provide strong evidence that phonon populations can be redistributed between different vibrational modes, and also confirm that an MoS2 resonator can be operated into the strong coupling regime. These observations further suggest that 2D materials could offer a platform for developing full quantum control of nanomechanics.

12:39PM T1.00008 Measuring nanoscale friction between 2D materials and SiO2: hBN, MoS2 and Phosphorene. JASON CHRISTOPHER, Boston University, STEVEN KOENIG, National University of Singapore, ANGELO ZILETTI, Boston University, BO WEN, ZHENG HAN, Columbia University, ALEX KITT, XIANYE WANG, LOGAN KAGEORGE, Boston University, CORY DEAN, Columbia University, BARBAROS OZYILMAZ, National University of Singapore, ANNA SWAN, BENNETT GOLDBERG, Boston University — Unlike their 3D counterparts, 2D materials can be tuned with strain, leading to “strain engineering” of electrical, optical and thermal properties. Control of the precise location, magnitude and direction of a strain field depends critically on characterizing and understanding any motion or sliding between the 2D material and its anchor points. With this goal in mind, we determine the friction between three different atomically thin materials and a SiO2 substrate. Our experimental setup consists of cylindrical, micro-chambers we etch into a SiO2 substrate and seal with a 2D material membrane. We pressurize the outside of the micro-chamber, causing the 2D material to deform and slide on the substrate. The resulting strain distribution and amount of sliding is mapped using high spatial resolution Raman spectroscopy from which we determine the friction, Grüneisen and shear deformation potentials. MoS2, hBN, and Phosphorene have been chosen because they are good candidates for strain engineering applications. Additionally, in the case of MoS2 and Phosphorene we measure the photoluminescence spectrum from which we determine the strain dependence of the band gap.

\[1\] J. Christopher thanks the NDSEG program for its support.
Here we report studies of 2D layers formed by depositing Si on silicene/ZrB$_2$ going from the mono- to multi-layer regime. Recent experiments studying multiple Si layers on Ag(111) have shown that, remarkably, the multilayers are more metallic than the monolayer[2]. In the past two years, there have been quite a few experimental attempts to grow silicene on Ag(111). However, there are still controversies about whether a silicene layer with massless Dirac fermions actually exists on Ag(111). Chen et al. [1] measured the interference patterns in the differential conductance map by scanning tunneling spectroscopy and found a linear dispersion relation as the evidence for the existence of massless Dirac fermions. On the other hand, Lin et al. [2] found no Landau level sequences appearing in the tunneling spectra under a magnetic field, concluding that the Si-Ag interaction is strong enough to break the symmetry of silicene. In order to resolve these conflicting experimental findings, we have studied various Si/Ag configurations on the surface and their related electronic structures using first-principles density-functional calculations. Comparisons with experimental results will be discussed. [1] Chen et al. Phys. Rev. Lett. 109, 056804 (2012). [2] Lin et al., Phys. Rev. Lett. 110, 076801 (2013).

1:15PM T1.00011 Heterostructures by inserting Oxygen Monolayers in Si: 2D Nanolattice Growth, Electronic properties and MOSFET Device Characteristics 1, SUSEENDRAN JAYACHANDRAN, KOEN MARTENS, AUGUSTIN LU, imec / KULeuven, KENGO NISHIO, AIIST, GEOFFREY POURTOIS, imec / KULeuven, ANNELIES DELABIE, MATTY CAYMAX, imec, MARC HEYNS, imec / KULeuven — We discuss how heterostructures can be created in silicon by inserting oxygen monolayers, as well as what Density Functional Theory simulations predict in terms of electronic properties of these 2D nanolattices. We also discuss the experimental electrical characteristics of Metal-Oxide-Semiconductor Field Effect Transistors with 2D nanolattices channels. By using short (up to 500ms) low temperature O$_2$ reaction on H-terminated Si, the deposited O content can be controlled near the monolayer level, as demonstrated by SIMS measurements. Epitaxial deposition of Si on an O layer and 2D nanolattices with up to 5 periods have been achieved by CVD using SiH$_4$ at 500C. We discuss the structural and electronic properties calculated with density functional theory and give an overview of the most promising Si superlattices in terms of anticipated mobility enhancement. We report on the electrical device characteristics of 2D nanolattice Schottky diodes, MOS capacitors and MOSFETs. We discuss the impact of defectivity on electrical characteristics and the impact of the 2D nanolattices on MOSFET carrier mobility.

1:27PM T1.00012 Intrinsic magnetism, band gap opening and optical absorption in bilayer silicene 1, XINQUAN WANG, ZHIGANG WU, Department of Physics, Colorado School of Mines, WU’S CONDENSE MATTER GROUP TEAM — It has been long known to create magnetism out of simple non-magnetic materials like silicon. Here we show that intrinsic magnetism exists in bilayer silicene with no need to cut, etch, or dope. Unlike bilayer graphene, strong covalent interlayer bonds formed in bilayer silicene breaks the original π-networking of each layer, leaving the un-bonded electrons unpaired and localized to carry magnetic moments. These magnetic moments then couple ferromagnetically within each layer while antiferromagnetically across layers, giving rise to an infinite magnetic sheet with structural integrity and magnetic homogeneity. Our ab initio many-body calculations using the GW approach reveals that the unique magnetic ordering results in a fundamental band gap of 0.55 eV. Furthermore, we computed absorption spectrum by solving the Bethe-Salpeter equation, and our results suggest very strong absorption near the absorption edge. The integration of intrinsic magnetism and spontaneous band gap opening makes bilayer silicene attractive to future nanoelectronics as well as spin-based computation and data storage. This material could also be used as excellent light absorber, and its small band gap and one-dimensional confinement might be employed for efficient multi-exciton generation.

This work was supported by a U.S. DOE Early Career Award (Grant No. DE-SC0006433).

1:39PM T1.00013 Structural and electronic properties of 2D Si layers formed by deposition of Si on silicene / ZrB$_2$ 1, CYRUS F. HIRJIBEHEDIN, TOBIAS G. GILL, BEN WARNER, HENNING PRUESER, UCL, UK, KOHEI AOYAGI, RAINER FRIEDELIN, ANTOINE FLEURÉNCE, JAIST, Japan, JERZY SADOWSKI, Brookhaven National Laboratory, USA, YUKIKO YAMADA-TAKAMURA, JAIST, Japan — Silicene has been predicted to share many interesting properties with graphene. These are significantly modified by interactions with the metallic substrates in existing epitaxial silicene systems[1]. For many 2D layered materials, like graphene and MoS$_2$, these properties can change dramatically when going from the mono- to multi-layer regime. Recent experiments studying multiple Si layers on Ag(111) have shown that, remarkably, the multilayers are more metallic than the monolayer[2]. Here we report studies of 2D layers formed by depositing Si on silicene/ZrB$_2$. Using LEED, STM, and ARPES, we find that the deposition of very small amounts of Si cause structural changes to the silicene monolayer without strongly modifying its electronic properties. Additional deposition of Si causes structural changes to the first Si layer and results in a different structural domain and is more metallic. This trend continues for 3 ML up to the deposition of 10 ML. These result illustrate the rich array of properties that can be manifested in novel 2D Si nanostructures and highlight the dramatic variation in Si phases that can be seen on different substrates. [1] A. Fleurence et al., PRL 108, 245501 (2012) [2] P. Vogt et al., APL 104, 021602 (2014)

1:51PM T1.00014 Silicene on Silver: fundamental physical properties and integration in Field-Effect Transistors 1, EUGENIO CINQUANTA, Laboratorio MDM, IMM-CNR, via C. Olivetti 2, Agrate Brianza, I-20864, Italy, LI TAO, Microelectronics Research Center, The University of Texas at Austin, Texas 78758, USA, GUIDO FRATESI, ETSF and Dipartimento di Fisica, Università degli Studi di Milano, Milano, Italy, CARLO GRAZIANETTI, MARCO FANCIULLI, Laboratorio MDM, IMM-CNR, via C. Olivetti 2, Agrate Brianza, I-20864, Italy, GIOVANNI ONIDA, ETSF and Dipartimento di Fisica, Università degli Studi di Milano, Milano, Italy, DEJJ AKINWANDE, Microelectronics Research Center, The University of Texas at Austin, Texas 78758, USA, ALESSANDRO MOLLE, Laboratorio MDM, IMM-CNR, via C. Olivetti 2, Agrate Brianza, I-20864, Italy — To date, Silicene encountered different bottlenecks as reliable option in the framework of two-dimensional materials beyond graphene. Its physical properties are not completely unveiled and this, combined with its environmental instability, limits its possible integration into devices. Here we show a comprehensive characterization of Silicene by combining ab-initio calculations with optical spectroscopies. We elucidate the role of Ag in determining the electronic band structure and the optical response of differently oriented Silicene superstructures. We also show how these fundamental properties reflect in devices by presenting the experimental evidence of the ambipolar electrical transport in Silicene based field effect transistor.
The linewidth of the quasi-particle states. The impact of temperature on the exciton states is also addressed. We discuss the bandgap dependence on the temperature, and the change in the framework of the GW method we calculate the contribution of the electron-phonon coupling to the self-energy. This allows us to calculate the zero-point density of states and a step-function turn on in the density of modes. The largest radius of the ring of states occurs for a single monolayer of each material. In one to four monolayers of the group-III chalcogenides (GaS, GaSe, InS, InSe) and Bi$_2$Se$_3$ the valence band undergoes a band inversion from a parabolic to an inverted Mexican hat dispersion as the film thickness is reduced from bulk to a single monolayer. The band inversion is robust against changes in stacking order, omission or inclusion of spin-orbit coupling and the choice of functional. The Mexican hat dispersion results in a $1/\sqrt{E}$ singularity in the two-dimensional density of states and a step-function turn on in the density of modes. The largest radius of the ring of states occurs for a single monolayer of each material. The dispersion with the largest radius coincides with the maximum power factor and ZT for a material at room temperature. Ab-initio electronic structure calculations are used with a Landauer approach to calculate the thermoelectric transport coefficients. Analytical models of the Mexican hat and the parabolic dispersions are used for comparison and analysis. Vertically biased bilayer graphene could serve as an experimental test-bed for measuring this effect since the radius of the Mexican hat band edge increases linearly with vertical electric field.

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**Ming-wei Wu, University of Science and Technology, China**

11:15AM T2.00001 ABSTRACT MOVED TO W1.00010 —

11:27AM T2.00002 Electronic and thermoelectric properties of Mexican hat bands in van-der-Waals materials$^1$, DARSHANA WICKRAMARATNE, University of California - Riverside, FERDOWS ZAHID, The University of Hong Kong, Hong Kong SAR, China, ROGER LAKE, University of California - Riverside — Mexican hat dispersions are relatively common in few-layer two-dimensional materials. In one to four monolayers of the group-III chalcogenides (GaS, GaSe, InS, InSe) and Bi$_2$Se$_3$ the valence band undergoes a band inversion from a parabolic to an inverted Mexican hat dispersion as the film thickness is reduced from bulk to a single monolayer. The band inversion is robust against changes in stacking order, omission or inclusion of spin-orbit coupling and the choice of functional. The Mexican hat dispersion results in a $1/\sqrt{E}$ singularity in the two-dimensional density of states and a step-function turn on in the density of modes. The largest radius of the ring of states occurs for a single monolayer of each material. The dispersion with the largest radius coincides with the maximum power factor and ZT for a material at room temperature. Ab-initio electronic structure calculations are used with a Landauer approach to calculate the thermoelectric transport coefficients. Analytical models of the Mexican hat and the parabolic dispersions are used for comparison and analysis. Vertically biased bilayer graphene could serve as an experimental test-bed for measuring this effect since the radius of the Mexican hat band edge increases linearly with vertical electric field.

$^1$Support by the NSF and SRC-NRI project 2204.001 (NSF-ECCS-1124733), FAME, one of six centers of STARnet, a SRC program sponsored by MARCO and DARPA and the use of XSEDE NSF grant # OCI-1053575.

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**11:39AM T2.00003 Ab-initio study of the temperature effects on the optical properties of transition metal dichalcogenides** , ALEJANDRO MOLINA-SANCHEZ, Physics and Material Sciences Research Unit, University of Luxembourg — MAURIZIA PALUMMO, Dipartimento di Fisica, University of Rome Tor Vergata, Italy, ANDREA MARINI, Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, Monterotondo, Italy, LUDGER WIRTZ, Physics and Material Sciences Research Unit, University of Luxembourg — Research on ultra-thin two-dimensional materials has been booming since the discovery of graphene along with its interesting physical properties. The transition metal dichalcogenides as MoS$_2$ are gaining considerable industrial attention due to their potential application in photovoltaics and nanoscale transistors. The optical properties of these layered materials depend strongly on the number of layers. The paradigmatic example is the transition from indirect to direct bandgap when we change from multi-layer to single-layer MoS$_2$. In this work, we study the effects of the electron-phonon interaction on the optical properties of single-layer MoS$_2$. In the framework of the GW method we calculate the contribution of the electron-phonon coupling to the self-energy. This allows us to calculate the zero-point re-normalization of the quasi-particle energies and to include temperature effects. We discuss the bandgap dependence on the temperature, and the change in the linewidth of the quasi-particle states. The impact of temperature on the exciton states is also addressed.

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**11:51AM T2.00004 Interaction and Correlation Effects in Quasi Two-dimensional Materials$^2$** , STEVEN G. LOUIE, Univ of California - Berkeley and Lawrence Berkeley National Lab — Experimental and theoretical studies of atomically thin quasi-two-dimensional materials (typically related to some parent van der Waals layered crystals) and their nanostructures have revealed that these systems can exhibit highly unusual behaviors. In this talk, we discuss some theoretical studies of the electronic, transport and optical properties of such systems. We present results on graphene and graphene nanostructures as well as other quasi-2D systems such as monolayer and few-layer transition metal dichalcogenides (e.g., MoS$_2$, MoSe$_2$, W$_2$S$_2$, and WSe$_2$) and metal monochalcogenides (such as GaSe and FeSe). Owing to their reduced dimensionality, these systems present opportunities for unusual manifestation of concepts and phenomena that may not be so prominent or have not been seen in bulk materials. Symmetry and many-body interaction effects often play a critical role in shaping qualitatively and quantitatively their properties. Several quantum phenomena are discussed, including novel and dominant exciton effects, tunable magnetism, electron supercollimation by disorder, unusual plasmon behaviors, and possible enhanced superconductivity in some of these systems. We investigate their physical origins and compare theoretical predictions with experimental data.

$^2$This work was supported by DOE under Contract No. DE-AC02-05CH11231 and by NSF under Grant No. DMR10-1006184. I would like to acknowledge collaborations with members of the Louie group and the experimental groups of Crommie, Heinz, Wang, and Zhang.

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**12:27PM T2.00005 Atomic model for excitons: Capturing Strongly Bound Excitons in Monolayer Transition-Metal Dichalcogenides$^3$** , FRANK TSENG, Naval Research Laboratory, ERGUN SIMSEK, George Washington University, DANIEL GUNLYCKE, Naval Research Laboratory — Monolayer transition-metal dichalcogenides form a direct bandgap predicted in the visible regime making them attractive host materials for various electronic and optoelectronic applications. Due to a weak dielectric screening in these materials, strongly bound electron-hole pairs or excitons have binding energies up to at least several hundred meV’s. While the conventional wisdom is to think of excitons as hydrogen-like quasi-particles, we show that the hydrogen model breaks down for these experimentally observed strongly bound, room-temperature excitons. To capture these non-hydrogen-like photo-excitations, we introduce an atomistic model for excitons that predicts both bright excitons and dark excitons, and as hydrogen-like quasi-particles, we show that the hydrogen model breaks down for these experimentally observed strongly bound, room-temperature excitons. For strongly bound exciton states, the lattice potential significantly distorts the envelope wave functions, which affects predicted exciton peak energies. The combination of large binding energies and non-degeneracy of exciton states in monolayer transition metal dichalcogenides may furthermore be exploited in room temperature applications where prolonged exciton lifetimes are necessary.

$^3$This work has been funded by the Office of Naval Research (ONR), directly and through the Naval Research Laboratory (NRL). F.T. and E.S acknowledge support from NRL through the SRC-NRI project 2204.001 (NSF-ECCS-1124733), FAME, one of six centers of STARnet, a SRC program sponsored by MARCO and DARPA and the use of XSEDE NSF grant # OCI-1053575.
12:39PM T2.00006 Observation of Rapid Exciton–Exciton Annihilation in Monolayer Molybdenum Disulfide, DEZHENG SUN, Departments of Physics and Electrical Engineering, Columbia University, YI RAO, Temple University, GEORG REIDER, Photonics Institute, TU Wien, GUGANG CHEN, Honda Research Institute USA, Inc., YUMENG YU, Departments of Physics and Electrical Engineering, Columbia University, LOUIS BREZIN, Laboratoire d’Optique Appliquée, ENSTA, CNRS, Ecole Polytechnique, AVETIK HARUTYUNYAN, Honda Research Institute USA, Inc., TONY HEINZ, Departments of Physics and Electrical Engineering, Columbia University — In this paper, we present ultrafast pump-probe spectroscopy results for monolayer MoS2 crystals in which we explore exciton dynamics as a function of exciton density. After a femtosecond excitation pulse of near-resonant radiation to create A excitons, we have monitored the temporal evolution of the exciton density using a continuum probe pulse. We observe a decay rate as long as 100 ps for samples at room temperature and at relatively low exciton density. The decay rate increases strongly with increasing exciton density. We are able to fit the entire set of density-dependent exciton dynamics using a simple model in which the dominant decay channel is an exciton-exciton annihilation process. From these measurements, we infer an exciton-exciton annihilation rate of \( (4.3 \pm 1.1) \times 10^7 \text{cm}^2/\text{s} \). We compare this rate with that observed in other nanostructured materials.

12:51PM T2.00007 GW-BSE calculations on two-dimensional MXene phases, ZHENGLI LI, Department of Physics, University of California at Berkeley; Materials Sciences Divisions, Lawrence Berkeley National Laboratory, LIANG HONG, Department of Physics, University of Illinois at Chicago, FELIPE JORNADA, TING CAO, Department of Physics, University of California at Berkeley; Materials Sciences Divisions, Lawrence Berkeley National Laboratory, SERDAR OGUZ, Department of Physics, University of Illinois at Chicago, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley; Materials Sciences Divisions, Lawrence Berkeley National Laboratory — MXene is a promising candidate for new useful two-dimensional (2D) crystals. Experimentally, few-layer samples have been made from the bulk, and they demonstrate many excellent properties for electric and thermal transport, as well as other novel physics. In this work, we have performed GW-BSE calculations based on first-principles calculations to study some of the MXene family. We find that monolayer Ti3C2 possesses insulating properties. Furthermore, the 2D screening effect is very strong, resulting in a GW band gap correction of almost 1 eV. Based on these initial results, we expect that optical properties of these materials will also have strong excitonic effects.

1:03PM T2.00008 Bright Interlayer Exciton Dynamics in MoSe2–WSe2 Heterostructures, PASQUAL RIVERA, KYLE SEYLER, JASON ROSS, JOHN SCHAIBLEY, UNIV OF WASHINGTON, HONGYI YU, UNIV OF Hong Kong, JON ELL, MARIE SCOTT, Uniu of Washington, JIAQIANG YAN, DAVID MANDRUS, Oak Ridge National Laboratory / Uniu of Tennessee, WANG YAO, Uniu of Hong Kong, XIAODONG XU, Uniu of Washington — Monolayer transition metal dichalcogenide heterostructures have recently demonstrated type-II band alignment, prompting great interest in characterizing the properties of this new material system. In the monolayer MoSe2–WSe2 heterostructure, bright spatially indirect excitons with dramatically extended lifetimes have been demonstrated. Since the interlayer excitons are permanent electrical dipoles, they allow for electrical and optical control. Here, we report on the investigation of interlayer exciton emission energy, lifetime, and in-plane spatial diffusion, as a function of electric field and exciton density, in the MoSe2–WSe2 heterostructure.

1:15PM T2.00009 Giant bandgap renormalization and excitonic effects in a monolayer transition metal dichalcogenide semiconductor, AARON BRADLEY, MIGUEL M. UGEDA, SU-FEI SHI, Physics Dept. UC Berkeley, FELIPE H. DA JORNADA, Physics Dept. UC Berkeley; MSD LBNL, YI ZHANG, ALS LBNL; SLAC, DIANA Y. QIU, Physics Dept. UC Berkeley; MSDLBNL, WEI RUAN, Physics Dept. UC Berkeley; Physics Dept. Tsinghua Univ., SUNG-KWAN YEH, KA HONG, ALS LBNL, ZHI-XUN SHEN, SLAC, Geballe Lab. Adv. Mater. Stanford, FENG WANG, Physics Dept. UC Berkeley; MSDLBNL, Kavli Nanosciences Inst., STEVEN G. LOUIE, Physics Dept. UC Berkeley; MSDLBNL, MICHAL F. CROMMIE, Physics Dept. UC Berkeley; MSDLBNL; Kavli Nanosciences Inst. — Reduced screening in 2D has been predicted to result in dramatically enhanced Coulomb interactions that should cause giant bandgap renormalization and exotic excitonic effects in single-layer TMD semiconductors. Here we present a direct experimental observation of extraordinarily high exciton binding energy and bandgap renormalization in a single-layer of a semiconducting MoSe2, grown on bilayer graphene, using high-resolution scanning tunneling spectroscopy and photoluminescence spectroscopy. We have measured both the quasiparticle electronic bandgap and the optical transitions, obtaining an exciton binding energy of 0.55 eV—a value orders of magnitude larger than in conventional 3D semiconductors. We have also studied the influence of external dielectric screening by repeating measurements on MoSe2/HOPG. These results are important for room-temperature optoelectronic devices involving 2D TMDs, as well as more complex layered heterostructures.

1:27PM T2.00010 Electron excitations in two-dimensional buckled honeycomb lattices, PO-HSIN SHIH, PhD. Candidate, Department of Physics, National Cheng Kung University, YU-HUANG CHIU, Professor of Department of Applied Physics, National Pingtung University, MIN-FA LIN, Professor of Department of Physics, National Cheng Kung University — The two-dimensional buckled honeycomb lattices system exhibits the rich Coulomb excitation spectra, being dominated by the free carrier density, band structure, and transferred momentum (q). There are two kinds of plasmon peaks in the energy loss spectra, calculated from the random phase approximation. They are, respectively, revealed at low and middle frequencies. The former, which arises from the free carriers, belongs to acoustic mode. It’s frequency depends on \( \sqrt{q} \) at long wavelength limit. On the other hand, the latter is due to all the \( n \)-electronic collective excitations is an optical mode. Whether such plasmon can service is mainly determined by q. The frequencies and intensities of plasmon peaks are very different among graphene, silicene, germanene, and Tin.

1:39PM T2.00011 SPEELEM Studies on the Electronic Structure of MoS2/Graphene Heterostructure, WENCAN JIN, PO-CHUN YEH, NADER ZAKI, DANIEL CHENET, GHIDEWON AREFE, YUFENG HAO, Columbia University, ALESSANDRO SALA, TEVFIK MENTES, ANDREA LOCATELLI, Elettra Sincrotrone Trieste, JAMES HONE, RICHARD OSGOOD, Columbia University, COLUMBIA UNIVERSITY COLLABORATION, — Two-dimensional layered materials have been realized through the use of van der Waals heterostructures composed of weakly interacting layers. Among them, MoS2/graphene heterostructures can combine the advantages of high carrier mobility in graphene with the direct band gap of MoS2, which leads to potential applications in nanoelectronic devices with various functionalities. In this work, we study the influence of interlayer twist angle on the electronic structure of a MoS2/graphene heterostructure using Spectroscopic Photoemission and Low Energy Electron Microscopy (SPEELEM) system. MoS2/graphene heterostructures are prepared by transferring chemical-vapor-deposition (CVD)-grown monolayer MoS2 on top of CVD-grown graphene. Twist angles are characterized using the micro-LEED and the electronic structures are directly measured using micro-ARPES.
1:15PM T2.00012 Environment-Dependent Quasiparticle Bandgap of Monolayer MoS2. YONG-SUNG KIM, Korea Research Institute of Standards and Science. JI-YOUNG NOH, HANCHUL KIM, Sookmyung Women's University, MINKYU PARK, University of Science and Technology, K.C. SANTOSH, K.J. CHO, UT Dallas — 2D semiconductors are manifested by strong Coulomb interaction inside. The strong Coulomb interaction gives remarkable effects on various properties of the 2D semiconductors, including (i) large exciton binding energy (electron-hole), (ii) large quasi-particle self-energy (electron-electron), (iii) large scattering cross section in carrier transports by charged defects (electron-charged defects), (iv) deep defect transition level (bound electron-charged defects), and (v) strong interaction between charged defects (charged defects-charged defects). The ground state, optical, and transport properties are then largely affected by the dielectric environments surrounding the 2D semiconductors, because the Coulomb interaction is effectively screened by the dielectrics. We investigate the electronic band structures of a single-layer MoS2, as a prototype 2D semiconductor, with a variety of dielectric environments by using density-functional-theory (DFT) and GW calculations.

2:03PM T2.00013 The effects of surface polarity and dangling bonds on the electronic properties of MoS2 on SiO2. HA-JUN SUNG, DUK-HYUN CHOE, KEE JOO CHANG, Korea Adv Inst of Sci & Tech — MoS2 has recently attracted much attention due to its intriguing physical phenomena and possible applications for the next generation electronic devices. In pristine monolayer MoS2, strong spin-orbit coupling and inversion symmetry breaking allow for an effective coupling between the spin and valley degrees of freedom, inducing valley polarization at the K valleys. However, the spin-valley coupling disappears in bilayer MoS2 because the inversion symmetry is restored. In this work, we investigate the effects of surface polarity and dangling bonds on the electronic properties of MoS2 on α-quartz SiO2 through first-principles calculations. In monolayer MoS2, a transition can take place from the direct-gap to indirect-gap semiconductor in the presence of O dangling bonds. In bilayer MoS2, O dangling bonds induce dipole fields across the interface and thus break the inversion symmetry, resulting in the valley polarization, similar to that of pristine monolayer MoS2. Based on the results, we discuss the origin of the valley polarization observed in MoS2 deposited on SiO2.

Thursday, March 5, 2015 11:15AM - 1:39PM –
Session T3 FPS GSNP: Invited Session: Network and Grid Resilience 002AB - Micah Lowenthal, National Academy of Science

11:15AM T3.00001 Electric Distribution Grid Resilience R&D by the U.S. DOE, DAN TON, U.S. Department of Energy — The U.S. Department of Energy’s Smart Grid Research and Development Program is undertaking R&D to modernize the distribution portion of the electricity delivery system. Key characteristics of a modernized electric distribution grid include reliability, efficiency, affordability, flexibility, and resilience of electricity delivery for all end uses. To address resilience, the Program has established a focused R&D area in FY15 aiming to reduce social consequences (economic, safety, and security) from extreme weather threats. This focus area was developed as the result of an established process in which the Program engaged national labs, universities, utilities, and other industry stakeholders to jointly envision the future state of a resilient grid, to identify R&D areas and activities of priority, and to define performance metrics and associated targets. This presentation will cover the development of the electric distribution grid R&D focus area to date, including its key elements in resilience metrics, enhanced system designs, improved preparedness and mitigation measures, and improved system response and recovery. Key findings from a stakeholder workshop and the year-one Quadrennial Energy Review (QER) report by federal agencies will be summarized presented. Further, examples of ongoing projects in this focus area supported by the Program will be featured. The presentation will conclude with highlighting some key activities planned by the Program for the near future.

11:51AM T3.00002 Designing Resilient Electrical Distribution Grids—R&D Challenges, SCOTT BACKHAUS, Los Alamos National Laboratory — Natural disaster such earthquakes, hurricanes, and other extreme weather pose serious risks to modern critical infrastructure including electrical distribution grids, as evidenced by recent events like Superstorm Sandy. To improve resilience to these events, recent U.S. government studies suggest that component and system-level hardening and resilience upgrades are needed, including adding redundant circuit segments, hardening transformers and other exposed components, adding switching and microgrid generation for flexibility. All of these upgrades are expensive. New methods are needed to design cost-efficient, high-performance combinations of upgrades. A network-centric resilience design approach is described and used to highlight several areas in need of fundamental research to improve the functionality of this and related resilience design tools.

12:27PM T3.00003 Resiliency of Distribution Systems: State-of-the-Art and the Future, CHEN-CHING LIU, Washington State University — Recent development of the smart grid significantly enhanced the level of automation in the distribution grids. With a higher level deployment of remote-controlled switches, distribution feeders can be restored more efficiently after power outages. In this presentation, computational algorithms for feeder restoration will be summarized together with their practical implementations. The traditional analytical techniques, however, are not designed for extreme events in the distribution systems. The same is true for widely adopted reliability indices. New thinking of design and operation for resilient distribution systems will be important. Resiliency for a power distribution system depends not only on the electrical and communication connectivity but also the availability and physical capability of the distribution systems to deliver power. The physical behavior of the distribution systems during an extreme operating condition will be discussed. This presentation will cover technical methods and open research issues related to resilient distribution systems. Simulation results using a 4-feeder 1069-node test system with microgrids will be used to validate the feasibility of the proposed methods.

1:03PM T3.00004 Resilience of Large-Scale Power Distribution: Modeling and Real Data, CHUANYI JI, ECE, Georgia Tech — Severe weather events are extreme but realistic scenarios of large-scale disruptions to power distribution, the last mile of our energy infrastructure. The impact of severe weather is significant: Each major disruption previously occurred caused power failures to millions of customers in large geographical areas for extended durations. A resilient power grid is called for in the nation, which poses a numerous fundamental questions. For example, how to quantify the resilience? How resilient is large-scale power distribution to severe weather? In this talk, we first discuss technical challenges for quantifying resilience that involve heterogeneous factors from power distribution to services. We then show that these factors can be modeled, in a network setting, through spatial-temporal random processes. A dynamic resilience metric is then derived from the model. The model and the metric guide us to learn resilience from real data. We will present a study, using large-scale real data on failures and recoveries, to understand how resilient power distribution is to severe-weather disruption. Joint work with Yun Wei and Henry Mei (Georgia Tech), in collaboration with utilities and policy makers, and supported by NYSEDA.

Thursday, March 5, 2015 11:15AM - 2:15PM –
Session T4 FEd FIAP: Focus Session: Building New Pathways in Physics Innovation and Entrepreneurship Education Mayor Cockrell Room 004 - Bahram Roughani, Loyola University Maryland
11:15AM T4.00001 Tinker, Thinker, Maker and CEO: Reimagining the Physics Student as Engineer, Inventor, and Entrepreneur, CRYSTAL BAILEY, American Physical Society APS — We live in an era of immense opportunity for physics graduates: their scientific training helps to make them key members of industry teams developing new technologies, or translating cutting-edge research into viable products. Physics as a discipline stands to make tremendous gains by implementing new educational approaches which provide training for success in what is increasingly the largest employment base for physicists: the private sector. In this talk, I will examine the role of physicist as innovator and how this role intersects with other similar STEM disciplines (such as engineering), and provide some insight into how implementing physics innovation and entrepreneurship (PIE) education will benefit both physics departments and the students they serve, regardless of students’ eventual career choices. I will also talk about some exciting new PIE related developments in the physics community, and provide information about how educators can get involved in this growing movement.

11:27AM T4.00002 Practical skills of the future innovator, VITALIY KAUROV, Wolfram Research — Physics graduates face and often are disoriented by the complex and turbulent world of startups, incubators, emergent technologies, big data, social network engineering, and so on. In order to build the curricula that foster the skills necessary to navigate this world, we will look at the experiences at the Wolfram Science Summer School [1] that gathers annually international students for already more than a decade. We will look at the examples of projects and see the development of such skills as innovative thinking, data mining, machine learning, cloud technologies, device connectivity and the Internet of things, network analytics, geo-information systems, formalized computable knowledge, and the adjacent applied research skills from graph theory to image processing and beyond. This should give solid ideas to educators who will build standard curricula adapted for innovation and entrepreneurship education.


11:39AM T4.00003 Fostering Innovation through Physics, 52 Technologies, and Wide Participation, RANDALL TAGG, University of Colorado Denver — We have created in a single site a workspace called the Innovation Hyperlab. It organizes 52 technologies into 3-technology work bays and houses appropriate supplies, tools, and instrumentation. Key to the operation is a supporting web site (for open release in summer 2015) with modular instruction in individual technologies. The instruction emphasizes underlying physical principles but provides direct engagement with key devices and methods in a given technology. The aim is to support learning on-demand in the midst of design projects as well as formal courses. The physical and virtual sides of the lab are designed to serve a wide range of participants, from high school students to graduate students. Most experience to date has been through using the space to support undergraduate-mentored high school student research and innovation teams pursuing projects as wide ranging as helicopter rescue and neurological rehabilitation.

11:51AM T4.00004 Your Higgs number – how fundamental physics is connected to technology and societal revolutions, SUZY LIDSTRÖM, Physica Scripta, Royal Swedish Academy of Sciences and Uppsala University, ROLAND E. ALLEN, Texas A&M University — Fundamental physics, as exemplified by the recently discovered Higgs boson, often appears to be completely disconnected from practical applications and ordinary human life. But this is not really the case, because science, technology, and human affairs are profoundly integrated in ways that are not immediately obvious. We illustrate this by defining a “Higgs number” through overlapping activities. Following three different paths, which end respectively in applications of the World Wide Web, digital photography, and modern electronic devices, we find that most people have a Higgs number of no greater than 3. Specific examples chosen for illustration, with their assigned Higgs numbers, are: LHC experimentalists employing the Worldwide Computing Grid (0) - Timothy Berners-Lee (1) - Marissa Mayer, of Google and Yahoo, and Sheryl Sandberg, of Facebook (2) - users of all web-based enterprises (3). CMS and ATLAS experimentalists (0) - particle detector developers (1) - inventors of CCDs and active-pixel sensors (2) - users of digital cameras and camcorders (3). Philip Anderson (0) - John Bardeen (1) - Jack Kilby (2) - users of personal computers, mobile phones, and all other modern electronic devices (3).

12:03PM T4.00005 Methods to Implement Innovation and Entrepreneurship in Physics, DOUGLAS ARION, Carthage College and Galileoscope LLC — The physics community is beginning to become aware of the benefits of entrepreneurship and innovation education: greater enrollments, improved students satisfaction, a wider range of interesting research problems, and the potential for greater return from more successful alumni. This talk will suggest a variety of mechanisms by which physics departments can include entrepreneurship and innovation content within their programs – without necessarily requiring earth-shattering changes to the curriculum. These approaches will thus make it possible for departments to get involved with entrepreneurship and innovation, and grow those components into vibrant activities for students and faculty.

12:15PM T4.00006 Enlarging the ‘knowledge toolbox’: helping students prepare for an innovation-driven world, ELIZABETH NILSEN, VentureWell — Physics students graduate from their course of studies to enter the “world of work.” While for many years that transition meant joining a large corporation for a life-long career, this is no longer the case. Today’s graduates will find their career with a series of organizations – often start-ups and small to mid-sized organizations – whose future depends on the ability to rapidly leverage technical knowledge into useful products and services. This session will discuss the value of preparing physics students to be innovators and entrepreneurs, both as a strategy to prepare them for future careers, as well as an opportunity to fully engage students in seeing the relevance of physics to “real world” challenges. The session will feature three case studies: 1) embedding core knowledge and skills within a technical content course; 2) building learning experiences around a team-based start-up exploration; 3) engaging an entire department in considering how to comprehensively include innovation & entrepreneurship themes in the curriculum. The session will conclude with information about how faculty members and institutions can access resources for adopting this approach to their course offerings.

12:27PM T4.00007 PANEL DISCUSSION —

Thursday, March 5, 2015 11:15AM - 2:03PM —

Session T5 DMP DCOMP: Focus Session: Disorder in Fe-based Superconductors Juan Gorman

Room 005 - Gregory Stewart, University of Florida
11:15AM T5.00001 Visualizing the atomic-scale influence on superconductivity and vortex pinning of high-energy ion irradiation in FeSeTe

PETER SPRAU, Cornell University, FREEK MASSEE, Brookhaven National Laboratory, Cornell University; YONGLEI WANG, Argonne National Laboratory; J. C. SEAMUS DAVIS, Brookhaven National Laboratory, Cornell University, University of St. Andrews, Kavli Institute at Cornell for Nanoscale Science, GENDA GU, Brookhaven National Laboratory, WAI-KWONG KWOK, Argonne National Laboratory — The maximum sustainable supercurrent density, JC, may be greatly enhanced by preventing dissipative motion of quantized vortices. Irradiation of superconductors with heavy ions is often used to create nanoscale defects with deep pinning potential for the vortices and this approach holds great promise for high current applications of iron-based superconductors. We have shown that two different atomic-scale interplay between the crystal damage from high-energy ion, the superconducting order parameter, and the vortex pinning processes. Here, we visualize the atomic-scale effects of irradiating FeSe0.45Te0.55 with 249 MeV Au ions and find two distinct forms of damage: compact regions of crystal disruption ascribable to the actual ion trajectory along with single atomic-site ‘point’ defects. We show directly that the superconducting order is virtually annihilated within the former while it is still altered by the latter. Simultaneous atomically-resolved images of the crystal defects, the superconducting density-of-states, and the vortex cores, then reveal how the vortex pinning evolves with increasing field in irradiating FeSe0.45Te0.55.

11:27AM T5.00002 Experimentally tuning the ground state of BaFe2As2 by orbital differentiation

PRISCILA ROSA, University of California at Irvine, CRIS ADRIANO, THALES GARITEZI, University of Campinas, TED GRANT, ZACHARY FISK, University of California at Irvine, RICARDO URBANO, PASCOAL PAGLIUSO, University of Campinas — The role of structural parameters in layered systems, such as iron pnictides/chalcogenides (Fe-Pn/Ch), cuprates and heavy fermions, has become crucial for the understanding of their properties. In this talk, I will discuss this subject using a combination of macroscopic and microscopic techniques to study Ba1−εEu1−εFe2−yMyAs2 single crystals (M = Co, Cu, Mn, Ni, and Ru). Interestingly, a close connection arises between the spin-density wave (SDW) phase suppression and local distortions in the structure. Furthermore, these changes in the Fermi surface by an increase of anisotropy and localization of the Fe 3d bands at the FeAs plane. Our results suggest that such increase in the planar (xσ/zw2−yγ) orbital symmetry seems to be a favorable ingredient for the emergence of superconductivity in this class of materials.

1This work was supported by FAPESP, CNPq, CAPES-Brazi and AFOSR MURI.

11:39AM T5.00003 FORC Evidence for Splitting of the Magnetostructural Transition in Fe1+y2 Te

MILES FRAMPTON, JOHN CROCKER, DUSTIN GILBERT, KAI LIU, RENA ZIEVE, Univ of California - Davis, GENDA GU, Brookhaven National Lab — Iron-based superconductors Fe1+y2 Te and CaFe2As2 both have simultaneous magnetic and structural transitions, at 67K and 170K, respectively. We have investigated these transitions using the First-Order Reversal Curve (FORC) method, which provides a detailed mapping of any heterogeneities and irreversible switching events. In this work, electrical resistance FORC measurements have been performed in the presence of external magnetic fields to deconvolute the phase transition. In Fe1+y2 Te the phase transition actually consists of two separate transitions, which is sensitive to the external field for H > 2T, as revealed by the FORC distribution. The different responses of these separate transitions to the magnetic field suggest that, at a minimum, the coupling to the field is different for each phase. In contrast, CaFe2As2 shows no sign of a split transition, with or without the magnetic field. In both cases the magnetic field is shown to shift the distribution, suggesting a change in the energy landscape and highlighting the coupling between the magnetic and structural transition. This work has been supported by the NSF (DMR-1008791).

11:51AM T5.00004 Unexpected impact of magnetic disorder on multiband superconductivity

DMITRI EREFROM, IWF- Dresden, Germany, MAXIM KORSHUNOV, Kirensky Institute of Physics, Krasnoyarsk, Russia, ALEXANDER GOLYUBOV, University of Twente, The Netherlands, OLEG DOLOGV, Max Planck Institute, Stuttgart, Germany — We analyze how the magnetic disorder affects the properties of the two-band s± and s±± models, which are subject of hot discussions regarding iron-based superconductors and other multiband systems like MgB2. We show that there are several cases when the transition temperature Tc is not fully suppressed by magnetic impurities in contrast to the Abrikosov-Gor’kov theory, but a saturation of Tc takes place in the regime of strong disorder. These cases are: (1) The purely interband impurity scattering, (2) impurity scattering purely in one of the bands, (3) the unitary scattering limit. We show that a transition between s±± and s± states may occur with increasing magnetic disorder.

12:03PM T5.00005 Modulation of Pairing Symmetry with Bond Disorder in Iron-based Superconductors

DAO-XIN YAO, YAO-TAI KANG, School of Physics and Engineering, Sun Yat-Sen University, WEI-FENG TSAI, Department of Physics, National Sun Yat-sen University — We study a simple two-orbital t-J1-J2 model for iron-based superconductors in the presence of a bond disorder (via nearest-neighbor bond-dilution). By using Bogoliubov-de Gennes approach, we self-consistently calculate the local pairing amplitudes and the corresponding density of states, which demonstrate a change of dominant pairing symmetry from the s+ wave to d-wave as long as J2 J1. Although the system exhibits spatially inhomogeneous pairing in weak correlations with a given realization of disorder, it is still in sharp contrast to the case with potential disorder, where the superconducting islands and the insulating sea are both present in the strong disorder regime. Moreover, from the detailed examination of the pairing gap as well as the superfluid density, the superconducting transition here is suggested to be beyond the conventional Abrikosov-Gor’kov consideration.

1Supported by NBRPC-2012CB821400, NSFC-11074310, NSFC-11275279, Fundamental Research Funds for the Central Universities, and the NSC in Taiwan under Grant No.102-2112-M-110-009.

12:15PM T5.00006 Low-energy magnetic defects at nano- and meso-scale in Fe-based superconductors

AFTAB ALAM, Department of Physics, Indian Institute of Technology Bombay, Powai, Mumbai 400076 Maharashtra, SUFIAN N. KHAN, DUANE D. JOHNSON, Ames Laboratory, Ames, Iowa 50011, USA — In Fe-based superconductors, “ordered” moments of Fe (0.3–0.5 μB) measured by neutron scattering in the antiferromagnetic groundstate are half (∼1.6 μB) of that estimated from density-functional theory (DFT), while other experiments are closer to DFT — a puzzle not yet understood. Structural and magnetic planar defects proliferate over differing length scales, and could be key to any moment description. Thus, we study via DFT the stability and magnetic properties of antiphase and domain boundaries, twins, and nanotwins, which exhibit low-moment states confined near defect boundaries. A single local-moment picture is thus inappropriate for long-range magnetic order. While the nanoscale defects are very low in energy, twins remain so at the mesoscale, where estimated distances between twin boundaries coincide with the observed magnetic correlation length. All these defects can be weakly mobile and/or have fluctuations that will lower assessed “ordered” moments from longer spatial and/or time averaging.

1Ames Laboratory is operated for the U.S. DOE by Iowa State University under contract DE-AC02-07CH11358. A thanks startup seed grant from IIT Bombay.

12:27PM T5.00007 NMR Investigations of Inhomogeneous glassy spin fluctuations in Doped BaFe2As2

NICOLAS CURRO, University of California, Davis — We present 77As and 31P NMR data in a series of Ba(Fe1−x−yM)x+yAs2 (M=Ni, Cu, Co) and BaFe2(As1−xFes)x2 crystals that reveal the large inhomogeneous distribution of glassy spin dynamics, as well as the coexistence of frozen antiferromagnetic domains in superconducting samples. In underdoped samples, the glassy dynamics turns on below temperatures on the order of 100K, persists in magnetic fields up to 30 Tesla, and is unrelated to a competition between antiferromagnetism and superconductivity. Rather, the glassy spin dynamics are driven by inhomogeneous nematic fluctuations.
1:03PM T5.00008 Competition between the spin fluctuations and disorder in an iron-pnictide superconductor. XIAO-JIA CHEN, YONG-HUI ZHOU. Center for High Pressure Science and Technology Advanced Research, Shanghai 201203, China, ZHU-AN XU, Department of Physics, Zhejiang University, Hangzhou 310027, China, VIKTOR STRUZHKIN, HO-KWANG MAO, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20051, USA. — The evolution path of superconductivity with pressure in an optimally doped iron pnictide BaFe$_{1.9}$Ni$_{0.1}$As$_2$ is examined by resistance measurements. We find that the superconducting transition temperature $T_c$ of this compound first increases with a maximum at around 5 GPa and then decreases with increasing pressure and eventually vanishes at around 12.5 GPa. The change of the strength of the spin fluctuations, derived from the analysis of the temperature-dependent resist ance, behaves in a similar way to $T_c$. After the destruction of superconductivity, the compound enters an insulating state due to the disorder-induced localization effect. These findings unveil that the superconductivity is controlled by the competition between the spin fluctuations and disorder and pin down the nature of the electron scattering and pairing in iron-based superconductors.

1:15PM T5.00009 Effects of Swift Particle Irradiations in (Ba,K)Fe$_2$As$_2$. TSUYOSHI TAMEGAI, TOSHIHITO TAEN, FUMIAKI OHTAKE, YUE SUN, SUNSENG PYON, MASATAKA MORIMOTO, The University of Tokyo, SATÔRÔ OKAYASU. Japan Atomic Energy Agency, HISASHI KITAMURA, National Institute of Radiological Sciences — Iron-based superconductors are believed to be good candidates for practical applications at high fields. Knowledge of the pinning mechanism of vortices is essential to achieve a large critical current density at high fields. Irradiations of swift particles are established way to introduce defects that pin vortices under the action of Lorentz force due to large current. We have systematically investigated the effects of swift particle irradiations on high-temperature superconductors (Ba,K)Fe$_2$As$_2$ family of compounds. The coherent combination of detailed structural information with an in-depth analysis of the electronic structure allows us to disentangle very sensitively “doping” effects from “substitutional” effects. This balance between substitution and doping turns out to be crucial for an understanding of magnetism and superconductivity in iron pnictides.

1:27PM T5.00010 Of substitution and doping: Spatial and electronic structure in iron pnictides. S. SCHUPPLER, P. SCHWEISS, P. NAGEL, M.-J. HUANG, R. EDER, TH. WOLF, H. V. LÖHNEYSEN, M. MERZ, Karlsruhe Institute of Technology (KIT) — A highly intriguing aspect in iron-pnictide superconductors is the composition-dependent electronic structure, in particular the question if and how charge carriers are introduced to the system upon substitution of Ba by alkali metals or of Fe by other transition metals, TM. We report on a systematic study of spatial structure and electronic states by x-ray diffraction and x-ray absorption, performed on a large number of compositions in the (Ba,K)Fe$_2$As$_2$ family of compounds. The coherent combination of detailed structural information with an in-depth analysis of the electronic structure allows us to disentangle very sensitively “doping” effects from “substitutional” effects. This balance between substitution and doping turns out to be crucial for an understanding of magnetism and superconductivity in iron pnictides.

1:39PM T5.00011 Superconductivity of Ba$_{1-x}$K$_x$Fe$_2$As$_2$ with and without artificial disorder over the entire doping range. SERAFIM TEKNOVJOYO, KYUL CHO, MAKARY A. TANATAR, RUSLAN PROZOROV, YONG LIU, THOMAS LOGRASSO, Ames Laboratory and Iowa State University, USA, MARCIN KONCZYKOWSKI, LSI, Ecole Polytechnique, France. — Effects of electron irradiation on superconducting transition temperature and in-plane London penetration depth were studied in single crystals of Ba$_{1-x}$K$_x$Fe$_2$As$_2$ ($x = 0.22, 0.34, 0.47, 0.56, 0.65, 0.80, 0.82, 0.90, 0.92, 1.0$). Electron irradiation introduces point-like disorder that gives insight into the superconducting gap structure by studying the effects of increasing scattering. We studied the entire superconducting “dome” and find distinctly different behaviours in underdoped, optimal, and overdoped compositions and unusual behaviour near $x = 0.7 - 0.8$.

Thursday, March 5, 2015 11:15AM - 2:15PM — Session T6 DMP: Focus Session: Iridates and Osmates 006A - Saicharan Aswartham, University of Kentucky

11:15AM T6.00001 A tale of three double perovskites: Ba$_2$XOs$_6$ (X=Na,Ca,Y)¹. SHRUBA GAN-GOPADHYAY, WARREN PICKETT, University of California - Davis — High valent Os based double perovskites are one center of current interest because they display extremely large spin orbit coupling and strong electronic correlation. We present electronic and magnetic structures of three cubic Os based double perovskites with Os$^{5+}$($d^5$), Os$^{5+}$($d^4$), Os$^{6+}$($d^1$). For these first principles based calculation we used an onsite hybrid exchange only on Os(5d), as implemented in Wien2k. While Ba$_2$NaOsO$_6$ is a ferromagnetic Mott insulator, the other two show antiferromagnetic ordering. For comparison purposes we have investigated only the ferromagnetic ordered phase of these three materials. A metal-insulator transition by changing spin orbit coupling direction is found in all three materials, however each double perovskite is metallic for different magnetic directions. Surprises from looking at the radial charge densities will be discussed. We provide a resolution to the riddle: why, despite d1 configuration, does Ba$_2$NaOsO$_6$ remain cubic. This material introduces a new class of J=3/2 Mott insulator.

¹DOE Stockpile Stewardship Academic Alliance Program

11:27AM T6.00002 Trigonal crystal field effect in spin-orbit Mott insulating Sr$_2$NiIrO$_6$. JUN OKAMOTO, WEN-BIN WU, HIROFUMI ISHII, KANG-LI YU, NOZOMU HIROAKA, RU-PAN WANG, Natl Synchrotron Rad Res Ctr, DENG-MING JUO, National Chiao Tung University, JUIN CHEN, National Pingtung University of Education, VIVEKA SINGH, GUANG-YU GUO, National Taiwan University, QINGHUI JIANG, Postech, SANG-WOOK CHEONG, Rutgers University, KU-DING TSUEI, DI-JING HUANG, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20051, USA. — The evolution path of superconductivity with pressure in an optimally doped iron pnictide BaFe$_{1.9}$Ni$_{0.1}$As$_2$ is examined by resistance measurements. We find that the superconducting transition temperature $T_c$ of this compound first increases with a maximum at around 5 GPa and then decreases with increasing pressure and eventually vanishes at around 12.5 GPa. The change of the strength of the spin fluctuations, derived from the analysis of the temperature-dependent resistance, behaves in a similar way to $T_c$. After the destruction of superconductivity, the compound enters an insulating state due to the disorder-induced localization effect. These findings unveil that the superconductivity is controlled by the competition between the spin fluctuations and disorder and pin down the nature of the electron scattering and pairing in iron-based superconductors.

11:53PM T6.00013 Competition between the spin fluctuations and disorder in an iron-pnictide superconductor. XIAO-JIA CHEN, YONG-HUI ZHOU. Center for High Pressure Science and Technology Advanced Research, Shanghai 201203, China, ZHU-AN XU, Department of Physics, Zhejiang University, Hangzhou 310027, China, VIKTOR STRUZHKIN, HO-KWANG MAO, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20051, USA. — The evolution path of superconductivity with pressure in an optimally doped iron pnictide BaFe$_{1.9}$Ni$_{0.1}$As$_2$ is examined by resistance measurements. We find that the superconducting transition temperature $T_c$ of this compound first increases with a maximum at around 5 GPa and then decreases with increasing pressure and eventually vanishes at around 12.5 GPa. The change of the strength of the spin fluctuations, derived from the analysis of the temperature-dependent resistance, behaves in a similar way to $T_c$. After the destruction of superconductivity, the compound enters an insulating state due to the disorder-induced localization effect. These findings unveil that the superconductivity is controlled by the competition between the spin fluctuations and disorder and pin down the nature of the electron scattering and pairing in iron-based superconductors.

1:15PM T5.00009 Effects of Swift Particle Irradiations in (Ba,K)Fe$_2$As$_2$. TSUYOSHI TAMEGAI, TOSHIHITO TAEN, FUMIAKI OHTAKE, YUE SUN, SUNSENG PYON, MASATAKA MORIMOTO, The University of Tokyo, SATÔRÔ OKAYASU. Japan Atomic Energy Agency, HISASHI KITAMURA, National Institute of Radiological Sciences — Iron-based superconductors are believed to be good candidates for practical applications at high fields. Knowledge of the pinning mechanism of vortices is essential to achieve a large critical current density at high fields. Irradiations of swift particles are established way to introduce defects that pin vortices under the action of Lorentz force due to large current. We have systematically investigated the effects of swift particle irradiations on high-temperature superconductors (Ba,K)Fe$_2$As$_2$ family of compounds. The coherent combination of detailed structural information with an in-depth analysis of the electronic structure allows us to disentangle very sensitively “doping” effects from “substitutional” effects. This balance between substitution and doping turns out to be crucial for an understanding of magnetism and superconductivity in iron pnictides.
11:39 AM T6.00003 Magnetism and anisotropy of Ir$^{5+}$ based double perovskites Sr$_2$CoIrO$_6$ and Sr$_2$FeIrO$_6$. JASMINKA TERZIC, S.J. YUAN, Center for Advanced Materials, Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506, USA, W.H. SONG, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei, China, S. ASWARTHAM, G. CAO, Center for Advanced Materials, Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506, USA — We report on structural, thermodynamic and transport study of single-crystal double perovskites Sr$_2$CoIrO$_6$ and Sr$_2$FeIrO$_6$. The isostructural Sr$_2$CoIrO$_6$ and Sr$_2$FeIrO$_6$ feature a cubic crystal structure with pentavalent Ir$^{5+}$ (5d$^6$) which are anticipated to have J=0 singlet ground states in the strong spin-orbit coupling limit. Here we observe magnetic coupling between 5d and 3d (Co, Fe) elements, which result in antiferromagnetic order at high temperatures in both double perovskites. Of the two, Sr$_2$CoIrO$_6$ displays antiferromagnetic metallic behavior with a pronounced magnetic anisotropy; in sharp contrast, the isostructural Sr$_2$FeIrO$_6$ exhibits an antiferromagnetic, insulating ground state without discernible magnetic anisotropy. The data will be discussed and presented with comparisons drawn with similar systems.

1This work was supported by NSF via Grant DMR 1265162.

11:51 AM T6.00004 Spin-orbit coupling, magnetic anisotropy and hard magnetism in Sr$_3$NiIrO$_6$. VIVIEN ZAPF, National High Magnetic Field Laboratory, MPA-CMMS, Los Alamos National Lab — Strong spin-orbit coupling is a pre-requisite for hard magnetism with high coercive magnetic fields. Magnetic oxides containing 5d ions such as Ir$^{4+}$ should show significant spin-orbit coupling due to the high Z value. Furthermore, in 5d ions, the comparable energy scales of crystal-electric field splitting, Coulomb repulsion and spin-orbit interactions create unusual electronic ground states that can entangle spins and orbits, mix t$_{2g}$ and e$_{g}$ levels and drive magnetic exchange anisotropy. Another set of interesting electronic ground states can arise when 5d orbitals overlap 3d orbitals. In the compound Sr$_3$NiIrO$_6$, electronic structure calculations predict that the 3d orbitals of the Ni$^{3+}$ ion directly overlap 5d orbitals of the Ir$^{4+}$ ion. In addition to a “Jeff = 1/2” Ir$^{4+}$ ground state that mixes t$_{2g}$ and e$_g$ levels, the Ni$^{3+}$ should show strong single-ion anisotropy [1-3]. We present magnetization measurements of Sr$_3$NiIrO$_6$ to high magnetic fields. [4] We demonstrate magnetic hysteresis with a record 55 Tesla coercive magnetic field and long stability over time in some crystals. More generally, the A$_3$BB’O$_6$ family of compounds shows hard magnetism as B’ ion goes from 3d to 4d to 5d. Further complexities to do with evolving magnetic order and magnetic frustration also present in this family.

3 X. Ou and H. Wu, arXiv:1312.7411

12:27 PM T6.00005 Novel Magnetic and Charge Orders in Dimer-Chain Iridate Ba$_5$AlIrO$_{11}$. FENG YE, J. TERZIC, J.C. WANG, Center for Advanced Materials, Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506, USA, W.H. SONG, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei, China, S.J. YUAN, S. ASWARTHAM, G. CAO, Center for Advanced Materials, Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506, USA — We report a novel magnetic state coexisting with a charge ordering state in a dimer-chain system Ba$_5$AlIrO$_{11}$. This newly synthesized single-crystal iridate features both tetravalent Ir$^{4+}$ and pentavalent Ir$^{5+}$ ions in each of dimers that are only linked via AlO$_4$-tetrahedra along the b-axis. Despite the evident one-dimensional characteristic, the dimer-chains undergo an unexpected long-rang order at $T_c$ = 4.5 K with a large magnetic anisotropy. The magnetic transition is unusually resilient to magnetic field up to 14 T but more susceptible to even modest hydrostatic pressure up to 10 kbar. Furthermore, a subtle structural change discerned at $T_S$ =200 K marks a charge ordering that accompanied a huge enhancement in the dielectric constant and changes in the electrical resistivity. It is evident that the strong SOC imposes a j=1/2 (Ir$^{4+}$) and singlet j=0 (Ir$^{5+}$) states in each dimer, which critically hinges on the orbital and lattice degrees of freedom.

1This work was supported by NSF via Grant DMR 1265162.

12:39 PM T6.00006 Giant spin-phonon coupling in a 5d NaOsO$_3$. STUART CALDER, JUN HEE LEE, MATTHEW STONE, MARK LUMSDEN, Oak Ridge National Lab, JONATHAN LANG, APS, MIKHAIL FEYGENSON, Oak Ridge National Lab, YOUGUO SHI, CAS, YIN SUN, YOSHIHIRO TSUGIMOTO, KAZUNARI YAMAURA, NIMS, ANDREW CHRISTIANSON, Oak Ridge National Lab — The coupling of distinct properties offers avenues to multifunctional materials. A limiting factor, however, is the degree that one parameter has to be modified to sufficiently alter the coupled property. Through a neutron scattering and first-principles density functional theory study of the 5d perovskite NaOsO$_3$ we reveal that from only a 0.1% lattice change an unprecedentedly large coupling emerges. The manifestation is a “giant” spin-phonon coupled mode shift of $\Delta J = 40$ cm$^{-1}$, the largest observed in any material. By identifying the dominant phonon as the octahedral breathing mode we show isosymmetric ordering and cooperation between the lattice and the exotic magnetically driven Slater metal-insulator transition in this material. The occurrence of the dramatic spin-phonon-electronic coupling in NaOsO$_3$ is due to a property common to all 5d materials: the large spatial extent of the 5d ion. Consequently examining 5d materials in a new light offers novel routes for multifunctional devices with enhanced coupled phenomena.

1A portion of this research at ORNL’s High Flux Isotope Reactor and Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

12:51 PM T6.00007 Metal-insulator transitions in effective J=1/2 insulating iridates. HONGBIN ZHANG, Rutgers University — The competition between spin-orbit coupling, crystal field splitting and electron correlations with comparable magnitude gives rise to many interesting phenomena. For instance, the so-called effective J=1/2 state has been observed in many iridates compounds, e.g., Ruddlesden-Popper (RP) Sr$_{n+1}$Ir$_n$O$_{3n+1}$ and pyrochlore RE$_2$Ir$_2$O$_7$ (RE=Bi, Pr, Nd, Sm, Eu, Y) iridates, where metal-insulator transitions occur driven by the interplay of electron correlations with magnetic ordering. Using first-principles methods, for correlated solids based on density functional theory and dynamical mean field theory (DMFT+DMFT), we have investigated the metal-insulator transitions in both classes of iridates. We explore the robustness of the effective J=1/2 state against band effects due to itineracy, structural distortion, and strain. We show how single-particle spectra, optical conductivities, and orbital and spin moments change with strain, and we demonstrate that the ground state can be well characterized in terms of an effective energy-dependent J = 1/2 state. For RP compounds, we demonstrate that the crystal field splittings induced by local structural distortions and hybridization are critical to understand previous experimental results. For pyrochlore compounds, the total energies obtained using charge self-consistent DFT+DMFT method reveal that the all-in-all-out magnetic ordering is stable at low temperature in late rare earth pyrochlores, while a bad metallic state is found in early rare earth pyrochlores, in agreement with experiments.

1This work was supported by NSF Grant No. DMRF-12-33434.
1:27PM T6.00008 Unquenched $e_g^1$ orbital moment in the Mott insulating antiferromagnet KOsO$_4$ $^1$, KWAN-WOO LEE, YOUNG-JOON SONG, KYO-HOON AHN, Department of Applied Physics, Graduate School, Korea Univ, Sejong, Korea, WARREN E. PICKETT, Department of Physics, Univ. of California, Davis, CA, USA — In condensed matter physics, spin-orbit coupling (SOC) has many important consequences, including some recent hot topics such as topological insulators, unconventional metal-insulator transitions, so-called relativistic Mott insulators, large orbital moments, and of course magnetic anisotropy. Whereas SOC in a $e_g$ manifold has been intensively discussed recently, SOC in an $e_g$ manifold has rarely been considered due to the conventional (usually correct) wisdom that an orbital moment is completely quenched in the $e_g$ subshell. In this presentation, using correlated band theory including SOC, we will address effects of SOC in an $e_g^1$ of KOsO$_4$, which contains OsO$_4$ tetrahedra such that the $e_g$ subshell is partially occupied. In contrast to the conventional wisdom, our results show very definite magnetocrystalline anisotropy and unquenched orbital moments of substantial size in KOsO$_4$ (half that of the Os spin moment). We have analyzed and interpreted the origin of the orbital moment on the basis of a small crystal splitting and symmetry breaking (crystalline, and additionally due to SOC itself).

$^1$This research was supported by Grant No. NRF-2013R1A1A2A10008946 (KU), by U.S. National Science Foundation Grant DMR-1207622-0 (K.W.L.), and by U.S. Department of Energy Grant DE-FG02-04ER46111 (W.E.P).

1:39PM T6.00009 Hierarchical stripe phases in IrTe$_2$ driven by competition between Ir dimerization and Te bonding $^2$, WEIIDA WU, JIXIA DAI, KRISTJAN HAULE, Department of Physics and Astronomy, Rutgers University, JUNJIE YANG, Laboratory for Pohang Emergent Materials and Department of Physics, Pohang University of Science and Technology, YOON SEOK OH, SANG WOOK CHEONG, Department of Physics and Astronomy, Rutgers University — Iridium di-telluride (IrTe$_2$) belongs to the family of transition metal dichalcogenides (TMD), but it distinguishes from the traditional TMDs due to the existence of multi-step single-q charge-density wave like phase transitions. Despite of intensive studies, there is still no consensus on the physical origin of the stripe phases or even the ground state modulation for this 5d material. In this study, we present atomic-resolving images and spectroscopic measurements from scanning tunneling microscopy and spectroscopy (STM/STS). We show that the ground state of IrTe$_2$ is a q=1/6 stripe phase, identical to that of the Se-doped compound. Furthermore, our data suggest that the multi-step transitions and the stripe phases are driven by the intralayer Ir-Ir dimerization that competes against the interlayer Te-Te bonding. This competition results in a unified phase diagram with a series of hierarchical modulated stripe phases.

$^2$This work is supported by NSF grant # DMR-0844807.

1:51PM T6.00010 Optical evidence for bonding-antibonding splitting in IrTe$_2$ $^3$, DIPANJAN MAZUMDAR, Southern IL Univ-Carbondale,USA, KRISTJAN HAULE, Rutgers University, Piscataway, USA, J.J. YANG, Laboratory for Pohang Emergent Materials and Department of Physics, Korea, G.L. PASCUT, Rutgers University, Piscataway, USA, B.S. HOLINSWORTH, K.R. O’NEAL, University of Tennessee, Knoxville, USA, VALERY KIRYUKHIN, SANG WOOK CHEONG, Rutgers University, Piscataway, USA, J.L. MUSFELDT, University of Tennessee, Knoxville, USA, DEPARTMENT OF CHEMISTRY, UNIVERSITY OF TENNESSEE, KNOXVILLE, USA TEAM, DEPARTMENT OF PHYSICS AND ASTRONOMY, RUTGERS UNIVERSITY, PISCATAWAY, USA TEAM, LABORATORY FOR POHANG EMERGENT MATERIALS AND DEPARTMENT OF PHYSICS, POHANG, KOREA TEAM, RUTGERS CENTER FOR EMERGENT MATERIALS, RUTGERS UNIVERSITY, USA TEAM, SOUTHERN ILLINOIS UNIVERSITY, CARBONDALE, USA TEAM — We combined optical spectroscopy with first principles calculations to reveal the electronic signatures of Ir dimer formation in the 1/5th phase of IrTe$_2$. Our measurements uncover two interband transitions into the unoccupied anti-bonding orbitals, one from mixed Iridium/Tellurium bands, the other from the dxy bonding orbital of the dimerized Ir centers. The bonding-antibonding splitting demonstrates that Iridium, not Tellurium, plays the dominant role in stabilizing the low temperature phase of IrTe$_2$ through localized bonding orbital formation.

2:03PM T6.00011 Spectroscopic evidence for negative electronic compressibility in a quasi-three-dimensional spin-orbit correlated metal $^4$, JUNFENG HE, T. HOGAN, THOMAS MION, Boston College, H. HAFIZ, Northwestern University, Y. HE, Stanford, J.D. DENLINGER, S.-K. MO, ALS, C. DHITAL, X. CHEN, QISEN LIN, Boston College, Y. ZHANG, Peking University, M. HASHIMOTO, SSRL, H. PAN, Boston College, D.H. LU, SSRL, M. ARITA, K. SHIMADA, HISOR, R.S. MARKIEWICZ, Northwestern University, Z. WANG, K. KEMPA, M.J. NAUGHTON, Boston College, A. BANSIL, Northwestern University, S.D. WILSON, RUI-HUA HE, Boston College — In quantum materials consisting of multiple mutually-coupled subsystems, the effective compressibility of one subsystem can be negative when it is countered by the positive compressibility of other subsystems. Manifestations of such negative compressibility in quantum materials have so far been limited to low-dimensional dilute electron systems. The origin of such negative compressibility has been commonly attributed to a dominance of the exchange energy over kinetic energy of electrons. Here we present evidence from ARPES for negative electronic compressibility in a quasi 3D spin-orbit correlated metal, (Sr$_{13}$Ir$_{17}$)$_2$O$_{40}$, which is driven by a dominance of the correlation energy of electrons at a relatively high density. Increased electron filling results in both an expansion of the electron Fermi pockets and an anomalous decrease of the chemical potential. This anomaly, suggestive of negative electronic compressibility, is made possible by a concomitant rapid lowering in energy of the correlated conduction band on which the chemical potential is defined, unveiling a new band picture of doping Mott insulators.

$^4$This work is supported by ARO Grant No. W911NF-09-10527, NSF Grant No. DMR-0955778, and DARPA grant No. D13AP00052. TACC provides computational resources.

Thursday, March 5, 2015 11:15AM - 2:15PM – Session T7 DMP DCMP: Focus Session: Dirac, Weyl Semimetals, Kondo Insulators 006B - Kai Sun, University of Michigan

11:15AM T7.00001 First Principles Prediction of Topological Phases in Thin Films of Pyrochlore Iridates $^1$, Xiang HU, The University of Texas at Austin, ZHICHENG ZHONG, Vienna University of Technology, GREGORY A. FITE, The University of Texas at Austin — We make materials-specific predictions for topological phases using density functional theory combined with Hartree-Fock theory that includes the full orbital structure of the relevant iridium $d$-orbitals and the strong but finite spin-orbit coupling strength. We find $Y_2$Ir$_2$O$_7$ bilayer and trilayer films grown along the [111] direction can respectively support a $Z_2$ topological metallic phase and a Chern metallic phase with a direct gap of up to 0.02 eV. These results could potentially bring transition metal oxides to the fore as a new class of topological materials with potential applications in oxide electronics.

$^1$Funded by ARO Grant No. W911NF-09-10527, NSF Grant No. DMR-0955778, and DARPA grant No. D13AP00052. TACC provides computational resources.
Furthermore, by in-situ doping, we were able to tune its Fermi-energy, making it a flexible platform for exploring exotic physical phenomena and application potentials.

In addition, the detected Berry phase is found to vary from nontrivial to trivial at different field directions, revealing a fierce competition between the orbit-coupled field strength and the field-generated mass term. Our results demonstrate a feasible path to generate a Weyl semimetal phase based on the TDSs by breaking TRS.

Motivated by recent experiments on Pr$_2$Ir$_2$O$_7$, we provide a theory of quantum oscillations in a minimal model for pyrochlore iridates. Focusing on the conduction electron degrees of freedom with strong spin-orbit coupling and considering the electronic structure near the Fermi level, we compute quantum oscillation signals in the paramagnetic state of the model. We compare our theoretical results with existing experimental data on Pr$_2$Ir$_2$O$_7$ and discuss implication to future experiments.

In-situ synchrotron X-ray and single crystal resistance measurements find that Cd$_3$As$_2$ single crystals under high magnetic fields shows a sign change from negative to positive around 50K upon cooling. R$_H$ peaks and becomes nonlinear in field around 10K then tend to saturate in value below 10K. Two samples with different geometries (thickness and lateral dimensions) show contrasting behaviors below and above 50K, which indicates a surface origin of the low temperature carriers.

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Quantum oscillations in magnetically doped SmB$_6$

I.15PM T7.00010 Quantum oscillations in magnetically doped SmB$_6$, GANG LI, COLIN TINSMAN, BENJAMIN LAWSON, FAN YU, TOMOYA ASABA, University of Michigan, XIANGFENG WANG, JOHNPIERRE PAGLIONE, University of Maryland, LU LI, University of Michigan — Quantum oscillation study on pure SmB$_6$ has revealed two-dimensional Fermi Surfaces in both crystalline (001) and (101) surface planes. On the (101) surface plane, only one area of Fermi surface is observed, consistent with theoretical prediction of surface state protected by time-reversal symmetry. It has been further predicted that for the system there is not only time reversal symmetry reservation but also crystalline mirror symmetry reservation that could give rise to protected surface states. By introducing magnetic impurities such as 1% Fe or 1% Ni into SmB$_6$, the magnetic ground state is altered and no longer has the time reversal symmetry. However, quantum oscillations are still observed for both Fe$_x$SmB$_6$ and Ni$_x$SmB$_6$ at higher field, the dispersive angular dependence of frequency will be discussed with comparison to SmB$_6$.

Electronic gap in SmB$_6$ studied by Raman spectroscopy

1:39PM T7.00011 Electronic gap in SmB$_6$ studied by Raman spectroscopy, MICHAEL VALEN'TINE, SEYED KOOPHAYEH, Johns Hopkins University, XIANGFENG WANG, YASUYUKI NAKAJIMA, JOHNPIERRE PAGLIONE, University of Maryland, COLLIN BROHOLM, WILLIAM PHELAN, TYREL MQUEEN, NATALIA DRICHKO, Johns Hopkins University — SmB$_6$ is a mixed valence compound which is suggested to be a topological Kondo insulator. Studies of insulating vs metallic properties of the bulk and the nature of the surface conduction are still ongoing. Using Raman scattering, we follow the opening of an electronic gap in samples of pure SmB$_6$ and SmB$_6$ with Al and C impurities. In all of the samples we observe an electronic gap in the range of 50-65 meV, confirming insulating state in the bulk. The gap appears in the A$_{1g}$+E$_g$ spectra as a suppression of low-frequency electronic scattering and a shift of the spectral weight to frequencies above the gap below approximately 100 K. The size of the gap and presence of electronic states in the gap depend on the method of growth (floating zone vs Al flux), and the chemical composition of the sample. We discuss a dependence of these parameters on the impurities and Sm valence.

Work at JHU was supported by the US Department of Energy, office of Basic Energy Sciences, Division of Material Sciences and Engineering under grant DE-FC02-08ER46544.

Effect of magnetic and non-magnetic substitution in topological Kondo insulator SmB$_6$

2:03PM T7.00013 Effect of magnetic and non-magnetic substitution in topological Kondo insulator SmB$_6$, XIANGFENG WANG, YASUYUKI NAKAJIMA, SHANTA SAHA, JOHNPIERRE PAGLIONE, University of Maryland, College Park, JEFF SONIER, Simon Fraser University, PROF. JOHNPIERRE PAGLIONE TEAM, PROF. JEFF SONIER TEAM — The topological Kondo Insulator SmB$_6$ is believed to be the first realization of a topological insulator with true bulk insulating properties that coexist with a robust conducting surface state that mounting evidence suggests is non-trivial. Here we report of a systemic study of the magnetic and non-magnetic doping effect TKI SmB$_6$, in particular the effect of iron inclusion as well as both magnetic and non-magnetic rare earth substitution in Sm$_1$-RxB$_6$. We will present our careful investigations of crystal structure, transport properties and magnetization, as well as muon spin rotation studies that together suggest a very profound effect on both the bulk and surface state properties.
play an important role for smaller sizes. A. Manjavacas and F.J Garcia de Abajo, Nat. Commun. (2014).

functions. Both approaches result in an excellent agreement for nanodisks with diameters above 13 nm, although quantum confinement and nonlocal effects based on the random-phase approximation (RPA), which we compare with classical simulations obtained solving Maxwell's equations using tabulated dielectric functions. The physical reason for the above behaviors is non-conservation of optically-excited plasmonic carriers is very different in metal nanocrystals with large and small sizes. We found that the hot-electron generation is efficient only for nanocrystals with very small sizes or in nanocrystals with plasmonic hot spots. The level of smearing is controlled by external electric field. The dispersion and electromagnetic field profile of SPs is calculated numerically for different asymmetric smearings. At some point near the smeared interfaces, where dielectric constant is close to zero, strong enhancement of electric field is predicted. Asymmetry of interface smearings breaks the P-symmetry of the system that leads to frequency splitting of SPs. The dispersion and electromagnetic field profile of SPs interfaces is studied for nano-width metallic films with accounting for interface smearing. Smearing is modelled by electron cloud with density decaying exponentially from the metal surface. The level of smearing is controlled by external electric field. The dispersion and electromagnetic field profile of SPs is calculated numerically for different asymmetric smearings. At some point near the smeared interfaces, where dielectric constant is close to zero, strong enhancement of electric field is predicted. Asymmetry of interface smearings breaks the P-symmetry of the system that leads to frequency splitting of SPs. The dispersion and electromagnetic field profile of SPs interfaces is studied for nano-width metallic films with accounting for interface smearing. Smearing is modelled by electron cloud with density decaying exponentially from the metal surface.

The support of the Australian Research Council is kindly acknowledged.

11:39AM T8.00003 Tailoring the surface plasmon propagation in subwavelength cylindrical structures, HUI KIN KWOK, KIN WAH YU, Department of Physics, The Chinese University of Hong Kong — Tailoring the propagation of surface plasmon polaritons (SPPs) in waveguides is useful for subwavelength focusing in photonic circuits. We have studied the wave propagation in an array of subwavelength dielectric cylinders and hollow cylinders immersed in a metallic host. Motivated by Prodan et al.(2003) who proposed the hybridization model for the plasmonic response of cylindrical nanostructures, we extend the study to non-zero off-plane wave number to assess the effect of the hybridization of SPP modes on the wave propagation in cylindrical structures. The hybridization of SPP modes of cylindrical multi-layer or multi-array geometry allows us to tailor the SPP propagation through the proper separation of the dielectric components as well as their sizes. By means of the electro-optic effect, the tunable refractive index of the material increases the flexibility on the operating frequency range of the dispersion relation.

11:51AM T8.00004 Effect of dielectric spacer layers and substrate on SERS with Au nanoparticle arrays, XIN ZHANG, ROBERT M. BRIBER, ODED RABIN1, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742 — The optical response of a plasmonic nanostructure is often highly dependent on the nature of the underlying substrate. To study the effect of the substrate on surface enhanced Raman scattering (SERS), a series of SERS substrates were fabricated consisting of a hexagonal array of Au nanoparticles self-assembled on block copolymer films, a silicon oxide (dielectric) layer and a silicon substrate or an Au substrate. The inter-particle distance and the dielectric layer thickness were controlled. The SERS Enhancement Factors (EF) were calculated by comparing the Raman spectra of 4-aminophenol adsorbed on the surface of the Au nanoparticles and in a standard solution. The SERS EF were found to be strongly affected by the inter-particle distance and silicon oxide thickness. Changing the inter-particle spacing induced a 102 variation in the EF, changing the oxide thickness increased EF values by an factor of 10, and changing substrate from Si to Au increased EF by a factor of 10. Maximal enhancement factors were found with oxide layer thicknesses between 30 nm and 50 nm beneath the 30 nm polymer film with Au substrates. This geometry both improves the resonance condition with the probe laser and reduced the absorption by the substrate. This work illustrates that optimization of plasmonic-based sensors should consider both the metallic and the surrounding structures.

1 The Institute for Research in Electronics and Applied Physics (IREAP), University of Maryland, College Park, MD 20742

12:03PM T8.00005 Surface plasmon propagation along smeared metal-dielectric interfaces, ANDRII BOZHKO, VLADIMIR DRACHEV, ARKADII KROKHIN, University of North Texas — Propagation of surface plasmons (SPs) along metal-dielectric interfaces is studied for nano-width metallic films with accounting for interface smearing. Smearing is modelled by electron cloud with density decaying exponentially from the metal surface. The level of smearing is controlled by external electric field. The dispersion and electromagnetic field profile of SPs is calculated numerically for different asymmetric smearings. At some point near the smeared interfaces, where dielectric constant is close to zero, strong enhancement of electric field is predicted. Asymmetry of interface smearings breaks the P-symmetry of the system that leads to frequency splitting of SPs. The dispersion and electromagnetic field profile of SPs interfaces is studied for nano-width metallic films with accounting for interface smearing. Smearing is modelled by electron cloud with density decaying exponentially from the metal surface.

12:15PM T8.00006 Generation of hot plasmonic carriers, thermal effects and plasmonic photochemistry in metal nanocrystals, ALEXANDER GOVOROV, Ohio University, HUI ZHANG, Rice University, LUCAS VÁZQUEZ, Ohio University, YURI GUN’KO, University of Dublin, Ireland, MIN OUYANG, University of Maryland — We investigate the effects of generation of hot plasmonic carriers and heat in metal and hybrid nanostructures. In our approach, the problem of hot-electron generation is calculated using the quantum-mechanical approach based on the DFT method and the equation of motion of the density matrix [1], whereas the problem of heat release is treated classically. The energy distribution of optically-excited plasmonic carriers is very different in metal nanocrystals with large and small sizes. We found that the hot-electron generation is efficient only for nanoparticles with very small sizes or in nanocrystals with plasmonic hot spots. The physical reason for the above behavior is non-conservation of momentum in a nanocrystal. Using the newly-developed kinetic DFT theory, we also describe the effect of breaking of the plasmonic resonance into multiple peaks in small nanocrystals. Finally, the generation of plasmonic holes via the interband transitions leads to efficient photochemistry [2]. The results obtained in this study can be used to design a variety of plasmonic nanodevices for photocatalysis and photodetectors.


12:27PM T8.00007 Tunable plasmons in atomically thin gold nanodisks, ALEJANDRO MANJAVacas, Rice University, JAVIER GARCIA DE ABAJO, ICFO-The Institute of Photonic Sciences — The ability to modulate light at high speeds is of paramount importance for telecommunications, information processing, and medical imaging technologies. This has stimulated intense efforts to master optoelectronic switching at visible and near-infrared (vis-NIR) frequencies, although with current computer speeds in integrated architectures still remains a major challenge. Here [1] we show that atomically thin noble metal nanoslands can extend optical modulation to the vis-NIR spectral range. We find plasmons in thin metal nanodisks to produce similar absorption cross-sections as spherical particles of the same diameter. Using realistic levels of electrical doping, plasmons are shifted by about half their width, thus leading to a factor-of-two change in light absorption. These results are supported by a microscopic quantum-mechanical calculations based on the random-phase approximation (RPA), which we compare with classical simulations obtained solving Maxwell’s equations using tabulated dielectric functions. Both approaches result in an excellent agreement for nanodisks with diameter above 13 nm, although quantum confinement and nonlocal effects play an important role for smaller sizes. [1] A. Manjavacas and F.J Garcia de Abajo, Nat. Commun. (2014).

1 A.M. acknowledges financial support from the Welch foundation through the J. Evans Attwell-Welch Postdoctoral Fellowship Program of the Smalley Institute of Rice University (Grant L-C-004).
12:39PM T8.00008 Plasmon-induced Hot Carriers in Metallic Nanoparticles1, JUN LIU, ALEJANDRO MANJAVacas, VIKRAM KULKARNI, PETER NORDLANDER, Rice Univ, LANP TEAM — Plasmon-induced hot carrier formation is attracting an increasing research interest due to its potential for applications in photocatalysis, photodetection and solar energy harvesting. Here [1] we develop a theoretical model for the plasmon-induced hot carrier process and apply it to spherical silver nanoparticles and nanoshells. We show that the inclusion of many-body interactions has only a minor influence on the results. Using the model we calculate the rate of hot carrier generation, finding that it closely follows the spectral profile of the plasmon. Our analysis reveals that particle size and hot carrier lifetime play a central role in determining both the production rate and the energy distribution of the hot carriers. We characterize the efficiency of the hot carrier generation process by introducing a figure of merit that measures the number of high energy carriers generated per plasmon. Furthermore, we analyze the spatial distribution and directionality of these excitations. [1] A. Manjavacas, J. G. Liu, V. Kulkarni, P. Nordlander ACS Nano (2014)

3 We acknowledge financial support from the Welch foundation through the J. Evans Attwell-Welch Postdoctoral Fellowship Program of the Smalley Institute of Rice University (Grant No. L-C-004).

12:51PM T8.00009 Bi-anisotropy in a metallic nanoparticle ring1, LIUYANG SUN, TZUHSUAN MA, SEUNG-CHEOL YANG, The University of Texas at Austin, JINWEI SHI, Beijing Normal University, IRVING MARTINEZ, The University of Uexas at El Paso, GAEHANG LEE, Korea Basic Science Institute, GI-RA YI, Sungkyunkwan University, GENNADY SHVETS, XIAOQIN LI, The University of Texas at Austin — Optical bi-anisotropy refers to magnetoelectric coupling effect, where electric (magnetic) polarization is excited by magnetic (electric) field of the incident light, and the induced polarization and incident field are at different directions. In the field of metamaterials, bi-anisotropy effects have been previously examined in various systems with broken symmetry, such as split rings and Pi-shaped or S-shaped resonators. We investigate bi-anisotropy in the visible frequency range in an asymmetric nano-ring system consisting of four nearly identical gold nanoparticles, in which electric and magnetic dipoles interact with each other. We arrange the nanoparticles into a designed ring geometry using atomic force microscopy manipulation method. Using dark field scattering spectroscopy, we observe that the magnetic dipole is either enhanced or suppressed under different excitation conditions. These results are relevant in designing negative index metamaterials, nano-sensors and other plasmonic devices.

1We acknowledge NSF and AFOSR

1:03PM T8.00010 Non-reciprocal Bands by Symmetry Breaking in One-way Magnetized Plasmonic Double Chain System, CHI WAI LING, KIN HUNG FUNG, The Hong Kong Polytechnic University — Non-reciprocity is a key component to provide one-way propagation in one dimensional (1D) optical waveguides, which enables applications like isolators and switches. Plasmonic chains, formed by spatial periodic metal nanoparticles, are subwavelength 1D optical waveguides. Coupled plasmon modes on the chains are characterized by dispersion relation ω(k), in which k is the wave vector. It has been shown that the spectral reciprocity ω(−k) = ω(k) can be protected by either time reversal (T) or inversion (P) symmetry. However, breaking of (P) and (T) symmetries are not sufficient to achieve ω(−k) ≠ ω(k). We use a magnetized plasmonic double chain system to show that breaking pi-rotation time-reversal (RT) symmetry is also a necessary condition.

1:15PM T8.00011 Controlling spontaneous emission rates of quantum dots with plasmonic nanopatch antennas, THANG HOANG, GLEB AKSELROD, CHRISTOS ARGYROPoulos, JIANI HUANG, DAVID SMITH, MAIKEN MIKKELSEN, Center for Metamaterials and Integrated Plasmonics, Duke University — The radiative processes associated with quantum emitters can be strongly controlled by intense electromagnetic fields created by plasmonic nanostructures. Here, we experimentally demonstrate large enhancements of the spontaneous emission rate of colloidal quantum dots coupled to single plasmonic nanopatch antennas. The antennas consist of silver nanocubes (75 nm) coupled to a gold film separated by a thin polyelectrolyte spacer layer (~1 nm) and core-shell CdSe/ZnS quantum dots (~6 nm). By optimizing the size of the nanopatch antenna, the plasmonic mode is tuned to be in resonance with the quantum dot emission. We show an increase in the spontaneous emission rate by a factor of 880 (Purcell factor) and a 2300-fold enhancement in the total fluorescence while maintaining a high radiative quantum efficiency of ~50 %. The nanopatch antenna, as demonstrated here, offers highly directional and broadband radiation that can be tailored for emitters from the visible to the near infrared, providing a promising approach for the spontaneous emission control of single quantum emitters.

1:27PM T8.00012 Probing plasmons in three dimensions in a scanning transmission electron microscope1, JORDAN HACHTEL, Vanderbilt University, ANAS MOUTI, Oak Ridge National Laboratory, DANIEL MAYO, CLAIRE MARVINNEY, Van- derbilt University, RICHARD MU, Fisk University, RICHARD HAGLUND, Vanderbilt University, STEPHEN PENNYCOOK, University of Tennessee, MATTHEW CHISHOLM, Oak Ridge National Laboratory, SOKRATES PANTELIDES, Vanderbilt University — The optical behavior of nanostructured materials is of significant interest across many fields. Surface plasmons and their interactions with emitters in nanoscale devices allow us to control light below the coherence limit. By understanding the nature of plasmonics at the local level we can move towards unlocking the full potential of photonic devices. To this end, we examine plasmonic Ag nanoparticles suspended on insulating nanowires by combining cathodoluminescence spectroscopy, electron energy loss spectroscopy, and high resolution annular dark field imaging in a scanning transmission electron microscope. The complementary nature of CL and EELS allow us to extract optical data from a randomly shaped and oriented nanoparticle, and understand its plasmonic behavior in all three spatial dimensions.

1This work was sponsored by the US Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, as well as NSF-EPS-1004083 and NSF-TN-SCORE

1:39PM T8.00013 Band modulation and in-plane propagation of surface plasmons in composite nanostructures, REN-HAO FAN, DI-HU XU, KUN ZHANG, RU-WEN PENG, MU WANG, Nanjing University — In this work, we have experimentally and theoretically studied band modulation and in-plane propagation of surface plasmons (SPs) in composite nanostructures with aperture arrays and metallic gratings. It is shown that the plasmonic band structure of the composite system can be significantly modulated because of coupling between the aperture and the grating. By changing the relative positions between these optical components, the resonant modes would shift or split. And the resonant SP modes launched on the structure surface can be effectively modified by the geometric parameters. Further, we provide an experimental observation to directly show the SP in-plane propagation by using far-field measurements. Our study offers a convenient way for observing the SP propagation in far field, and provides unique composite nanostructures for possible applications in subwavelength optodevices, such as optical sensors and detectors.


1:51PM T8.00014 ABSTRACT WITHDRAWN
2:03PM T8.00015 Study on electrostatic resonance of nanoprisms with sharp corners. WAI SOEN CHAN, KA KI NG, KIN WAH YU, Department of Physics, The Chinese University of Hong Kong — We have studied the electrostatic resonance of metal nanoprisms with sharp corners numerically. We consider an infinite metal cylinder with polygonal base, e.g. square. The incident electric field lies in the plane of cross-section of the cylinder. Yu and co-workers proposed Green’s function formalism (GFF) to numerically calculate the electric potential and field distribution in plasmonic systems. We will adopt the scheme to demonstrate the effect of sharp corners, particularly on the effect of electrostatic resonance spectrum, as in the spectral analysis proposed by Bergman and Milton. Hetherington and Thorpe investigated the conductivity of a sheet containing dilute inclusion with sharp corners, they made use of a conformal mapping approach to calculate the conductivity from circular inclusions. Helsing, McPhedran and Milton also investigated the optical properties of a metamaterial lattice with inclusions having sharp corners. We study the possibility of improving numerical accuracy by combining the conformal mapping approach and GFF. We may extend similar approach to investigate the properties of plasmonic systems, for examples nanobottles and nanostars.

Thursday, March 5, 2015 11:15AM - 2:15PM
Session T9 FLAP: Physics and Applications of Photonics and Lasers 006D - Aleksei Zheltikov, Texas A&M University

11:15AM T9.00001 Formation of a single attosecond pulse from the resonant XUV radiation on a steep front edge of a strong IR field. TIMUR AKHMEDZHANOV, Department of Physics and Astronomy, Texas A&M University and Institute for Quantum Studies and Engineering, College Station, TX, VLADIMIR ANTONOV, Institute of Applied Physics of the Russian Academy of Sciences, Nizhny Novgorod, Russia, OLGA KOCHAROVSKAYA, Department of Physics and Astronomy, Texas A&M University and Institute for Quantum Studies and Engineering, College Station, TX — Formation of isolated attosecond pulses is one of the key aims of modern optics. Such pulses with the carrier frequency below the threshold of atomic ionization would provide a tool for studying ultrafast bound dynamics of atoms and molecules. Recently, a mechanism to form a single attosecond pulse from an incident XUV radiation via abrupt interruption of its resonant interaction with hydrogen-like atoms on a steep front edge of a strong IR field was proposed [Phys. Rev. Lett. 110, 213903 (2013)]. If the front edge of the IR field is steep enough, the atoms, essentially unaffected by the IR field during one half-period, can be completely ionized during subsequent half-period of the IR field. Thus, the transient multifrequency atomic response to the XUV radiation is limited to an ultrashort time interval, providing the possibility for attosecond pulse formation. In this contribution, we present the results of solution of time-dependent Schrodinger equation for H atoms simultaneously irradiated by the resonant XUV field and a pulse of strong IR field with steep front edge, which show the possibility to form an isolated attosecond pulse with duration on the order of few hundred attoseconds under the experimentally feasible conditions.

11:27AM T9.00002 Optical breakdown criterion for single-cycle laser pulses. PETER ZHOKHOV, ALEKSEI ZHELTIKOV, Physics & Astronomy Department, Texas A&M University — The Keldysh theory of photoionization in solids is generalized to the case of arbitrarily short driving pulses of any shape or polarization. We derive a closed-form solution for the nonadiabatic ionization rate and field-driven currents in the solid-state electron-hole plasma. Using this framework, we propose a new criterion for optical breakdown of solids that depends on the pulse shape and is applicable to laser pulses as short as a single optical cycle.

11:39AM T9.00003 Large Optical Nonlinearity Induced by Singlet Fission in Pentacene Films1, YUNLONG LIU, CHUNFENG ZHANG, Nanjing Univ, MIN XIAO, Nanjing Univ; University of Arkansas — By creating two triplet excitons from one photoexcited singlet exciton, singlet fission in organic semiconductors has drawn tremendous attention for its potential application in boosting the efficiency of solar conversion. Here, we show that this carrier-multiplication effect can be used to dramatically improve the nonlinear optical response in organic materials. With the technique of dual-wavelength optical Kerr effect (OKE), we have observed large optical nonlinearity with a magnitude of $\chi^{(3)}$ up to $10^{-9}$ esu in pentacene films, which is further shown to be a result of singlet fission as demonstrated by the detailed temporal dynamics and wavelength dependence experiment. Through the use of optical heterodyne detected OKE experiment, we have determined both the sign and value of $\chi^{(3)}$ of the pentacene film. Such efficient third order nonlinear optical response has been successfully applied to demonstrate the all-optical switching. The results observed in this work indicate that the singlet fission could be served as an effective strategy to promote the optical nonlinearity in organic molecule systems.

This work is supported by the National Basic Research Program of China (2013CB932903 and 2012CB921801, MOST), the National Science Foundation of China (91233103, 61108001, 11227406 and 11321063)

11:51AM T9.00004 Incorporation of C in Cu for the Fabrication of Transparent Electrodes1, ROMAINE ISAACS, HONG LI ZHU, COLIN PRESTON, PETER ZAVALLI, University of Maryland, AZZAM MANSOUR, Naval Surface Warfare Center, MELBS LEMIEUX, LIANGBING HU, LOURDES SALAMANCA-RIBA, University of Maryland — The incorporation of carbon nanostructures into the copper lattice has the potential to improve the current density of copper to meet the ever-increasing demands of nanoelectronic devices. We report on the structure and properties of a new material formed by the incorporation of carbon in concentrations up to 10 wt% into the crystal structure of copper that we refer to as "Cu covetic". The carbon does not phase separate after subsequent melting and re-solidification despite the absence of a predicted solid solution at such concentrations in the binary phase diagram. Bulk samples, as well as thin films grown at room temperature and high temperature are investigated. X-ray photoelectron spectroscopy (XPS) confirmed that C incorporates in the bulk of the Cu. Transmission Electron Microscopy (TEM) shows that C forms a modulated structure in the crystal lattice, and Electron Energy Loss Spectroscopy (EELS) indicates that C-K edge is graphicitic nature with sp2 bonding. Copper covetic films exhibit greater transparency, higher conductivity, and resistance to oxidation than pure copper films of the same thickness, making them a suitable choice for transparent conductors.

1Supported by DARPA/ARL under Grant No. W911NF-13-1-0058 and ONR under grant N000141410042.

12:03PM T9.00005 Reflective Optical Limiter Based on Resonant Transmission1, ELEANA MAIKRI, TSAMPIKOS KOTTOS, Department of Physics, Wesleyan University, Middletown CT-06459, USA, ILYA VITEBSKIY, Air Force Research Laboratory, Sensors Directorate, Wright Patterson AFB, OH 45433 USA — Optical limiters transmit low-level radiation while blocking electromagnetic pulses with excessively high energy (energy limiters) or with excessively high peak intensity (power limiters). A typical optical limiter absorbs most of the high-level radiation which can cause its overheating and destruction. Here we introduce the novel concept of a reflective energy limiter which blocks electromagnetic pulses with excessively high total energy by reflecting them back to space, rather than absorbing them. The idea is to use a defect layer with temperature dependent loss tangent embedded in a low-loss photonic structure. The low energy pulses with central frequency close to that of the localized defect mode will pass through. But if the cumulative energy carried by the pulse exceeds certain level, the entire photonic structure becomes highly reflective (not absorptive!) within a broad frequency range. The underlying physical mechanism is based on self-regulated impedance mismatch which increases dramatically with the cumulative energy carried by the pulse.

1AFOSR MURI FA9550-14-1-0037
12:15PM T9.00006 Coupling control based on Adiabatic elimination for densely integrated nano-photonics — MICHAEL MREJEN, HAIM SUCHOWSKI, TAIKI HATAKEYAMA, CHIH-HUI WU, LIANG FENG, KEVIN O’BRIEN, YUAN WANG, XIANG ZHANG, NSF Nanophotonics Science and Engineering Center (NSEC), 3112 Etcheverry Hall, University of California, Berkeley — The ever growing need for energy-efficient and fast communications is driving the development of highly integrated photonic circuits where controlling light at the nanoscale becomes the most critical aspect of information transfer. Here we develop a unique scheme of adiabatic elimination (AE) modulation to actively control the coupling among waveguides for densely integrated photonics. Analogous to atomic systems, AE is achieved by applying a decomposition on a three waveguide coupler, where the two outer waveguides serve as an effective two-mode system with an effective coupling of \( V_{eff} = \left[ (V_{1}^{*} + V_{2}^{*} + V_{3}^{*})^2 / 2 \right] [n_1 - V_1 + V_2]/2 \), and the middle waveguide is the equivalent to the intermediate level ‘dark state’. We experimentally demonstrate the first all optical AE modulation and its ability to control the coupling between the two waveguides by manipulating the mode index of the decoupled middle one. In addition, we show that the strong modes interactions allowed at the nano-scale offer a unique configuration of zero-coupling between all the waveguides, a phenomena that paves the way for ultra-high density photonic integrated circuits where small footprint is of crucial importance.

12:27PM T9.00007 A Moiré Cavity Plasmonic Dye Laser — ERTUGRUL KARADEMIR, Department of Physics, Bilkent University, 06800 Ankara, Turkey, SINAN BALCI, Department of Astronautical Engineering, University of Turkish Aeronautical Association, 06790 Ankara, Turkey, COSKUN KOCABAS, ATILLA AYDINLI, Department of Physics, Bilkent University, 06800 Ankara, Turkey — From its first conception [1] to its first demonstration, [2] plasmonic lasers have been an intriguing topic of research. In this work, Moiré gratings which manifest a cavity state in the SPP dispersion curve [3]. We used a reverse Kretschmann setup to decouple the amplified light component of SPPs. We employed a Moiré cavity with 250 nm periods and four period structures, respectively, with a peak wavelength of 614 nm in the four period device. Since each layer of a period has a different refractive index, constructive interference from the total reflected portion of light can be investigated to create effective reflectors. The DBR's can be made to act as optical mirrors to enhance certain wavelengths of light to be highly reflected. Due to the high refractive optical structure can be paired with a superpartner with similar guided wave and scattering properties. As a result, the guided mode spectra of these optical waveguide systems can be judiciously engineered so as to realize new families of mode filters and mode division multiplexers and demultiplexers. Here we show that the concept of supercavity can be used to synthesize scattering settings with identical scattering properties, thus giving rise to an entirely new class of transformation optics. By systematically eliminating all bound states, scattering arrangements with a low refractive index contrast can be designed to faithfully mimic the scattering behavior of high-contrast structures. Similar strategies can be used to replace negative-permittivity domains, thus avoiding unwanted optical losses.

12:39PM T9.00008 Supersymmetry and transformation optics — MOHAMMAD-ALI MIRO, MATTHIAS HEINRICH, DEMETRIOS CHRYSTODOLIDES, CRÉOL. The College of Optics and Photonics, University of Central Florida, NONLINEAR WAVE GROUP TEAM — Supersymmetry (SUSY) originated within the framework of quantum field theory as a means to treat fermions and bosons on an equal footing. While the verification of such theories remain an ongoing challenge in particle physics, some of their fundamental notions have been successfully adapted to other fields. As shown recently, optics can provide a versatile platform where the implications of supersymmetric transformations can be studied and observed. In this regard, any optical structure can be paired with any other structure with similar guided wave and scattering properties. As a result, the guided mode spectra of these optical waveguide systems can be judiciously engineered so as to realize new families of mode filters and mode division multiplexers and demultiplexers. Here we show that the concept of supercavity can be used to synthesize scattering settings with identical scattering properties, thus giving rise to an entirely new class of transformation optics. By systematically eliminating all bound states, scattering arrangements with a low refractive index contrast can be designed to faithfully mimic the scattering behavior of high-contrast structures. Similar strategies can be used to replace negative-permittivity domains, thus avoiding unwanted optical losses.

12:51PM T9.00009 Controlling modal interactions in lasers for frequency selection and power enhancement — LI GE, College of Staten Island/Graduate Center, CUNY — The laser is an out-of-equilibrium non-linear wave system where the interplay of the cavity geometry and non-linear wave interactions determines the self-organized oscillation frequencies and the associated spatial field patterns. Using the correspondence between nonlinear and linear systems, we propose a simple and systematic method to achieve selective excitation of lasing modes that would have been dwarfed by more dominant ones. The key idea is incorporating the control of modal interaction into the spatial pump profile. Our proposal is most valuable in the regime of spatially and spectrally overlapping modes, which can lead to a significant enhancement of laser power as well.

1:03PM T9.00010 Retrieval of contaminated information using random lasers — JINWEI SHI, DAHE LIU, Beijing Normal University, LIBIN CUI, Beijing Normal University and Beijing University of Technology — Data retrieval is an important information processing task. The most commonly used method in optical information processing is spatial filtering based on Fourier optics. However, these methods are very difficult to implement in practical applications. Over the last two decades, random lasers due to its cavity free property have attracted widespread attention. Some potential applications have been proposed; however, few actual applications were reported. Here we develop an information retrieval method based on random lasers, where the spatial frequency spectrum of a contaminated Fourier transform hologram can be obtained by detecting the temporal frequency spectrum information from random lasing. The hologram information can be reconstructed from an inverse Fourier transform of the spatial frequency spectrum obtained after data processing. It is shown that random lasers can be used for information retrieval, and may potentially find applications in information optics and optical data storage.

1:15PM T9.00011 Reflectivity Calculations on Hybrid-layered CdS/PVK Distributed Bragg Reflectors — JAVIER HASBUN, AJITH DESILVA, University of West Georgia — In this study we apply the Born theory [1] of wave propagation on a stratified medium to obtain the reflectivity and transmissivity of a series of distributed Bragg reflectors (DBR). The DBR's are made of pairs of identical alternating layers. Each pair of layers is referred to as a period. Thus, we grow DBR's of one, two, three, and four periods and study their reflectivity properties. Since each layer of a period has a different refractive index, constructive interference from the total reflected portion of light can be investigated to create effective reflectors. The DBR's can be made to act as optical mirrors to enhance certain wavelengths of light to be highly reflected. Due to the high refractive index difference between polyvinyl carbazole (PVK), index 1.853 and cadmium sulfide CdS (index 2.5), a greater reflectivity can be obtained from the structure for fewer periods. The constructed DBR data show theoretically fitted reflectivities with reflectances of about 27%, 51%, 64%, and 80% for the one, two, three, and four period structures, respectively, with a peak wavelength of 614 nm in the four period device.


The authors wish to thank the UWG-UWISE minigrant program for their support.
which forms a natural multilayer heterostructure consisting of a TI and an ordinary insulator. For heterostructures is a new promising strategy for manipulating the topological states and realizing exotic quantum phenomena. In this work, with recently discovered topological phase transition in (Bi$_2$Se$_3$)$_m$ and insulating bulk. If it is possible to manipulate the two coexisting states, then it should form an ideal laboratory for realizing a topologically tunable Fano system. The asymmetric Fano profile, suggesting potentials toward optically controllable topological Fano systems. By engineering the spatial overlap between surface Dirac electrons and bulk phonon, we continuously tune, abruptly switch, and dynamically modulate the sequence of layers or insert different building blocks into the crystal. We have performed angle-resolved photoemission spectroscopy on (PbSe)$_2$(Bi$_2$Se$_3$)$_3$ to test this hypothesis. The results demonstrate that utilizing of TI heterostructures is a new promising strategy for manipulating the topological states and realizing exotic quantum phenomena.

**Thursday, March 5, 2015 11:15AM - 2:15PM**

**Session T10 DCMP: Topological Insulators: Synthesis**

007A - Yasuyuki Nakajima, University of Maryland

**11:15AM T10.00001 Manipulation of topological states in a topological-insulator heterostructure** — YUSUKE TANAKA, KOSUKE NAKAYAMA, TAKAFUMI SATO, Department of Physics, Tohoku University, SEIGO SOUMA, WPI-AIMR, Tohoku University, TAKASHI TAKAHASHI, Department of Physics, Tohoku University, KAZUMA ETO, SATOSHI SASAKI, KOJI SEGAWA, YOICHI ANDO, ISIR, Osaka University — The Dirac fermions in the Topological insulators (TIs) are immune to backward scattering by nonmagnetic impurities or disorder. While experimental realizations of novel topological phenomena depend crucially on the inherent robustness of the topological surface states against perturbations, it turned out to be difficult to maintain stable surface properties under ambient atmosphere. This situation has been a hindrance for realizing novel topological phenomena and device applications of TIs. We present a novel approach to solve this problem— the heterostructure engineering where one can alter the stacking sequence of layers or insert different building blocks into the crystal. We have performed angle-resolved photoemission spectroscopy on (PbSe)$_2$(Bi$_2$Se$_3$)$_3$ to test this hypothesis. The results demonstrate that utilization of TI heterostructures is a new promising strategy for manipulating the topological states and realizing exotic quantum phenomena.

**11:27AM T10.00002 Topologically tunable ultrafast Fano interference dynamics** — SANGWAN SIM, School of Electrical and Electronic Engineering, Yonsei University, Korea, NIKESH KOIRALA, MATTHEW BRAHLEK, Department of Physics and Astronomy, Rutgers the State University of New Jersey, USA. JUN PARK, SOONYOUNG CHA, School of Electrical and Electronic Engineering, Yonsei University, Korea, SEONGSHIK OH, Department of Physics and Astronomy, Rutgers the State University of New Jersey, USA. HYUNYONG CHOI, School of Electrical and Electronic Engineering, Yonsei University, Korea — Asymmetric Fano resonance arises from interference between continuum and discrete state. The asymmetric profile has attracted strong interests in understanding light-induced optoelectronic responses and corresponding applications. In conventional solids, however, the tunability of Fano resonance is generally limited by material’s intrinsic property. Topological insulator is unique class of matters embodying both conducting Dirac surface and insulating bulk. If it is possible to manipulate the two coexisting states, then it should form an ideal laboratory for realizing a topologically tunable Fano system. In this work, with recently discovered topological phase transition in (Bi$_2$Se$_3$)$_m$, we report novel Fano interference phenomena. By engineering the spatial overlap between surface Dirac electrons and bulk phonon, we continuously tune, abruptly switch, and dynamically modulate the Fano profile. Ultrafast optical-pump terahertz-probe spectroscopy reveals that the controlled spatial overlap is responsible for the picosecond tunability of the asymmetric Fano profile, suggesting potentials toward optically controllable topological Fano systems.
11:39AM T10.00003 Adsorption and dissociation of H2O molecules on the topological insulator surface, Bi2Se3 (111)1, EUN-HA SHIN, HANCHUL KIM, Sookmyung Women’s University — Three-dimensional strong topological insulators (TIs) such as Bi2Se3, Bi2Te3 and Bi2SBi are intriguing for their surface metallicity in contrast to the insulating bulk. The metallic surface states of TI are known to be topologically protected and robust for impurities and disorders. In this work, we report first-principles calculations on the adsorption and dissociation of H2O molecules on Bi2Se3 (111) to understand the chemical reactivity and the effect of oxidation on the surface metallicity. On the pristine (111) surface, H2O molecule is found to chemisorb on a subsurface Bi atom and form two additional hydrogen bonds with neighboring surface Se atoms. The adsorbed H2O molecule can be dissociated into a hydroxyl (OH) and H. The dissociated OH takes a surface Se site, and pushes up the Se atom that is bonded with the dissociated H. We examined a subsequent dissociation reaction of OH. The final reaction products are a substitutional O (Osub) and an H2Se molecule floating in the vacuum. By examining the electronic structure, we found that the chemisorbed OH induces n-type doping. On the other hand, the Osub and the adsorbed H2O result in p-type doping. Throughout the whole chemical processes studied, the metallic surface state remains intact.

1This work was supported by a National Research Foundation of Korea grant (No. 20100012231) and the EDISON program (No. 2012M3C1A6035684) funded by the Korea government(MEST), and by the Supercomputing Center at KISTI (No. KSC-2014-C3-042).

11:51AM T10.00004 Flexible Thermoelectric Fabrics Based on Layered Topological Insulator Bi2Se3 Nanoplates/Polyvinylidene Fluoride Composite1, CHAOCHAO DUN, COREY HEWITT, HUIHUI HUANG, DAVID CARROLL, Center for Nanotechnology and Molecular Materials, Department of Physics, Wake Forest University, Winston-Salem, NC 27109, U. S. — We report a highly-flexible and ultrathin thermoelectric fabrics based on topological insulator (TI) Bi2Se3 Nanoplates/PVDF Composite, which show a room temperature Seebeck coefficient, electrical conductivity, and figure of merit ZT ∼ 0.2 W/(mK), 5000 S/m, 0.02, respectively. This results demonstrate that Bi2Se3 Nanoplates/PVDF composite exhibit favorable thermoelectric characteristics, which opens a new avenue to fabricate highly-flexible and lightweight sustainable energy sources that could be compatible with portable/wearable electronic devices. The low thermal conductivity of the composites (∼ 0.42 W/(mK)) suggests the nonconducting host polymer matrix PVDF serves to bind the conducting topological insulator (TI) Bi2Se3, while still maintaining an adequate power factor and figure of merit. The flexible thermoelectric fabrics based on layered topological insulator Bi2Se3 Nanoplates/PVDF composite that with comparable thermoelctrical efficiency is only a typical example that showing the promising of the present method for further applications of 2D topological insulator like Bi2Se3, Bi2Te3 and Sb2Te3. At their current performance, if enough thermal energy is available, the composites could be used to provide sufficient thermoelectric power for low powered personal and portable electronics.

1This study was conducted under support from the Air Force Office of Scientific Research Grant Number FA 9550-13-1-0085.

12:03PM T10.00005 Fermi level tuning and weak localization/weak antilocalization competition of bulk single crystalline Bi1−xSb2xTe compounds, WONHYUK SHON, JONGSOO RHYE, Kyung Hee Univ — In the investigation of the electrical transport properties of single crystalline Bi1−xSb2xTe (x = 0.0, 0.6, 0.8, 1.0, 1.2, and 1.4) compounds, we observed a systematic change of the Fermi level from n-type metallic (x = 0.0, 0.6) or small-gap semiconducting (x = 0.8) to p-type semiconducting (x = 1.0) and metallic (x = 1.2, 1.4), respectively, with increasing Sb-substitution concentration from the temperature-dependent electrical resistivity ρ(T) and Hall resistivity ρxy(T) measurements, respectively. The parent compound Bi2Te3 exhibits linear negative magnetoresistance measurements at low temperatures. From the Hikami-Larkin-Nagaoka analysis of the compounds (x = 0.8 and 1.0), we found that there is a competing behavior between WL and WAL in terms of Sb-doping and magnetic field strength.

12:15PM T10.00006 Emergence of Decoupled Surface Transport Channels in Bulk Insulating Bi2Se3 Thin Films, MATTHEW BRAHLEK, NIKESH KOIRALA, MARYAM SALEHI, NAMRATA BANSAL, SEONGSHIK OH, Rutgers Univ — In ideal topological insulator (TI) films the bulk state, which is supposed to be insulating, should not provide any electric coupling between the two metallic surfaces. However, transport studies on existing TI films show that the topological states on opposite surfaces are electrically tied to each other at thicknesses far greater than the direct coupling limit where the surface wave functions overlap. Here, we show that as the conducting bulk channels are suppressed, the parasitic coupling effect diminishes, and the decoupled surface channels emerge as expected for ideal TIs. In Bi2Se3 thin films with fully suppressed bulk states, the two surfaces, which are directly coupled below ∼10 QL, become gradually isolated with increasing thickness and are completely decoupled beyond ∼ 20 QL. On such a platform, it is now feasible to implement transport devices whose functionality relies on accessing the individual surface layers without any deleterious coupling effects.

12:27PM T10.00007 ABSTRACT WITHDRAWN —

12:39PM T10.00008 Epitaxial Growth of Artificial Graphene on Conventional Semiconductor Surface towards Room Temperature Topological Quantum States1, MIAO ZHOU, WENMEI MING, ZHENG LIU, ZHENGFEI WANG, FENG LIU, University of Utah — Graphene is a 2D hexagonal lattice made of sp2 hybridized carbon. Fundamental understanding of graphene has recently spurred a surge of searching for 2D topological quantum phases in solid-state materials. Here we demonstrate the epitaxial growth of artificial graphene, in which the carbon atoms are replaced by other elements, on conventional semiconductor surface to realize large-gap topological quantum phases. We show that Si(111) surface functionalized with 1/3 monolayer of halogen atoms [Si(111)-3√3×√3X (X=C1, Br, I)] exhibiting a trigonal superstructure, provides an ideal template for epitaxial growth of heavy metals, such as Bi, which self-assemble into a hexagonal lattice with high kinetic and thermodynamic stability. Remarkably, the Bi overlayer show the feature of a (Osub)2 and an H2Se molecule floating in the vacuum. By examining the electronic structure, we found that the chemisorbed OH induces n-type doping. On the other hand, the Osub and the adsorbed H2O result in p-type doping. Throughout the whole chemical processes studied, the metallic surface state remains intact.

1This research was supported by DOE (Grant No: DEF02-04ER46148).

12:51PM T10.00009 Population dynamics of Floquet-Bloch states on the surface of a topological insulator, FAHAD MAHMOOD, DILLON GARDNER, Massachusetts Inst of Tech-MIT, YEW SAN HOR, Missouri University of Science and Technology, YOUNG LEE, NUH GEDIK, Massachusetts Inst of Tech-MIT — Floquet-Bloch bands emerge in solid-state systems due to a coherent interaction between light and matter. Using time and angle resolved photoemission spectroscopy; we demonstrate that intense ultrashort midinfrared pulses hydrbide with the surface Dirac fermions of a topological insulator to form states periodic in both momentum and energy. These states exhibit band gaps at avoided crossings which are dependent on the incident light polarization and the electron momentum. Circularly polarized light induces an additional gap at the Dirac point by naturally breaking time reversal symmetry. We further characterize these bands as a function of the incident light intensity and pump-probe delay time to understand the excitation and decay mechanisms of electrons in the Floquet-Bloch states.
1:03PM T10.00010 Surface and interface states of Bi$_2$Se$_3$ thin films investigated by second harmonic generation. SUN YOUNG HAMH, SOON-HEE PARK, JONG SEOK LEE, Department of Physics and Photon Science, Gwangju Institute of Science and Technology, Gwangju 500-712, Korea, JEONG HEUM JEON, SE-JONG KHANG, Department of Physics, Korea University, 136-713, Korea, KWANGNAM YU, ENJIP CHOI, Department of Physics, University of Seoul, Seoul 130-743 Korea, SEONGSHIK OH, Department of Physics and Astronomy, Rutgers, the State University of New Jersey, Piscataway, New Jersey 08854, USA, SUNG KIM, SUK-HO CHOI, Department of Applied Physics, College of Applied Science, Kyung Hee University, Yongin 446-701, Korea, JOONBUM PARK, JUN SUNG KIM, Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea — Topological insulators (TIs) behave as a charge-gapped insulator in its interior, but hosting a spin-momentum-locked Dirac state at the surface. When the Fermi level crosses over conduction/valence band, undesirable bulk charge transport disturbs to explore the surface nature, so that thin film TIs have been highlighted as a method to reduce bulk carrier effect due to large surface to volume ratio. In this presentation, we discuss surface and/or interface states for Bi$_2$Se$_3$ in form of field by exploiting second harmonic generation technique. Based on nonlinear susceptibility deduced from the model fitting, we investigate the details of band bending such as its direction and strength which were further addressed by examining terahertz field profile emitted from the sample. Finally, we discuss the evolution of these properties as a function of film thickness.

1:15PM T10.00011 Investigation of the Dirac states in a topological insulator, Bi(2)Se(3). DEEPNARAYAN BISWAS, SANGEETA THAKUR, KHADIZA ALI, Tata Institute of Fundamental Research, G. BALAKRISHNAN, University of Warwick, KALOBARAN MAITI, Tata Institute of Fundamental Research. — Topological insulators are bulk insulators with metallic surface states protected by time reversal symmetry. These surface states are spin-polarized, backscattering free and exhibit Dirac cone in their energy band structure, and thus are potential candidates for technological advances and realizing exotic phenomena. However, experiments show appearance of such topological order on the surface of metallic bulk and instability of the Dirac states in most of the materials studied. Thus, doping foreign elements to engineer the electronic states and get access to the surface states has become an outstanding problem. We studied the detailed electronic structure of Bi$_2$Se$_3$ using ARPES and DFT calculations and observe different behavior for different surface terminations. Se terminated surface exhibits an electron doping scenario with aging in contrast to the hole doped scenario in Bi terminated surface. The Dirac cone on Bi terminated surface is found to be most stable even in presence of impurities and is most suitable to observe different behavior for different surface terminations. In all devices, the upper and lower surface states are independently tunable to the Dirac point by the top and bottom gate electrodes. In thin devices, electric fields are found to penetrate through the bulk, indicating finite capacitive coupling between the surface states. A charging model allows us to use the penetrating electric field as a measure of the intersurface capacitance $C_{TT}$ and the surface state energy-density relationship $\mu(n)$, which is found to be consistent with independent angle-resolved photoemission spectroscopy measurements. At magnetic fields, increased field penetration through the surface states is observed, strongly suggestive of the opening of a surface state band gap due to broken time-reversal symmetry.

1:39PM T10.00013 A top-down approach to prepare bismuth bi-layer terminated Bi$_2$Se$_3$(0001). ROOZBEH SHOKRI, HOLGER, L. MEYERHEIM, SIMULAY ROY, KATAYÖN MOHSENEN, ARTHUR ERNST, Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle, Germany, MIKHAILO M. OTROKOV, EVGENI V. CHULKOV, Departamento de Física de Materiales UPV/EHU, Centro de Física de Materiales CFM · MPC and Centro Mixto CSIC-UPV/EHU, Spain, JÜRGEN KIRSCHNER, Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle, Germany — A bi-layer of bismuth (Bi) in the (111) plane possesses strong spin-orbit coupling and represents a prototype 2D topological insulator (TI). In this study, we propose a novel top-down approach to prepare Bi on 3D TI Bi$_2$Se$_3$(0001). Combining scanning tunneling microscopy, X-ray crystal truncation rod analysis and Auger electron spectroscopy we demonstrate that under controlled exposure of Bi$_2$Se$_3$ to atomic hydrogen flux the selenium is removed from the topmost quintuple layer and a flat Bi bi-layer terminated Bi$_2$Se$_3$, with Bi$_2$Se$_3$-terrace-size lateral extension is achieved. Our results suggest new perspectives to manipulate the electro-optical properties of both Bi and Bi$_2$Se$_3$ TIs.

1:51PM T10.00014 Efficient Dual-Gate Tuning of Fermi Level in Thin-Film Topological Insulator. ALEXEY TASKIN, FAN YANG, SATOSHI SASAKI, KOJU SEGAWA, YASUHIDE OHNO, KAZUHIKO MATSUMOTO, YOICHI ANDO, Osaka University, ISIR TEAM — Experimental studies of novel quantum phenomena predicted for three-dimensional (3D) topological insulators (TI) often require tuning of the Fermi level across the Dirac point. Both back gating and top gating techniques have been successfully applied to 3D TI thin films, however, with a single gate the chemical potential of only one surface can be controlled effectively, which is not sufficient for many applications. Recently, we have succeeded in developing a comprehensive method for fabricating dual-gated devices on TI thin films grown by molecular beam epitaxy. The method combines 1) the transfer of a high-quality bulk-insulating (Bi$_2$Se$_3$)$_x$(SiO$_2$)$_{1-x}$ thin film grown on sapphire onto a SiO$_2$/Si wafer, which serves as a back gate, and 2) the fabrication of a top gate by using a low-temperature deposition of SiN$_x$. We demonstrate that the dual gating allows effective tuning of the chemical potentials of the top and bottom surfaces across the Dirac point, which is manifested in a large peak of the sheet resistance accompanied by a sharp sign change of $R_{xy}$ upon sweeping the top and bottom gate voltages. This dual-gating method opens exciting opportunities for realization of various novel phenomena expected for 3D TIs.

2:03PM T10.00015 Air-Stable Electron Depletion of Bi$_2$Se$_3$ into the Topological Regime using Molybdenum Trioxide. JACK HELLERSTEEDT, Monash University and University of Maryland, MARK T. EDMONDS, Monash University, ANTON TADICH, Australian Synchrotron, ALAN SCHENK, Monash University, JARENE M. O’DONNELL, Australian Synchrotron, JACOB TOSADO, Monash University and University of Maryland, NICHOLAS P. BUTCH, National Institute of Standards and Technology, PAUL SYERS, JOHNPIERRE PAGLIONE, University of Maryland, MICHAEL S. FUHRER, Monash University and University of Maryland — Bismuth selenide (Bi$_2$Se$_3$) is a three-dimensional strong topological insulator of particular interest due to its relatively large bulk band gap (300 meV) and single set of topologically non-trivial surface states. However, persistent doping makes routine electronic access to the topological regime difficult. Here we explore surface transfer doping via molecular deposition as a route to bring the Fermi level into the topological regime and protect against ambient degradation. Bi$_2$Se$_3$ single crystals are cleaned in ultra-high vacuum and X-ray photoemission spectroscopy is used to measure the shifts in work function, Bi core levels, and charge state of Mo during deposition of MoO$_3$ molecules; the data indicate that MoO$_3$ can lower the Fermi level to within ∼100 meV of the Dirac point. Thin film transport measurements that ∼10$^{13}$ electrons can be depleted from the Bi$_2$Se$_3$ and that an MoO$_3$ capping layer is stable for days after exposure to ambient.

1Supported by JSPS (KAKENHI 25220708 and 25400328), MEXT (Innovative Area “Topological Quantum Phenomena” KAKENHI), AFOSR (A0ARD 124038), Inamori Foundation, and the Murata Science Foundation.

2Supported by the NSF grants DMR-11-05224 and DMR-05-20471 (Maryland MRSEC); MSF is supported by an ARC Laureate Fellowship.
Thursday, March 5, 2015 11:15AM - 2:15PM —
Session T11 DCMP: Superconductivity: Heavy Elements and Spin-Orbit Effects 007B - Valentin Taoufar, Ames Laboratory

11:15AM T11.00001 Fermi-surface instabilities in the presence of spin-orbit coupling  CHRISTIAN PLATT, MARIO FINK, WERNER HANKE, RONNY THOMALE, University of Wuerzburg — Besides its relevance in the formation of topological insulators, the effect of spin-orbit coupling also gives rise to novel types of superconductivity and unprecedented spin- and charge orders. Due to the progress in the fabrication of tailored materials and surfaces, these novel states-of-matter now become accessible and can be investigated by different experimental probes. Within the theoretical framework of functional renormalization group, we study the effect of spin-orbit coupling on the emergence of Fermi-surface instabilities. Starting from an ab-initio model input, we compare our results with recent experiments performed on the metallic surface states of half-Heusler compounds.

11:27AM T11.00002 Far-from-equilibrium dynamics of spin-orbit coupled superfluids  MUBARAK ALQAHTANI, MAXIM DZERO, Kent State University — We present the results of the theoretical study for the collisionless dynamics of the pairing amplitude in two-dimensional superfluid with strong spin-orbit coupling. We consider the cases when the dynamics is initiated by a sudden change of the coupling constant or an external magnetic field. Depending on the initial conditions and an amplitude of a quench, at long times the pairing amplitude dynamically vanishes, reaches a constant or periodically oscillates with time. We determine the corresponding steady state phase diagram exactly for generic quenches of the coupling constant and specific quenches of the magnetic field. We also study topological Floquet superfluidity which can be generated by the periodic oscillations of the pairing amplitude.

11:39AM T11.00003 Superconducting hyper-honeycomb lattice  ADRIEN BOUHON, ANNICA BLACK-SCHAFER, Uppsala Univ — Motivated by the recent discovery of the hyper-honeycomb β-Li2IrO3 studied in the context of Kitaev spin liquids, we investigate the possibility to realize superconductivity in the hyper-honeycomb lattice. Based on a t-J model we discuss the effect of the band structure and spin-orbit coupling on the most stable superconducting state.

11:51AM T11.00004 Superconductivity in R$_3$T$_4$Ge$_{13}$ (R = Y, Lu and T = Rh, Co, Os) single crystals  BINOD RAI, Rice University, IAIN OSWALD, University of Texas at Dallas, JIAKUI WANG, Rice University, GREGORY MCCANDLESS, JULIA CHAN, University of Texas at Dallas, EMILIA MOROSAN, Rice University — Single crystals of R$_3$T$_4$Ge$_{13}$ (R = Y, Lu and T = Rh, Co, Os) have been grown by flux methods and have been found to adopt the Fr$_3$Rh$_4$Sn$_{13}$ structure type. Magnetization and specific heat measurements confirm that all four compounds are bulk superconductors. Reduced superconducting gaps observed in the specific heat suggest that these may be multi-band superconductors. We observe an unusual increase of the electrical resistivity and a decrease of the charge carrier density on cooling in the normal state in all four reported compounds. However, band structure calculations reveal a metallic ground state in all four compounds, consistent with the emergence of superconductivity at low temperatures. We empirically show that large atomic displacement parameter ratios in R$_3$T$_4$Ge$_{13}$ compounds are correlated with the semiconducting behavior, resolving the contradiction between the experiment and the calculations.

1Work at Rice University was supported by Welch Foundation and AFO

12:03PM T11.00005 Unconventional superconductivity in U$_2$PtC$_2$  NICK WAKEHAM, ANDY MOUNCE, Los Alamos Natl Lab, NI NI, UCLA, MINGKANG KANG, Los Alamos Natl Lab, SANGYUN LEE, Sung Kyun Kwan University, ROMAN MOVSVOVICH, JIANXIN ZHU, Los Alamos Natl Lab, TUSON PARK, Sung Kyun Kwan University, ERIC BAUER, JOE THOMPSON, FILIP RONNING, Los Alamos Natl Lab — U$_2$PtC$_2$ has long been known to be a moderately heavy-fermion superconductor with transition temperature $T_c\sim 1.3$K. However, until recently little was known about the nature of the superconductivity. We will present a summary of our recent investigation into the superconductivity in this material through structural, transport, thermodynamic, and nuclear magnetic resonance measurements. Evidence for an unconventional gap structure comes from power law dependencies of the specific heat as a function of field and temperature in all four reported compounds. However, band structure calculations reveal a metallic ground state in all four compounds, consistent with the emergence of superconductivity at low temperatures. We empirically show that large atomic displacement parameter ratios in R$_3$T$_4$Ge$_{13}$ compounds are correlated with the semiconducting behavior, resolving the contradiction between the experiment and the calculations.

12:15PM T11.00006 ABSTRACT WITHDRAWN —

12:27PM T11.00007 Superconducting and normal state properties in Uranium-based materials from thermal and thermoelectric measurements  J.-PH. REID, J. BARRACLOUGH, University of St-Andrews, O. ENTWISLE, C. LITHGOW, D. SOKOLOV, W. WHITLEY, E. YELLAND, ANDREW HUXLEY, University of Edinburgh — Although it is clear that the interplay between superconductivity and magnetic or charge orders has a crucial role to the origin of superconductivity, it is not yet understood how and why that is. One of the best ways to shed light on this question is by measuring thermal conductivity and thermoelectricity. The former probes the zero-energy ($T \to 0$) quasiparticles and is very sensitive to the superconducting gap structure, whereas the latter is ideal to detect any change in the Fermi surface due to competitive orders. In this talk, a thermal and thermoelectric study will be presented and will focus on the ferromagnetic superconductor URhGe.

12:39PM T11.00008 Possible mechanism for s-wave superconductivity in heavy-fermion systems: Variational cluster study  KEISUKE MASUDA, Department of Physics, Waseda University, DAISUKE YAMAMOTO, Waseda Institute for Advanced Study, Waseda University — We study s-wave superconductivity in heavy-fermion systems, which cannot be easily understood due to the existence of the strong Coulomb repulsion between $f$ electrons. The key idea of our proposal is to consider the interorbital Cooper pairing between conduction electrons ($c$ electrons) and localized $f$ electrons, which we refer to as the “$c$-$f$ pairing.” We analyze the periodic Anderson model by means of the variational cluster approach in which all the three types of on-site pairing, namely intraorbital pairings between $c$ electrons and between $f$ electrons and the $c$-$f$ pairing, are taken into account. At half filling, the system exhibits the Kondo insulating or antiferromagnetic state, depending on the strength of the Coulomb repulsion. When electrons or holes are doped to the antiferromagnetic state, s-wave superconductivity appears coexisting with the antiferromagnetic long-range order. We also find that the magnetic order vanishes for further doping, and a pure s-wave superconducting state is formed for a certain range of doping concentration. We suggest the $c$-$f$ pairing as a possible mechanism for s-wave superconductivity in heavy-fermion systems.

1D.Y. is supported by KAKENHI from JSPS Grants No. 26800200.
12:51PM T11.00009 A comprehensive study of chemical substitution effects on superconductivity in LaPt$_4$Ge$_{12}$

E. KEVIN HUANG$^1$, DUYGU YAZICI, BENJAMIN WHITE, ALEXANDER BREINDEL, NAVEEN POUSE, Physics Department, University of Houston, LEI SHUI, Physics Department, Fudan University, BRIAN MAPLE, Physics Department, UC San Diego — The compound PrPt$_4$Ge$_{12}$ has attracted significant attention following observations of signatures of unconventional superconductivity such as time reversal symmetry breaking from μSR measurements. In contrast, LaPt$_4$Ge$_{12}$ is a conventional BCS-type superconductor, interestingly, with the same superconducting transition temperature, $T_c$, as PrPt$_4$Ge$_{12}$ ($T_c = 8$ K). To elucidate the properties of superconductivity in PrPt$_4$Ge$_{12}$, the system La$_{1-x}$Ce$_x$Pt$_4$Ge$_{12}$ was investigated and the results are compared to our previous work on Pr$_{1-x}$Ce$_x$Pt$_4$Ge$_{12}$. Measurements of magnetic susceptibility, electrical resistivity, and specific heat were performed demonstrating that $T_c$ is suppressed more rapidly in La$_{1-x}$Ce$_x$Pt$_4$Ge$_{12}$ than in Pr$_{1-x}$Ce$_x$Pt$_4$Ge$_{12}$. Specific heat measurements reveal a crossover in the temperature dependence of the superconducting state of La$_{1-x}$Ce$_x$Pt$_4$Ge$_{12}$, changing from a power law for $x = 0$ to an exponential for the Ce-substituted samples, possible evidence of a transition from a multiband to a single-band superconducting energy gap. This substitution for La did not produce the crossover.

$^1$Research at UC San Diego was supported by the US National Science Foundation under Grant No. DMR 0802478 and the US Department of Energy under Grant No. DE-FG02-04ER46105.

1:03PM T11.00010 Superconductivity at 600 mK in a novel ternary platinum phosphide SrPt$_4$P$_4$ $^1$, BENMAWA JAWDAT, BING LV, ZHENG WU, MELISSA GOOCH, KUI ZHAO, LIANGZI DENG, YIYU XUE, BERND LORENZ, Texas Center for Superconductivity and Department of Physics, University of Houston, ARNOLD GULOY, Texas Center for Superconductivity and Department of Chemistry, University of Houston, CHING-WU CHU $^2$, Texas Center for Superconductivity and Department of Physics, University of Houston — In the course of our search for new superconducting materials, we have synthesized a novel, metal-rich ternary platinum phosphide superconductor with a unique structure type, and an expected transition temperature greater than 1 K. The crystal structure was determined by single crystal X-ray diffraction, and features a unique three-dimensional anionic network of vertex-shared Pt$_4$P$_4$ trigonal prisms. Furthermore, we have investigated the superconductivity in this material resistively, magnetically, and calorimetrically. The results of these studies will be presented and discussed.

$^1$Present location: Fudan University

1:15PM T11.00011 Penetration depth and point-contact spectroscopy studies of exotic superconductivity in noncentrosymmetric half-Heusler YPtBi

HYUNSOO KIM, STEVEN ZIEMAK, KEFENG WANG, YASUYUKI NAKAJIMA, JOHNPRIERRE PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park, MD, USA, MAKARIY TANATAR, RUSLAN PROZOROV, Ames Laboratory, Department of Physics and Astronomy, Iowa State University, Ames, IA, USA — Strong asymmetric spin-orbit coupling in a noncentrosymmetric superconductor allows mixing of even and odd parity of the pairing interactions. Such an exotic pairing interaction has been suggested in some Pt-based noncentrosymmetric superconductors such as CePt$_3$Si and Li$_2$Pt$_3$B. More recently, we reported superconductivity below 0.8 K in YPtBi, a half-Heusler compound that lacks inversion symmetry. Here we present our studies of the superconducting energy gap in YPtBi using soft point contact spectroscopy and superconducting penetration depth measurements via tunnel diode resonator technique as a function of temperature and applied magnetic field. We will compare the morphology of our dI/dV energy gap spectra to previous theoretical and experimental results for triplet $p$-wave materials, and review our analysis of normalized superfluid density and theoretical current density and compare to various possible superconducting energy gap symmetries.

1:27PM T11.00012 Origins of charge density wave in novel Pt-based superconductors: SrPt$_3$As$_2$ and LaPt$_3$Si$_2$

SOORAN KIM, KYOO KIM, B.I. MIN, POSTECH — The intriguing coexistence of the charge density wave (CDW) and superconductivity in SrPt$_3$As$_2$ and LaPt$_3$Si$_2$ has been investigated by using the ab initio density functional theory band structure and phonon calculations. We have found that the local shift distortions in the [As-Pt-As] layers play an essential role in driving the five-fold supercell CDW instability as well as the phonon softening instability in SrPt$_3$As$_2$ than in LaPt$_3$Si$_2$. Specific heat measurements reveal a crossover in the temperature dependence of the superconductivity in SrPt$_3$As$_2$ and LaPt$_3$Si$_2$ different. The phonon calculations, however, suggest that the CDW and the superconductivity coexist in [X-Pt-X] layers (X = As or Si) in both cases.

1:39PM T11.00013 Superconductivity in AuBe $^1$

D.J. REBAR, J.F. DITUSA, P. ADAMS, D. BROWNE, I. VEKHTER, D. YOUNG, J. PRESTIGIACOMO, Louisiana State University — Metallic AuBe, which forms with the chiral B20 crystal structure, is a superconductor (SC) with a $T_c$ of approximately 3.2 K. Recent research on materials with this structure has revealed Skyrmion lattices, a topologically interesting magnetic state. We investigate the role the Dzyaloshinsky-Moriya interaction and spin-orbit coupling play in the superconductivity and normal state properties of this material. Samples were arc-melted in Ar atmosphere and characterized for structure and elemental composition. Magnetic susceptibility measurements revealed a full Meissner effect while the specific heat showed a sharp step at the transition temperature whose size is characteristic of a weakly-coupled SC. Measurements of the electrical resistivity at 1.8 K revealed a critical field that is five to six times that seen in the magnetization, far above the enhancement expected from a simple superconducting surface layer. In addition, we observed de Haas-van Alphen (dHvA) oscillations in these polycrystalline samples with two dominant frequencies indicating small spin-orbit split Fermi surfaces. We interpret the dHvA oscillations as emanating from a Dirac point approximately 0.4 eV below the Fermi level.

1:51PM T11.00014 Characterization of the Heavy Metal Pyrochlore Lattice Superconductor CaIr$_2$ $^1$

NEEL HALDOLAARACHCHIGE, QUINN GIBSON, LESLIE SCHOOPE, HUIXIA LUO, ROBERT CAVA, Princeton University — Compounds based on 5d transition metals are of recent interest because electron correlations and spin-orbit interactions play an important role in determining their electronic properties. Iridium oxides with the pyrochlore lattice, in particular, are predicted to host exotic electronic states, but these materials have not yet been shown to host superconductivity. A handful of Ir compounds are known to be superconducting, some more likely showing this property due to the presence of rare earths, but in other cases superconductivity is derived from Ir states at the Fermi Energy. Here we report the synthesis, experimental electronic characterization, and calculated electronic band structure of the cubic Laves phase superconductor CaIr$_2$. The inferred electron-phonon coupling constant show that CaIr$_2$ is a weakly coupled BCS-type superconductor. The electronic band structure calculations indicate that the Ir d states are dominant through the Fermi level. Given the profound effect of spin-orbit coupling on the electronic structure, it can be argued that the value of $T_c$ and possibly even the existence of superconductivity at all, is due to the heavy element character imparted to this material by the Ir pyrochlore lattice.

$^1$This work was supported by the Department of Energy, Division of Basic Energy Sciences, grant DE-FG02-98ER45706.
2:03PM T11.00015 The electron-phonon coupling and superconductivity for light-actinides on fcc structure: a first principles study\(^1\), OMAR DE LA PEÑA-SEAMAN, PAOLA GONZÁLEZ-CASTELAZO, Institute of Physics (IFUAP), Benemérita Universidad Autonoma de Puebla (BUAP), ROLF HEID, KLAUS-PETER BOHNMEN, Institute of Solid State Physics (IFP), Karlsruhe Institute of Technology (KIT) — We have studied the electronic structure, lattice dynamical properties, electron-phonon (\(\text{e-ph}\)) coupling and superconducting properties of the light-actinides (Ac, Th, Pa, U) on fcc structure. These systems have been studied within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method. The electronic density of states (DOS), full-phonon dispersion as well as the Eliashberg spectral function \((\alpha^2 F(\omega))\) and the electron-phonon coupling \((\lambda)\) parameter have been calculated with and without the inclusion of spin-orbit coupling (SOC). The observed effects of SOC on \(\alpha^2 F(\omega)\) for the light-actinides under study have its roots on the changes of two quantities: the full phonon dispersion and the \(\text{e-ph}\) coupling matrix elements. The observed influence of these two ingredients is different depending of the actinide, and it is analyzed together with the contribution of the different states on the DOS at the Fermi level. The superconducting critical temperature \((T_c)\) has been analyzed solving numerically the Eliashberg gap equations on the strong-coupling regime with the information provided from \(\alpha^2 F(\omega)\) for the entire series, analyzing the superconducting behavior of the light-actinides.

\(^1\)This research was supported by Conacyt-México under project No. 221807

Thursday, March 5, 2015 11:15AM - 2:15PM
Session T12 DMP: Focus Session: Non-Oxide Nanostructures and Artificially Structured Materials and Related Phenomena 007C - Pratibha Dev, Naval Research Laboratory

11:15AM T12.00001 ABSTRACT WITHDRAWN –

11:27AM T12.00002 Artificially-Engineered III-Nitride Digital Alloy for Solar Energy Harvesting\(^1\), WEI SUN, CHEE-KEONG TAN, NELSON TANSU, Center for Photonics and Nanoelectronics, Department of Electrical and Computer Engineering, Lehigh University — The pursuit of III-Nitride based solar cell has been primarily driven by the attribute of broad solar spectrum coverage through the use of InGaN material. However, the phase separation in high In-content InGaN alloy has been one of the largest barrier in the pursuit of nitride-based solar cells. Thus, a new approach in extending the bandgap coverage in nitride-based alloy needs to be pursued. In this work, we propose a novel artificially engineered III-Nitride based digital alloy structure to overcome the limitation presented by the epitaxy of phase-separated InGaN material with high In-content. The InGaN digital alloy structure is a short period superlattice that is formed by GaN and InN thin film layers alternately in which the thickness of each layer is represented by a number of monolayer (ML). By adjusting the thickness of GaN layer (\(n\) MLs) and InN layer (\(n\) MLs), the In-content and the band structure of InGaN digital alloy can be engineered correspondingly. The use of this digital alloys demonstrated suitability of this method in extending the bandgap coverage in nitride-based semiconductors.

11:39AM T12.00003 Simulation of Epitaxial Growth of DNA-nanoparticle Superlattices on Pre-patterned Substrates\(^1\), SAIJIE PAN, TING LI, MONICA OLVERA DE LA CRUZ, Northwestern Univ — DNA self-assembly is a well-developed approach towards the construction of a great variety of nanoarchitectures. E-beam lithography is widely used for high-resolution nanoscale patterning. Recently, a new technique combining the two methods was developed to epitaxially grow DNA-mediated nanoparticle superlattices on a pre-patterned surface\(^1\). Here we use multi-scale simulations to study and predict the formation and defects of the absorbed superlattice monolayer. We demonstrate that the epitaxial growth is enthalpy driven and show that the anisotropy of the DNA-mediated substrates leads to structure defects. We develop design rules to dramatically reduce defects of the attached layer. Ultimately, with the assist of our simulation, this technique will open the door for the construction of well-ordered, three-dimensional novel metamaterials. [1] H. Atwater, et al. Nano Lett. 2013, 13, 6084.

\(^1\)This work was supported by the the Air Force Office of Scientific Research (AFOSR) Multidisciplinary University Research Initiative (MURI) FA9550-11-1-0275.

11:51AM T12.00004 Theory of Energy Level Tuning in Quantum Dots by Surfactants, DANYLO ZHEREBETSKYY, LIN-WANG WANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, MATERIALS SCIENCES DIVISION, LAWRENCE BERKELEY NATIONAL LABORATORY TEAM — Besides quantum confinement that provides control of the quantum dot (QD) band gap, surface ligands allow control of the absolute energy levels. We theoretically investigate energy level tuning in PbS QD by surfactant exchange. We perform direct calculations of real-size QD with various surfactants within the frame of the density functional theory and explicitly analyze the influence of the surfactants on the electronic properties of the QD. This work provides a hint for predictable control of the absolute energy levels and their fine tuning within 3 eV range by modification of big and small surfactants that simultaneously passivate the QD surface.

12:03PM T12.00005 Crystalline \((\text{Al}_{1-x}\text{B}_x)\text{PSi}_3\) and \((\text{Al}_{1-x}\text{B}_x)\text{AsSi}_3\) tetrahedral phases via reaction of \(\text{Al(BH}_4)_3\) and \(\text{M(SiH}_3)_3\) \((\text{M}=\text{P, As})\)\(^1\), PATRICK SIMS, ANDREW WHITE, TOSHIHIRO AOKI, JOSE MENENDEZ, JOHN KOVETAKIS, Arizona State University — Crystalline \((\text{Al}_{1-x}\text{B}_x)\text{PSi}_3\) alloys \((x = 0.04-0.06)\) are grown lattice-matched on Si(100) by reactions of \(\text{P(SiH}_3)_3\) and \(\text{Al(BH}_4)_3\) using low-pressure CVD. The materials have been characterized by ellipsometry, XRD, XTEM, EELS and EDS, indicating the formation of single-phase monocrystalline layers with tetrahedral structures based on \(\text{AlPSi}_3\). The latter comprises interlinked \(\text{AlPSi}_3\) tetrahedra in which Al-P pairs are isolated within a Si matrix. Raman scattering of \(\text{Al}_{1-x}\text{B}_x\text{PSi}_3\) films support the presence of substitutional B in place of Al and provides evidence that B is bonded to P. The substitution of B atoms is desirable for promoting lattice matching, as required for Si-based solar cell designs. Analogous reactions of \(\text{As(SiH}_3)_3\) with \(\text{Al(BH}_4)_3\) produce \((\text{Al}_{1-x}\text{B}_x)\text{AsSi}_3\) in which the B incorporation is limited to doping concentrations at \(10^{20}\) cm\(^{-3}\). In both cases the \(\text{Al(BH}_4)_3\) efficiently delivers Al to create crystalline group IV-III-V materials comprising light, earth abundant elements with possible application in photovoltaics and light element refractory solids.

\(^1\)Supported by NSF-DMR 1309090
12:15PM T12.00006 Optical trends in InP polytypic superlattices¹, GUILHERME SIPAHI, TIAGO DE CAMPOS, PAULO EDUARDO DE FARIÁ JUNIOR, Universidade de São Paulo, State University of New York at Buffalo — Recent advances in growth techniques have allowed the fabrication of semiconductor nanostructures with mixed wurzite/zinc-blende crystal phases. Although the optical characterization of these polytypic structures is well reported in the literature, a deeper theoretical understanding of how crystal phase mixing and quantum confinement change the output linear light polarization is still needed. Here, we theoretically investigate the effects of these polytypic homojunctions on the interband absorption of an InP superlattice [1]. Using a single 8x8 k.p Hamiltonian that describes both crystal phases [1, 2] together with the effects of quantum and optical confinement we were able to explain the recent optical experimental results carried out on polytypic InP [3]. In summary, we have shown how the interplay of crystal phase mixing and quantum confinement can be used for light polarization engineering in polytypic homojunctions.


1FAPEP (No. 2011/19333-4, No. 2012/05618-0 and No. 2013/23993-8) and CNPq (No. 138457/2011-5, No. 245649/2012-2 and No. 149904/2013-4)

12:27PM T12.00007 Erbium doped Aluminum Nitride Nanoparticles for Nano-Thermometer Applications¹, SNEHA G. PANDYA, MARTIN E. KORDESCH, Department of Physics and Astronomy, Ohio University, Athens, OH-45701 — We have synthesized Nanoparticles (NPs) of Aluminum Nitride (AlN) doped in situ with Erbium (Er) using the inert gas condensation technique. These NPs have optical properties that make them good candidates for nanoscale temperature sensors. The Photoluminescence (PL) spectrum of Er³⁺ in these NPs shows two emission peaks in the green region at around 540 nm and 560 nm. The ratio of the intensities of these luminescence peaks is related to temperature. Using Boltzmann’s distribution, the temperature of the NP and its surrounding can be calculated. The NPs were directly deposited on (111) p-type Silicon wafers, TEM grids and glass cover slips. XRD and HRTEM study indicates that most of the NPs have crystalline hexagonal AlN structure. An enhancement of the luminescence from these NPs was observed after heating-in-air at 770 K for 3 hours. The sample was then heated in air using a scanning optical microscope laser. The corresponding change was in the range of 320-470 K. This temperature range is of interest for temperature sensors which are used for determining the potential at measure sidewall scattering. This is accomplished by acquiring spectra on a regularly spaced grid and then fitting the spectra to determine both the Schottky barrier height and the slope of the spectra. The position dependent maps of these two parameters are then related to the scattering at the interface due to the underlying pattern.

1The SNOM help provided by Prof. Hugh Richardson is gratefully acknowledged.

12:39PM T12.00008 Controlled formation of GeSi nanostructures on pillar-patterned Si substrate , TONG ZHOU, Fudan University, CENG ZENG, Huazhong University of Science and Technology, YONGLIANG FAN, ZUIMIN JIANG, Fudan University, JINSONG XIA, Huazhong University of Science and Technology, ZHENYANG ZHONG, Fudan University, FUDAN UNIVERSITY TEAM, HUAZHONG UNIVERSITY OF SCIENCE AND TECHNOLOGY COLLABORATION — GeSi quantum nanostructures (QNS) have potential applications in optoelectronic devices due to their unique properties and compatibility with the sophisticated Si technology. However, the disadvantages of poor quantum efficiency of the GeSi QNS on flat Si (001) substrates hinder their optoelectronic applications. Today, numerous growth strategies have been proposed to control the formation of GeSi QNS in hope of improving the optoelectronic performance. One of the ways is to fabricate GeSi QNS on patterned substrates, where the GeSi QNS can be greatly manipulated in aspects of size, shape, composition, orientation and arrangement. Here, self-assembled GeSi QNS on periodic Si (001) sub-micro pillars (SPMs) are systematically studied. By controlling the growth conditions and the diameters of the SPMs, different GeSi QNS, including circularly arranged quantum dots (QDs), quantum rings (QRs), and quantum dot molecules (QDMs), are realized at the top edge of SPMs. Meanwhile, fourfold symmetric GeSi QDMs can be also observed at the base edges of the SPMs. The promising features of self-assembled GeSi QNS are explained in terms of the surface chemical potential, which disclose the critical effect of surface morphology on the diffusion and the aggregation of Ge adatoms.

12:51PM T12.00009 ABSTRACT WITHDRAWN

1:03PM T12.00010 Utilizing Ballistic Electron Emission Microscopy to Study Sidewall Scattering of Electrons, WESTLY NOLTING, CHRIS DURCAN, ROBERT BALSANO, College of Nanoscale Science and Engineering, University at Albany, VINCENT LABELLA, Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute — Sidewall scattering of electrons in aggressively scaled integrated devices dramatically increases the resistance since the dimensions are approaching the mean free path of electrons in a metal ~ 40 nm. Ballistic Electron Emission Microscopy (BEEM) can be utilized to study hot electron scattering in metal films. In this presentation BEEM is performed on a lithographically patterned interface between a metal and a semiconductor to determine its potential at measure sidewall scattering. This is accomplished by acquiring spectra on a regularly spaced grid and then fitting the spectra to determine both the Schottky barrier height and the slope of the spectra. The position dependent maps of these two parameters are then related to the scattering at the interface due to the underlying pattern.

1:15PM T12.00011 Novel size effects on magneto-optics in the spherical quantum dots, M. KUSHWAHA, Rice University — We embark on investigating the magneto-optical absorption in spherical quantum dots completely confined by a harmonic potential and exposed to an applied magnetic field in the symmetric gauge. This is done within the framework of Bohm-Pines’ RPA that enables us to derive the Dyson equation that takes proper account of the Coulomb interactions. Intensifying the confinement or magnetic field and reducing the dot-size yields a blue-shift in the absorption peaks. However, the size effects are seen to be predominant in this role. The magnetic field tends to maximize the localization of the particle, but leaves the peak position of the radial distribution intact. The intra-Landau level transitions are forbidden.

1:27PM T12.00012 Silicene, germanene and tinene: Modeling of IR absorbance and topological states, FRIEDHELM BECHSTEDT, LARS MATTHES, Friedrich-Schiller-Universitaet Jena, OLIVIA PULCI, University Rome II Italy, PAOLA GORI, University Rome III Italy, BECHSTEDT/MATTHES TEAM, PULCI/GORI TEAM — The graphene-like but Si-, Ge- or Sn-derived group-IV honeycomb crystals [1] have attracted much attention due to their unique properties and their recent realization in experiments [2]. We study their electronic and optical properties by means of ab initio electronic-structure calculations. Conical valence and conduction bands and a vanishing electronic band gap have enormous consequences.

3. F. Bechstedt et al., APL 100, 261906 (2012)
5. L. Matthes, F. Bechstedt, PRB 90, 165431 (2014)
1:39PM T12.00013 Internal Strain in Nano-Diamond and Boron Nitride, WILLIAM MATTSON, DONALD JOHNSON, US Army Research Laboratory — Nanodiamond surfaces undergo reconstruction imposing stress on nanoparticle (NP) core and possibly storing strain energy. The unique way in which these NPs store energy may lead to useful applications, but a greater understanding of strain energy storage/release is needed. In the current work, density functional theory methods are employed to predict structural properties and energetics of C (diamond) and cubic-BN NPs. The goal is to quantify NP core stress and its relationship to surface rearrangement, particle size, and material composition. Initial results suggest different chemical factors drive surface rearrangement, leading to compressive stress in C and tensile stress in BN.

1:51PM T12.00014 Plasmon Enhanced Raman Scattering in Ag-CdTe Core-Shell Nanostructures1, SHENG WANG, DEXIONG LIU, JIANG ZENG, HUA ZHANG, DELIANG WANG, ZHENYU ZHANG, University of Science and Technology of China — Surface-enhanced Raman scattering (SERS) has been a powerful technique in investigating the properties of semiconductors. For semiconductor thin films, plasmon resonance and photoluminescence (PL) are two important factors in determining the signal of SERS. Here we carry out a combined experimental and theoretical study of the optical properties of metal-semiconductor hybrid nanosystems using SERS. First, we fabricate Ag-CdTe core-shell nanostructures by depositing CdTe on Ag nanoparticle arrays. By varying the thickness of the CdTe shell, one peak of plasmon is tuned to the wavelength of the incident light for resonant absorption, which is further verified by our finite-difference time-domain simulations. The coupling between the plasmons and excitons at the interface quenches the radiative PL process, while the non-radiative Raman scattering process is unaffected. Furthermore, the importance of multi-phonon resonance Raman scattering in these systems is investigated.

1 Chinese National Science Foundation

2:03PM T12.00015 Band Gaps in InN/GaN Superlattices: Polar and Nonpolar Growth Directions, NIELS CHRISTENSEN, Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, IZABELA GORCZYCA, KAMILA SKROBAS, TADEUSZ SUSKI, Institute of High Pressure Physics, UNIPRESS 01-142 Warsaw, Poland, AXEL SVANE, Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C — The electronic structures of short-period superlattices (SLs) consisting of \(m\)InN/\(n\)GaN unit cells with composition \((m,n)\) have been calculated within the density-functional theory including corrections for the “LDA gap error”. The variation of the gaps with SL composition and the dependence on the growth direction, the polar \((c)\) and nonpolar \((a,m)\) directions in the wurtzite structure, are compared. The band gaps calculated for the polar SLs are much smaller than those found for non-polar SLs due to the electric polarization fields in the \((c)\) SLs. For the \((1,m)\) class of polar samples photoluminescence measurements yield energy-gap values, which are much larger than the calculated values. The reason for this is that the structure of the samples differs from the assumed ideal composition. Transmission electron microscopy studies of the assumed polar \(In_{x}Ga_{1-x}N/GaN\) SLs show that the real structure is \(In_{1-x}Ga_{x}N/GaN\) with In-content \(x<0.33\). New calculations for such SLs in perfect agreement with photoluminescence experiments.


11:15AM T13.00001 Geometry and heterointerface engineered phases of nickelates1, JAK CHAKHALIAN, University of Arkansas — Deterministic control over the spatial arrangement atoms in a crystal is the backbone of its properties that, along with the interactions, defines its ground state. Following this notion, several theoretical proposals exist to utilize a few unit cells of a correlated oxide heterostructured along the pseudo-cubic \((111)\) direction. This geometrically engineered motif relies on the presence of correlated carriers placed on a buckled honeycomb \((i.e.,\) graphene-like) lattice, or dice lattices for bilayers and trilayers of ABO\(_3\) perovskites. The guiding principle is to use strong electronic correlations combined with quantum confinement and symmetry-breaking interfaces to enable access to new electronic band structures that may activate novel or latent quantum phases. In this talk, the current status of research in this field will be reviewed. The experimental challenges in realization and characterization of such heterostructures will be exemplified by rare earth nickelates heterostructures. Several promising examples of such geometrically engineered artificial Mott materials will be discussed.

1 Work supported by DOD-ARO under the Grant number 0402-17291 and funded in part by the Gordon and Betty Moore Foundation’s EPIQS Initiative through Grant GBMF4534.

11:51AM T13.00002 Tunable Charge and Spin Order in PrNiO\(_3\) Thin Films and Superlattices, MATTHIAS HEPTING, MATTEO MINOLA, ALEX FRANO, GEORG CRISTIANI, MENG WU, MARTIN BLUSCHKE, YI LU, HANS-ULRICH HABERMEIER, GENNADY LOGVENOV, EVA BENCKISER, MATHIEU LE TACON, BERNHARD KEIMER, MPI FKF Stuttgart — The rich phase diagram of transition metal oxides such as rare-earth nickelates heterostructures. Several promising examples of such geometrically engineered artificial Mott materials will be discussed.

12:03PM T13.00003 The effect of the interface termination on the atomic and electronic structure of LaNiO\(_3\)/PbZr\(_{0.2}\)Ti\(_{0.8}\)O\(_3\)1, ANDREI MALASHCHEVICH, MATTHEW S. J. MARSHALL, ANKIT S. DISA, FREDERICK J. WALKER, CHARLES H. AHN, SOHRAB ISMAIL-BEIGI, Center for Research on Interface Structures and Phenomena and Department of Applied Physics, Yale University — Thin film metal oxide/ferroelectric interfaces can exhibit dependence of conductivity on the polar state of the ferroelectric layer. This property has potential for technological applications in non-volatile field-effect devices. Recently, we demonstrated that ferroelectric PbZr\(_{0.2}\)Ti\(_{0.8}\)O\(_3\) (PZT) can be used to modulate conductivity of the \((001)\)-oriented LaNiO\(_3\)/PZT interface. We found that changes in conductivity result primarily from large mobility changes in the interfacial channel region. In this study, we investigate the effect of the LaNiO\(_3\) film termination \((LaO vs NiO\(_2\)) on the atomic structure and electronic properties of LaNiO\(_3\)/PZT. We present the results of the first-principles calculations of the atomic structure of the related LaNiO\(_3\)/PbTiO\(_3\) interface for both LaNiO\(_3\) terminations. For the analysis of the atomic structure and electronic properties of the ferroelectric PbTiO\(_3\) polar state and compare the results to the available experimental observations.

1This work is supported by the National Science Foundation through grant MRSEC NSF DMR-1119826
12:15PM T13.00004 Strain Control of Electronic Phase in Rare Earth Nickelates\textsuperscript{1}, ZHUORAN HE, ANDREW MILLIS, Dept. of Physics, Columbia Univ. — In this work, we use DFT+U methods to study the effects of strain on the electronic states and lattice structure of thin films of LuNiO$_3$. We model the effects of a substrate-induced strain by fixing the in-plane lattice parameter and relax both the c-axis lattice parameter and all internal coordinates. Both compressive and tensile strain destroy the charge order and create a metallic state. Tensile strain induces a staggered Jahn-Teller order. The staggered Jahn-Teller state is shown to compete with the charge-ordered state. The transitions are found to be first order, but the insulating gap in the charge-ordered phase varies substantially with applied strain. Implications for experiments are discussed.

\textsuperscript{1}Support: DOE ER-046169

12:27PM T13.00005 Comparative study of LaNiO$_3$/LaAlO$_3$ heterostructures grown by oxide MBE and PLD techniques\textsuperscript{1}, FRIEDERIKE WROBEL, GENNADY LOGVENOV, GEORG CHRISTIANI, EVA BENCHEKIER, Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany, ALISON F. MARK, WILFRIED SIGLE, PETER A. VAN AKEN, Max Planck Institute for Intelligent Systems, Heisenbergstr. 3, 70569 Stuttgart, Germany, BERNHARD KEIMER, Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — The physical properties of functional oxides can be altered by, e.g., dimensionality, strain, interfacial interaction and doping. Ozone assisted molecular beam epitaxy (oxide MBE) is a technique that gives wide access to all tuning parameters while having a low deposition energy. We succeeded in growing high-quality heterostructures based on LaNiO$_3$ with oxide MBE and pulsed laser deposition (PLD) and compared crystallinity, resistivity, x-ray absorption (XAS), orbital polarization and high-resolution transmission electron microscopy (HRTEM) images. Despite the difference in growth conditions, the samples show essentially the same physical properties: By reducing the layer thickness, LaNiO$_3$ turns from a paramagnetic metal into an antiferromagnetic insulator. XAS confirms the nickel +III oxidation state and that the orbital polarization is mainly controlled through substrate strain.

\textsuperscript{1}European Union Seventh Framework Program [FP/2007-2013] under grant agreement no 312483 (ESTEEM2)

12:39PM T13.00006 ABSTRACT WITHDRAWN —

12:51PM T13.00007 Orbital engineering of nickelates in three-component heterostructures, ANKIT DISA, DIVINE KUMAH, ANDREI MALASHEVICH, HANGHUI CHEN, SOHRAB ISMAIL-BEI GI, FRED WALKER, CHARLES AHN, Center for Research on Interface Structures and Phenomena and Department of Applied Physics, Yale University, ELIOT SPECHT, Materials Science and Technology Division, Oak Ridge National Laboratory, DARIO ARENA, National Synchrotron Light Source, Brookhaven National Laboratory — The orbital configuration of complex oxides dictates the emergence of a wide range of properties, including metal-insulator transitions, interfacial magnetism, and high-temperature superconductivity. In this work, we experimentally demonstrate a novel method for achieving large and tunable orbital polarizations in nickelates. The technique is based on leveraging three-component, atomically layered superlattices to yield a combination of inversion symmetry breaking, charge transfer, and polar distortions. In the system we studied, composed of LaTiO$_3$/LaNiO$_3$/LaAlO$_3$, we use synchrotron x-ray diffraction and spectroscopy to characterize these properties and show that they lead to fully broken orbital degeneracy in the nickelate layer consistent with a single-band Fermi surface. Furthermore, we show that this system is widely tunable and enables quasi-continuous orbital control unachievable by conventional strain and confinement-based approaches. This technique provides an experimentally realizable route for accessing and studying novel orbitally dependent quantum phenomena.

1:03PM T13.00008 Soft X-ray ARPES investigation of the nickelate Fermi surface in exchange biased LaNiO$_3$-LaMnO$_3$ superlattices, FLAVIO BRUNO, S. MCKEOWN WALKER, A. DE LA TORRE, A. TAMAI, M. GIBERT, S. CATALANO, J.-M. TRISCONE, University of Geneva, Switzerland, Z. WANG, F. BISTI, V. STROCOV, Swiss Light Source, PSI, Switzerland, F. BAUMBERGER, University of Geneva, Swiss Light Source PSI Switzerland and University of St Andrews UK — We investigate (111)-oriented superlattices consisting of paramagnetic LaNiO$_3$ (LNO) and ferromagnetic LaMnO$_3$ (LMO). The field dependence of the magnetization in these heterostructures was measured at 5 K after cooling the sample in the presence of a 0.4 T field. Surprisingly, a shift of 15 mT in the magnetization loop towards negative fields along the magnetic field axis was observed [1]. If the same measurement is repeated in a (111) LMO thin film, no exchange bias is observed which implies that LNO is the driving force for the biasing effect exhibited by the heterostructures. Since LNO is a well-known paramagnetic material, the existence of exchange bias in the superlattices implies the existence of an interface-induced magnetic order. Here we use soft x-ray angle resolved photoemission spectroscopy –SX ARPES- to study the electronic band structure of LNO layers in these heterostructures. Due to the increase in photoelectron escape depth in the 500 – 1000 eV energy range, we are able to map the LNO Fermi surface below 7 u.c. of LMO. In this talk we will discuss the similarities and differences in the electronic structure between thin films of (111)-LNO and buried LNO-LMO interfaces.


1:15PM T13.00009 Advanced electron microscopy characterization of tri-layer rare-earth oxide superlattices, PATRICK PHILLIPS, University of Illinois - Chicago, ANKIT DISA, SOHRAB ISMAIL-BEI GI, Yale University, ROBERT KLEIE, University of Illinois - Chicago, UNIVERSITY OF ILLINOIS - CHICAGO TEAM, YALE UNIVERSITY TEAM — Rare-earth nickelates are known to display complex electronic band structures and will be discussed at length. By combining both energy dispersive X-ray (EDX) and electronic energy loss (EEL) spectroscopies in an aberration-corrected (STEM)-based methods, properties such as interfacial sharpness, electron transfer, O presence, and local electronic structure can be probed at the atomic scale, and the energetic ordering of Ni d orbitals and 2D conduction, the present work focuses on the experimental characterization of thin film superlattice structures consisting of alternating layers of LaNiO$_3$ and LaAlO$_3$. Sandwiched between a dull insulator, LaAlO$_3$, the superlattice film is a single-layer superlattice, LaNiO$_3$-LaMnO$_3$. Using advanced scanning transmission electron microscopy (STEM)-based methods, properties such as interfacial sharpness, electron transfer, O presence, and local electronic structure can be probed at the atomic scale, and will be discussed at length. By combining both energy dispersive X-ray (EDX) and electronic energy loss (EEL) spectroscopies in an aberration-corrected STEM, it is possible to attain energy and spatial resolutions of 0.35 eV and 100 pm, respectively. Focus of the talk will remain not only on the aforementioned properties, but will also include details and parameters of the acquisitions to facilitate future characterization at this level.

1:27PM T13.00010 Measurement of the quantum capacitance of two-dimensional vanadium dioxide films, ZHE WU, TALBOT KNIGHTON, VINICIO TARQUINI, JIAN HUANG, Department of Physics and Astronomy, Wayne State University, NELSON SEPULVEDA, Department of Electrical and Computer Engineering, Michigan State University, DEPARTMENT OF PHYSICS AND ASTRONOMY, WAYNE STATE UNIVERSITY COLLABORATION, DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING, MICHIGAN STATE UNIVERSITY COLLABORATION — With a homebuilt ac bridge, we have performed capacitance measurement of quasi two-dimensional vanadium dioxide films grown on silicon-dioxide/p-doped silicon substrate. The out-phase-signal, which corresponds to the resistivity variation, is superior to the four-terminal measurement result below the critical temperature by four orders of magnitude, consistent with a Mott transition influenced by Peierls transition.
1:39PM T13.00011 Carrier Localization in Confined Vanadate Superlattices, CRAIG EATON, LEI ZHANG, ROMAN ENGEL-HERBERT, Penn State University — Perovskite oxide heterostructures have attracted attention due to the wealth of phenomena emerging at the interface, as well as the presence of strong electron correlations with potential applications as active electronic material for logic application utilizing the metal-to-insulator transition. Successful monolithic integration of perovskite oxides with Si makes them an ideal material choice. Here we present the growth of cubic SrTiO$_3$/SrVO$_3$/SrTiO$_3$ heterostructures on (La$_{0.3}$Sr$_{0.7}$)(Al$_{0.5}$Ta$_{0.5}$)O$_3$ substrates and orthorhombically distorted CaTiO$_3$/SrVO$_3$/CaTiO$_3$ heterostructures on (La$_{0.3}$Sr$_{0.7}$)O$_3$ substrates by hybrid molecular beam epitaxy, where alkaline earth metals were supplied using conventional effusion cells and the transition metals from the metal-organic precursor titanium-isopropoxide and vanadium tri-isopropoxide. Here, the interfaces are non-polar and carrier confinement in the correlated vanadate metals (d$^1$ configuration, 1 electron per unit cell) is achieved using insulating titanates as barrier material. Growth challenges associated with optimizing conditions for cation and oxygen stoichiometry are discussed. Confined structures down to 2 ML have been studied to demonstrate the potential for tuning incipient 2D Mott transition from 3D correlated metal. Room temperature hall measurements revealed carrier concentration in SrVO$_3$ films are $2 \times 10^{22}$ cm$^{-3}$ in thick films and decreases to $8 \times 10^{19}$ cm$^{-3}$ at 3 ML confinement, revealing the onset of strong carrier localization. Direct comparison between SrVO$_3$ and CaTiO$_3$ structures are presented to elucidate the role of dimensional confinement and structural distortion.

1:51PM T13.00012 Emergent conductance and magnetism at metal oxide interfaces via internal charge transfer$^1$, HANGHUI CHEN, ANDREW MILLIS, CHRIS MARIANETTI, Columbia Univ — Internal charge transfer across the interface of transition metal oxides is proven to be a powerful approach to induce new electronic structure in metamaterials (PRL 111, 116403 (2013); arXiv:1408.0217 (2014)). Here we use ab initio calculations to demonstrate that while SrVO$_3$ is a paramagnetic metal and SrMnO$_3$ is an antiferromagnetic insulator, charge transfer in a SrVO$_3$/SrMnO$_3$ superlattice leads to both electronic and magnetic reconstructions on the Mn sites: the Mn $e_g$ states are electron doped and the Mn $t_{2g}$ core spins are ferromagnetically aligned. As a result, net magnetic moments are expected to emerge in the superlattice. Our work shows that charge transfer is a robust route to the design of novel two dimensional half metallic ferromagnets.

$^1$This research was supported by National Science Foundation under Grant No. DMR-1120296.

2:03PM T13.00013 DFT+DMFT study of strain and interface effects in $d^1$ and $d^2$ $t_{2g}$-perovskites, GABRIELE SCLAUZER, KRZYSZTOF DYMKOWSKI, CLAUDE EDERER, ETH Zurich — Metal-insulator transitions in thin films of early-transition metal correlated oxides are linked to both epitaxial strain and electronic reconstruction at the film/substrate interface. We separately address these two key factors for LaTiO$_3$ and LaVO$_3$ through density functional theory plus dynamical mean-field theory (DFT+DMFT). We find that mere epitaxial strain suffices to induce an insulator-to-metal transition in LaTiO$_3$ [1], but not in LaVO$_3$, in agreement with recent experiments [2]. We show that this difference can be explained by the combined effect of strain-induced changes in the crystal field splitting of $t_{2g}$ orbitals and different orbital filling in these two materials. The role of the interface is investigated through DFT+DMFT simulations of LaVO$_3$/SrTiO$_3$ heterostructures with varying superlattice periodicities and substrate terminations. Our aim is to assess whether the metallicity observed at the LaVO$_3$/SrTiO$_3$ interface could be driven by pure electronic reconstruction effects, rather than structural or stoichiometric reasons (such as, e.g., O-related defects). [1] Dymkowski and Ederer, Phys. Rev. B 89, 161109 (2014). [2] He et al., Phys. Rev. B 86, 081401 (2012).

Thursday, March 5, 2015 11:15AM - 2:15PM — Session T14 DMP FIAP: Focus Session: Dopants and Defects in TiO2, SrTiO3, and Other Oxides 008A - Kookrin Char, Seoul National University

11:15AM T14.00001 Structural and electronic defects in SrTiO$_3$ and TiO$_2$$^1$, ANDERSON JANOTTI, Materials Department, University of California Santa Barbara, CA 93106-5050 — Control of defects and charge carriers is key to the development of metal oxide semiconductors as electronic materials. As in any semiconductor, one of the main challenges is to control the conductivity by doping as well as to reduce the concentration of native defects and unintentional impurities that act as compensation centers or sources of deep level luminescence, thus minimizing their deleterious effects. Experiments indicate that defects such as oxygen vacancies easily form and strongly affect the electronic properties of many oxide semiconductors. In SrTiO$_3$, it has been proposed that oxygen vacancies simultaneously act as a shallow donor that contribute to n-type conductivity, and as a deep center that causes luminescence well below the band-gap energy. This seemingly paradoxical behavior has remained unresolved. In rutile TiO$_2$, it has been proposed that excess electrons, either from oxygen vacancies or donor impurities, form small polarons. Although the formation of small polarons explains prominent features observed in the optical absorption spectra, charge localization seems incompatible with the high electron mobilities determined in Hall measurements of single crystals. In this talk we will discuss results of first-principles calculations for native point defects and impurities in SrTiO$_3$ and TiO$_2$, as they are prototypes of a large class of transition-metal oxide semiconductors. We will address the impact of defects and small-polaron formation on the electrical and optical properties in each material, providing a framework for interpreting similar phenomena in other complex oxides.

$^1$This work was performed in collaboration with J. B. Varley, M. Choi, N. Umezawa, P. Rinke, C. Franchini, G. Kresse, and C. G. Van de Walle. We acknowledge support from the Army Research Office under grant number W911NF-11-1-0232.

11:51AM T14.00002 Oxygen vacancy and hole conduction in “leaky” amorphous TiO2 from first-principles calculations, HIEU PHAM, LIN-WANG WANG, Lawrence Berkeley National Laboratory — In the last decade, titanium dioxide (TiO$_2$) has been one of the most studied materials due to its low cost, lightweight, eco-friendliness and long-term stability to be used in energy applications. Specifically, it was found recently that amorphous TiO$_2$ could be used as a protection layer for photo-induced water splitting. While protecting the light-absorbing photoanodes from corrosion, it can conduct hole carriers, perhaps through some defect levels. Nevertheless, the exact mechanism for such hole conductivity is not clearly understood. In this work, an amorphous TiO$_2$ model is obtained from molecular dynamics employing the melt-and-quench technique. The electronic properties, polaronic states and hole conduction mechanism in amorphous structure were investigated by means of density functional theory. The formation of oxygen vacancy was found to reduce significantly (by a few eV) upon the amorphization. Our theoretical study suggested that the oxygen vacancies and their defect states provide hopping channels which are comparable with experimental observations and could be responsible for the hole conduction in the “leaky” TiO$_2$ recently discovered for the photochemical water-splitting applications.
12:03PM T14.00003 Negative $U$ behavior of TiO$_2$- Magnéli and Corundum phases

ANTONIO CLAUDIO PADILHA, Universidade Federal do ABC, Santo André, Brazil, ALEXANDRE ROCHA, Universidade Estadual Paulista, São Paulo, Brazil, HANNES RAEBINGER, Yokohama National University, Yokohama, Japan, GUSTAVO DALPIAN, Universidade Federal do ABC, Santo André, Brazil — The isolated oxygen vacancy is known to be a negative $U$ defect in rutile TiO$_2$. This effect manifests itself by a double donor level close to the conduction band. As oxygen is further removed, TiO$_2$ no longer remains in the rutile structure and the Magnéli phases Ti$_n$O$_{2n-1}$ ($4 \leq n \leq 37$) are obtained. Those structures are characterized by ordered planes of oxygen vacancies (so-called shear planes) between rutile-like layers. Further removal of oxygen leads to the formation of Ti$_2$O$_3$ and the corundum phase Ti$_2$O$_3$. In this work, we calculated using DFT+$U$ the formation energy of several of these systems and show that these systems also have a double donor transition per oxygen vacancy. This means that these compounds as such also have negative $U$ behavior, even though the vacancies are not isolated and the donor level is a broad delocalized impurity band close to the bottom of the conduction band. The relaxation energy for the doubly ionized system is larger than that of the singly ionized one, rendering the latter unstable.

1This work was supported by FAPESP and CNPq

12:15PM T14.00004 Termination-specific study of oxygen vacancy transition levels on SrTiO$_3$(001) surfaces by scanning tunneling spectroscopy

WATTAYA SITAPUTRA, NIKHIKL SIVADAS, MAREK SKOWRONSKI, DI XIAO, RANDALL FEENSTRA, Carnegie Mellon University — We have studied the surface electronic structure of oxygen vacancies on SrTiO$_3$(001) surfaces using scanning tunneling spectroscopy and DFT calculations with local spin density approximation (LSDA+$U$). With high dynamic range measurements, a mid-gap level associated with the surface oxygen vacancies was observed for SrO-terminated surfaces. TiO$_2$-terminated surfaces, on the other hand, did not exhibit observable mid-gap states (this lack of signal is believed to be due to the nature of defect wavefunction involved, as well as possibly involving transport limitations in the STS measurements). Both vacuum-cleaved and MBE-grown surface have been studied. For the former, the Fermi level is pinned near mid-gap owing to disorder-induced surface states. The amount of surface disorder can be controlled in the case of epitaxially grown surfaces. Rougher MBE-grown surfaces tend to exhibit similar spectral characteristics to the cleaved surfaces, while a shift of the Fermi level toward the conduction band was observed for flattened grown surfaces. Notably, with a decreasing number of disorder-induced surface states, the Fermi level is found to be pinned within the observed band of oxygen vacancy levels.

1This research was supported by AFOSR Grant No. FA9550-12-1-0479, and it used resources of the National Energy Research Scientific Computing Center, supported by the Office of Science, US Department of Energy under Contract No. DEAC02-05CH11231.

12:27PM T14.00005 Magnetism and metal-insulator transition in oxygen deficient SrTiO$_3$

ALEJANDRO LOPEZ-BEZANILLA, Argonne Natl Lab, P. GANESH, Oak Ridge National Lab, PETER LITTLEWOOD, Argonne Natl Lab — We report new findings in the electronic structure and magnetism of oxygen vacancies in SrTiO$_3$. By means of first-principles calculations we show that the appearance of magnetism in oxygen-deficient SrTiO$_3$ is not determined solely by the presence of a single oxygen vacancy but by the density of free carriers and the relative proximity of the vacant sites. While an isolated vacancy behaves as a non-magnetic double donor, manipulation of the doping conditions allows the stability of a single donor state with emergent local moments. Strong local lattice distortions enhance the binding of this state. Consequently we find that the free-carrier density and strain are fundamental components to obtaining trapped spin-polarized electrons in oxygen-deficient SrTiO$_3$, which may have important implications in the design of switchable magneto-optic devices.

1AL-B and PBL were supported by DOE-BES under Contract No. DE-AC02-06CH11357. PG was sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT- Battelle, LLC, for the US Department of Energy.

12:39PM T14.00006 The effect of oxygen vacancies and strain on the optical energy gap of strained SrTiO$_{3−δ}$ thin films

NATHAN STEINLE, BARRY KOEHNE, Undergraduate Assistant, RYAN COTTIER, Post-Doctoral, DANIEL CURRIE, Post-Graduate, NIKOLETA THEODOROPOULOU, Advisor — SrTiO$_{3−δ}$ (STO) films were grown on single crystal SrTiO$_3$ and p-Si (001) substrates using molecular beam epitaxy (MBE). The single-phase STO/Si films were of high crystalline quality as verified by x-ray diffraction (XRD) and atomic force microscopy (AFM) with an rms roughness of less than 0.5 nm. Oxygen vacancies were introduced by controlling the oxygen pressure (P(O$_2$): 10$^{-8}$ to 10$^{-7}$ torr) during growth. The lattice mismatch of STO on Si causes a 1.7% bi-axial, compressive strain. The oxygen vacancies cause a tensile strain because of the different Ti$^{4+}$ and Ti$^{3+}$ ionic radii. This agrees with our XRD measurements that show a decrease of the out of plane lattice constant as either the thickness or P(O$_2$) during growth increase. We used a Variable Angle Spectroscopic Ellipsometer M-2000 by Woolam and the VASE software to measure and model the optical properties of the films and substrates using Tauc-Lorentz and Gaussian oscillators for the STO layer. Our results show that the direct energy bandgap of STO at around 3.8 eV increases as either the thickness or P(O$_2$) decrease, in agreement with theoretical calculations. Additionally, absorption is observed in the 1.5-2 eV region for the films with increased Oxygen vacancies.

1Fundied by NSF Career Award DMR-1255629.

12:51PM T14.00007 Niobium doped strontium titanate: Effect of oxygen ambient on the doping mechanism

CHUN-FU CHANG, National Sun Yat-Sen University, Taiwan, Q.Y. CHEN, National Sun Yat-Sen University, Taiwan; University of Houston, USA, P.V. WADEKAR, University of Liverpool, UK, O. LOZANO, University of Namur, Belgium, M.S. WONG, National Dong-Hwa University, Taiwan, W.C. HSIEH, Y.S. WANG, Y.T. LIN, H.H. LIU, C.W. CHANG, H.C. HUANG, National Sun Yat-Sen University, Taiwan, H.H. LIAO, Enli Technology, Taiwan, W.K. CHU, University of Houston, USA, H.W. SEO, University of Arkansas, USA — Double doping in oxides, a scenario where free electrons are created by ordered planes of oxygen vacancies (so-called shear planes) between rutile-like layers. Further removal of oxygen leads to the formation of Ti$_2$O$_3$ and the corundum phase Ti$_2$O$_3$. In this work, we calculated using DFT+$U$ the formation energy of several of these systems and show that these systems also have a double donor transition per oxygen vacancy. This means that these compounds as such also have negative $U$ behavior, even though the vacancies are not isolated and the donor level is a broad delocalized impurity band close to the bottom of the conduction band. The relaxation energy for the doubly ionized system is larger than that of the singly ionized one, rendering the latter unstable.

1This work was supported by FAPESP and CNPq
1:03PM T14.00008 Small Polaronic and Point Defects in Barium Cerate\textsuperscript{1}, MICHAEL SWIFT, ANDERSON JANOTTI, CHRIS G. VAN DE WALL, Univ of California - Santa Barbara — Barium cerate (BaCeO\textsubscript{3}) is a well-known proton-conducting material. In applications, it is frequently doped (for instance with yttrium) to increase stability and promote hydrogen uptake. However, the microscopic mechanisms of ionic conductivity and the effects of doping and native defects are still not fully understood. Many of the obstacles to the theoretical study of this material stem from the nature of the conduction band, which is made up of cerium 4f states. These states present a challenge to first-principles techniques based on density functional theory within the standard approximations for exchange and correlation. Using a hybrid functional, we investigate the effects of hydrogen impurities and native defects on the electrical and optical properties of BaCeO\textsubscript{3}. We discuss the tendency of excess electrons or holes to localize in the form of small polarons. We also explore the interactions of polarons with hydrogen impurities and oxygen vacancies, and their impact on luminescence properties.

\textsuperscript{1}This work was supported by the DOE and ARO.

1:15PM T14.00009 Use of nonpolar BaHfO\textsubscript{3} gate oxide for field effect on the high mobility BaSnO\textsubscript{3}. CHULKWON PARK, USEONG KIM, YOUNG MO KIM, CHANGJONG JU, KOOKRIN CHAR, Department of Physics & Astronomy, Seoul National University — Recently, BaSnO\textsubscript{3} (BSO) has attracted attentions as a transparent conducting oxide and/or a transparent oxide semiconductor due to its novel properties: the excellent oxygen stability even at high temperature and the high electrical mobility at room temperature. We fabricated field effect transistors using La-doped BSO as the semiconducting channel on undoped BSO buffer layers on SrTiO\textsubscript{3} substrates. A non-polar perovskite BaHfO\textsubscript{3} was used as the gate insulator, and 4% La-doped BSO as the source, the drain, and the gate electrodes grown by pulsed laser deposition. We have measured the optical and the dielectric properties of the epitaxial BaHfO\textsubscript{3} gate oxide layer, namely the optical band gap, the dielectric constant, and the breakdown field. Using such BaHfO\textsubscript{3} gate oxide, we observed carrier modulation in the active layer by field effect. In this presentation, we will report on the performance of such field effect transistors: the output and the transfer characteristics, the field effect mobility, the ratios, and the subthreshold swing.

1:27PM T14.00010 Field effect transistors based on BaSnO\textsubscript{3} with AlO\textsubscript{x} and HfO\textsubscript{3} gate oxides. YOUNG MO KIM, CHULKWON PARK, USEONG KIM, KOOKRIN CHAR, Department of Physics and Astronomy, Seoul National University — La-doped BaSnO\textsubscript{3} (BSO) is a transparent perovskite oxide semiconductor with high electron mobility and excellent oxygen stability. We fabricated n-type field effect transistors (FETs) on undoped BaSnO\textsubscript{3} (BSO) buffer layers on SrTiO\textsubscript{3} (STO) substrates using BLSO as the semiconducting channels and amorphous AlO\textsubscript{x} and HfO\textsubscript{3} as the gate insulators. BSO buffer layers and BLSO channels were grown by pulsed laser deposition, while the AlO\textsubscript{x} and HfO\textsubscript{3} gate insulators were grown by atomic layer deposition (ALD). Sn\textsubscript{2}O\textsubscript{3} (ITO) was used as the source, the drain, and the gate electrodes. At room temperature, we achieved the field effect mobility value of 17.8 cm\textsuperscript{2}/Vs for the AlO\textsubscript{x} FET and 19.2 cm\textsuperscript{2}/Vs for the HfO\textsubscript{3} FET. The subthreshold swing was measured to be 3.2 V/dec for the AlO\textsubscript{x} FET and 1.2 V/dec for the HfO\textsubscript{3} FET.

1:39PM T14.00011 P-type Semiconducting Behavior of BaSn\textsubscript{1−x}Ru\textsubscript{x}O\textsubscript{3} system, HYUKWOO Kwon, JUYEON SHIN, KOOKRIN CHAR, Seoul National University — BaSnO\textsubscript{3} is a promising transparent perovskite oxide semiconductor due to its high mobility and chemical stability. Exploiting such properties, we have applied BaSnO\textsubscript{3} to the field effect, the 2-dimensional electron gas, and the pn-junction devices. In spite of the success of the K-doped BaSnO\textsubscript{3} as a p-type doped, its carrier density at room temperature is rather small due to its high activation energy of about 0.5 eV. In continuation of our previous study on SrSn\textsubscript{1−x}Ru\textsubscript{x}O\textsubscript{3} system, we studied the p-type semiconducting behavior of BaSn\textsubscript{1−x}Ru\textsubscript{x}O\textsubscript{3} system. We have epitaxially grown the BaSn\textsubscript{1−x}Ru\textsubscript{x}O\textsubscript{3} (0<\textless\textless0.12) thin films by pulsed laser deposition. X-ray diffraction measurements show that the films maintain a single phase over the entire doping range and the lattice constants of the system decrease monotonously as the Ru doping increases. Transport measurements show that the films are semiconducting and their resistivities dramatically decrease as the Ru doping increases. Hall measurement data show that the charge carriers are p-type and its corresponding mobility values vary from 0.3 ~ 0.04 cm\textsuperscript{2}/Vs, depending on the doping rate. The hole carrier densities, measured to be 10\textsuperscript{17} ~ 10\textsuperscript{19} /cm\textsuperscript{3}, are larger than those of K-doped BaSnO\textsubscript{3}. Using BaSn\textsubscript{1−x}Ru\textsubscript{x}O\textsubscript{3} and Ba\textsubscript{1−y}La\textsubscript{y}SnO\textsubscript{3} as p-type and n-type semiconductors, we will fabricate np-junctions and report its performance.

1:51PM T14.00012 Effect of a Ru doped SnO\textsubscript{2−x} buffer layer on thin-film transistors based on SnO\textsubscript{2−x} channel layer, HYOSIK MUN, HYEONSEOK YANG, KOOKRIN CHAR, Seoul National University — We report on studies of transparent thin-film transistor (TFT) devices based on SnO\textsubscript{2−x} thin film. SnO\textsubscript{2−x} thin films were prepared by pulsed laser deposition with and without Ru-doped SnO\textsubscript{2−x} buffer layer on r-plane sapphire substrates to investigate the effect of a Ru-doped SnO\textsubscript{2−x} buffer layer on the electrical properties of SnO\textsubscript{2−x} channel layer. The Ru-doped SnO\textsubscript{2−x} buffer layer was found to be very crystalline and insulating at the same time. Using such Ru-doped SnO\textsubscript{2−x} buffer layer made it possible for the SnO\textsubscript{2−x} channel layer to have both low carrier density and high mobility, probably due to reduction of the threading dislocation density. AlO\textsubscript{x} gate insulator layer was deposited by atomic layer deposition and ITO was used as the source, the drain, and the gate electrodes. We will compare the TFT performances with or without the Ru-doped SnO\textsubscript{2−x} buffer layer and discuss how such buffer layer enables the necessary device parameters for TFT.

2:03PM T14.00013 Aliovalently-Doped Garnets for Li Battery Solid State Electrolytes, DEREK K. SCHWANZ, ERNESTO E. MARINERO, Purdue University — We report on a new family of fast ionic conductivity electrolytes based on the garnet LiLaZ\textsubscript{2}O. Partial substitution of Zr by aliovalent atomic species through solid state solution synthesis results in ionic conductivities 2 orders of magnitude larger than the tetragonal phase of LiLaZ\textsubscript{2}O and comparable to that of its cubic phase. The synthesis temperature is 400°C, lower than that required for the cubic stabilization of LiLaZ\textsubscript{2}O. Ongoing improvements on microstructure and film density as well as optimization of the garnet stoichiometry are expected to yield ionic conductivities surpassing the highest values reported to-date on cubic doped LiLaZ\textsubscript{2}RO (Ta, Al, W, Nb).

Thursday, March 5, 2015 11:15AM - 2:03PM
Session T15 FlAP: Nanotechnology 008B - Samir Iqbal, University of Texas at Arlington

11:15AM T15.00001 Structural aspects of TiO\textsubscript{2} nanopowders, SERGEY MAMEDOV, Horiba Scientific — TiO\textsubscript{2} nanopowders obtained using different methods with the mean size of 5, 15, 30 and 40 nm have been investigated by Raman spectroscopy in wide spectral range. Nano-size of TiO\textsubscript{2} crystals lead to a shift and broadening of the first-order Raman lines through a relaxation of the q = 0 selection rule and effects on the position, width and asymmetry of a Raman bands. The details of the evolution of the 144 cm\textsuperscript{-1} Raman line shape on the size and distributions of the nanopowders are presented and discussed in frame of confined phonons model. Analysis of Raman spectra shows that structural characteristics of nanopowders may be different even size of the nanopowders is the same. Structural features of the material depend on preparation methods/conditions and can be extracted from Raman spectra of the material.
11:27AM T15.00002 Growth and Characterization of Coherently Strained Si-Si\(_{1-x}\)Ge\(_x\) Core-Shell Nanowire Heterostructures , DAVID DILLEN, KYOUNGHWAN KIM, EMANUEL TUTUC, Univ of Texas, Austin — The large valence band offset in Ge-Si-Si\(_{1-x}\)core-shell nanowires has provided an interesting platform for the study of quasi one-dimensional hole-confined systems, and has led to the demonstration of high-performance electronic devices. Progress in the development of electron-confined systems using Group-IV core-shell structures has, however, been much slower. Coherently strained Si-Si\(_{1-x}\)Ge\(_x\)core-shell nanowires represent one possible radial heterostructure where a positive shell-to-core conduction band offset, beneficial for quantum confinement of electrons in the Si core, may be realized. We discuss the growth of strained Si-Si\(_{1-x}\)Ge\(_x\)core-shell nanowires with tunable shell composition using vapor-liquid-solid growth for the Si nanowire core, followed in-situ by Si-Si\(_{1-x}\) Ge\(_x\)shell growth. Transmission electron microscopy reveals a single crystal nanowire structure, evincing an epitaxial shell growth. Raman spectroscopy reveals a red-shift of the core Si-Si Raman mode, which depends on the shell composition and nanowire thickness, indicating coherent tensile strain in the Si core.

11:39AM T15.00003 Gold Nanorod translocations and charge measurement through solid-state nano pores , REBECCA ENGLEKE, MEHDI ZANJANI, KIM VENTA, XINGCHEN YE, GOPINATH DANDA, CHRISTOPHER MURRAY, JENNIFER LUKES, MARJIA DRNDIC, Univ of Pennsylvania — We study translocations of gold nanorods through silicon nitride nanopores and present a method for determining the surface charge of nanorods from the magnitude of the ionic current change as nanorods pass through the pore. Positively-charged nanorods with average diameters 10 nm and average nanorod lengths between 44 and 65 nm were translocated through 40 nm thick nanorods with diameters between 19 and 27 nm in 1, 10, or 100 mM KCl solutions. The presented method based on comparing simulations with experiments predicts a surface charge of 26 mC/m\(^2\) for 44 nm long gold nanorods and 18 mC/m\(^2\) for 65 nm long gold nanorods.

11:51AM T15.00004 The Effects of Nanotexturing Microfluidic Platforms to Isolate Brain Tumor Cells\(^1\) , MUHYMIN ISLAM, ADEEL SAJID, YOUNG-TAE KIM, University of Texas at Arlington, SAMIR M. IQBAL, Nano-Bio Lab, Electrical Engineering, Bioengineering, University of Texas at Arlington — Detection of tumor cells in the early stages of disease requires sensitive and selective approaches. Nanotextured polydimethylsiloxane (PDMS) substrates were implemented to detect metastatic human glioblastoma (hGBM) cells. RNA aptamers that were specific to epidermal growth factor receptors (EGFR) were used to functionalize the substrates. EGFR is known to be overexpressed on many cancer cells including hGBM. Nanotextured PDMS was prepared by micro reactive ion etching. PDMS surfaces became hydrophilic uponnanotexturing. Nanotextured substrates were incubated in tumor cell solution and density of captured cells was determined. Nanotextured PDMS provided >300% cell capture compared to plain PDMS due to increased effective surface area of roughened substrates at nanoscale as well as more focal points for cell adhesion. Next, aptamer functionalized nanotextured PDMS was incorporated in microfluidic device to detect tumor cells at different flow velocities. The shear stress introduced by the flow pressure and heterogeneity of the EGFR overexpression on cell membranes of the tumor cells had significant impact on the cell capture efficiency of aptamer anchored nanotextured microfluidic devices. Eventually tumor cells were detected from the mixture of white blood cells at an efficiency of 73% using the microfluidic device. The interplay of binding energies and surface energies was major factor in this system.

\(^1\)Support Acknowledged from NSF through ECCS-1407990

12:03PM T15.00005 Nano-Storage Wires for the Controlled Release of Biochemical Materials , HANEUL YOO, DONGJUN LEE, EUNJI KIM, DAESAN KIM, JUHUN PARK, SEUNGHUN HONG, Seoul Natl Univ — We herein report "nano-storage wires" that can store chemical species and release them at a desired moment by electrical stimulations. Here, we utilized the electrodeposition process through an anodized aluminium oxide template to fabricate multi-segmented nanowires which consisted of a polypyrrole (PPy) segment containing adenosine triphosphate (ATP) molecules, a ferromagnetic nickel segment, and a conductive gold segment. We could drive and deposit the NSWs onto desired positions on electrode surfaces via external magnetic fields. When the external electric potential was applied from the electrodes, the NSWs released ATPs from the PPy segments, and the released ATPs could change the activities of motor proteins near the NSWs. Furthermore, through direct writing or magnetic manipulation strategies, we could print NSWs onto various substrates such as flexible or three-dimensional structured substrates to build versatile chemical storage devices. Since our strategy enables the controllable storage and release of chemicals, our development should open up various applications such as drug delivery systems, biosensors and biochips for the controlled release of chemicals to biosystems.

12:15PM T15.00006 Precise Fabrication of Nanowires with Diameters of Sub-1 nm to 3 nm Using Multilevel Pulse-voltage Injection , ITARU YANAGI, RENA AKAHORI, TAKAHIDE YOKOI, KEN-ICHI TAKEDA, Central Research Laboratory, Hitachi Ltd — To date, solid-state nanowires have been fabricated primarily through a focused-electronic beam via TEM. For mass production, however, a TEM beam is not suitable and an alternative fabrication method is required. Recently, a simple nanowire-fabrication method has been reported that is based on a dielectric breakdown phenomenon of a thin membrane. In this study, to stably fabricate nanowires with diameters of 1 to 2 nm (which is an essential size for distinguishing each nucleotide) via dielectric breakdown, a technique called multilevel pulse-voltage injection (MPVI) is proposed and demonstrated. MPVI uses pulse voltages for generating the nanowires, and the generation of the nanowires is verified by measuring the current through a membrane at low voltage. This method can generate nanowires with diameters of less than 1 nm in a 10-nm-thick Si\(_3\)N\(_2\) membrane with a probability of 90%. The diameter of the generated nanowires can be widened to the desired diameters (up to 3 nm) with sub-nanometre precision. The mean effective thickness of the fabricated nanowires was 3.7 nm. These findings are derived from TEM images of the fabricated nanowires and analyses of ionic-current blockades during single-stranded DNA translocation.

12:27PM T15.00007 Electrospaying in a complex electrical field: jet formation and characteristics of final product , SHEILA KHODADADI, KIRSTEN ROVERS, GABRIEL MEESTERS, Delft University of Technology, TUDELFT-DELFT PROJECT MANAGMENT TEAM — The electrohydrodynamic atomization (EHDA) of liquid solutions is a technique developed to produce micro and nanometer size droplets. It consists of breaking a liquid jet by applying electrical forces. EHDA is one of the most suitable techniques for drug delivery and bio-nanotechnology, when precise (nm-µm) particle size and narrow size distribution is needed. However there are some challenges facing application of this technique such as limitation in flow rate, characteristics of liquids (surface tension, conductivity,…) and, the possible droplet size reduction due to evaporation of the liquid and Coulomb fission. To tackle these challenges in an EHDA-based inhalation device, we explored different possibilities to reach a stable mode in terms of jet formation, droplet-particle size and size distribution. In this contribution, we demonstrate how device configuration and operational conditions influence the electrospayed liquid and final product. We will also discuss how our approach can be used to tailor morphological properties of nanostructured materials with identical chemical compositions.
Effect of processing temperature on the properties of Fe-Hydroxyapatite: 1
VINODI KATHIRIARACHCHI, THEODORA LEVENTOURI, Department of Physics, Florida Atlantic University, ADAM RONDINONE, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, KOREY SORGE, Department of Physics, Florida Atlantic University — Multi-substituted Hydroxyapatite (HAp), Ca$_5$(PO$_4$)$_3$OH, is the main mineral phase in physiological apatite. Fe is a minor substitution element in bone and enamel substituting Ca in the HAp structure. Crystal structure, magnetic and microstructure properties of Ca$_5-x$Fe$_x$(PO$_4$)$_3$OH depend on processing parameters. We present results from our research on the Ca$_5-x$Fe$_x$(PO$_4$)$_3$OH system (x = 0.0, 0.05, 0.1, 0.2 and 0.3) prepared at 37$^\circ$C, and 80$^\circ$C. Hydroxyapatite single-phase was detected for x <0.1 in both sets of samples, while hematite and/or maghemite develops starting at x = 0.1. Rietveld refinements of XRD and NPD patterns show that the a and c lattice constants decrease with increasing Fe concentration for both sets of samples. Pure HAp is diamagnetic but as x increases, Fe-HAp transitions from paramagnetic to weak ferromagnetic behavior. TEM images show spherical particles in samples prepared at 37$^\circ$C, and elongated particles in samples prepared at 80$^\circ$C. XRF studies confirm the iron substitution and show that the Ca/P stoichiometric ratio of 1.67 decreases with increasing the Fe concentration. Further, the Fe/Ca+Fe atomic ratios of samples prepared at 37$^\circ$C are greater than those prepared at 80$^\circ$C.

1TEM and XRF data were collected at the Center for Nanophase Materials Sciences which is a DOE Office of Science User Facility. NPD data were collected at the SNS of the ORNL.

Application of near infrared sensitive multifunctional nanophosphors in optical and photoacoustic imaging . FRANCISCO PEDRAZA, AJITH KUMAR, LAWRENCE MIMUN, JING YONG YE, DHIRAJ SARDAR, Univ of Texas, San Antonio — Though there are several contrast agents available in the biomedical industry for non-invasive imaging, many of them are not capable of providing in-depth information with high signal to noise ratio. Because of the extremely high scattering processes in the biological medium, most of the optical imaging techniques fail to provide sufficient resolution in deep tissue. An alternate way to circumvent this difficulty is to integrate multiple imaging modalities such as optical, magnetic, and photoacoustic (PA) in a single contrast agent. Trivalent rare earth doped inorganic phosphors are found to be the most suitable candidates for this purpose due to their excellent NIR spectral properties. In addition, by controlling the non-radiative processes through various emission channels, it is possible to generate strong PA signals that would help us explore the wavelength dependent PA imaging features. Furthermore, magnetic imaging can be added by incorporating paramagnetic (Gd) or ferromagnetic (Fe) ions suitable lattice positions. In this work we explore the NIR sensitive optical and PA imaging features of rare-earth doped phosphors and compare their capabilities with other metallic nanoparticle-based PA imaging agents.

Fabricating quench condensed lead thin film circuits using MEMS Fab on a Chip technology . MATTHIAS IMBODEN, HAN HAN, Boston University, PABLO DEL CORRO, Instituto Balseiro, Centro Atomico Bariloche, FLAVIO PARDO, CRISTIAN BOLLE, Bell Labs, Alcatel-Lucent, DAVID BISHOP, Boston University — We have developed a MEMS Fab on a Chip consisting of micro-sources, mass sensors/heaters/thermometers, shutters and a dynamic stencil. The fab only occupies a volume of a few cubic millimeters and consumes milliwatts of power, and hence can be operated in a cryostat. Thin film patterns of arbitrary shapes using multiple materials can be manufactured, while strongly suppressing thermal annealing effects. We demonstrate deposition of quench condensed lead films with fractions of a monolayer thickness control. Furthermore, using low deposition rates it is estimated that the surface temperature of the target heats by only 1.7 K. We study the effects of growing quench condensed films with different evaporation rates to demonstrate thermal annealing effects which occur during deposition. We measure the minimum conduction thickness (insulator to metal transition) as well as the superconducting transition temperature as a function of film thickness in order to shed light on growth of amorphous films and the transition to nanocluster formations. The Fab on a Chip will allow us to build nanocircuits made of ultra-thin materials. Annealing and doping is controlled and measurements occur in situ, without exposing the fabricated circuits to thermal fluctuations or foreign contaminants. This enables new types of experiments based on quantum circuits which cannot be fabricated using standard lithography techniques.

High speed electrical measurement for roll-to-roll nanomanufacturing . NATHAN ORLOFF, CHRISTIAN LONG, JAN OBRZUT, National Institute of Standards and Technology, LAURENT MAILLAUD, National Institute of Standards and Technology — Roll-to-roll processing of nanomaterials can produce high-quality coatings and filamentous continuously, enabling materials applications for electronics, fabrics, and wires. These applications often require specific electrical properties that are correlated to the material’s nanostructure. While several high-throughput structural characterizations techniques exist, there are relatively few contactless options for quantifying the electrical properties of materials for nanomanufacturing. Here, we demonstrate a microwave method for measuring complex permittivity (or geometry for samples of known dielectric properties) in a millisecond. The demonstrated measurement times are suitable for current industrial needs, allowing real-time materials characterization and in-line control of processing variables without disrupting production.

Development Characteristics of PMMA in alternative alcohol:water mixtures . LEONIDAS E. OCOLA, Argonne National Laboratory — The most widely used resist in electron beam lithography is polymethylmethacrylate (PMMA). The standard developers used are solution mixtures of isopropanol (IPA) and methyl isobutyl ketone (MIBK) in a ratio of 3:1 and mixtures of IPA and water (H2O) in a ratio of 7:3. The Globally Harmonized System (GHS) classification entry for IPA includes: Specific target organ toxicity - single exposure (Category 3). MIBK is much more hazardous than IPA. The only GHS classification entry for Ethanol is: Flammable liquids (Category 2), i.e. more environmentally safe. Using Ethanol/H2O as a developer will therefore enable lower hazardous waste disposal costs to cleanrooms. We find Ethanol/H2O at 85% volume (2.1 molar) exhibits excellent lithography results as good as with IPA/H2O, and better contrast and sensitivity than IPA/H2O and MIBK/IPA developers. Lithographic data shows trends similar to published cosolvency data, but differ too much to be explained by it. In addition, unusual development at 50% volume concentrations for both IPA and Ethanol in H2O show dramatic pohotolite formation instead of uniform thickness loss found in standard contrast curve exposures. We believe local pockets of concentrated alcohol water molar mixtures are responsible for such behavior.

This work was supported by the Department of Energy under Contract No. DE-AC02-06CH11357. Use of the Center for Nanoscale Materials was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

ABSTRACT WITHDRAWN —
of strong electron interactions within the fractal Hofstadter spectrum. Exploiting nano-scale interfacial effects between graphene and hexagonal boron nitride substrates, together with application of extremely high magnetic fields.

The discovery of the quantum Hall effect gave birth to an expansive field of research into 2D electronic systems in the presence of a magnetic field, however, direct application of such techniques and a real-space Kubo-Greenwood approach [2]. Such a breaking of the sublattice symmetry leads to the appearance of a true band gap in graphene protected by boron nitride. The device is enabled by a top-gated, solid electrochemical cell designed with calcium fluoride (CaF$_2$), which facilitates the tuning of these films by choice of substrate or chemical functionalization. Such parameters are generally selected during fabrication, and therefore remain static during device operation. However, the possibility of dynamic chemistry in a tunable solid-state system will enable the development of new devices which fully leverage the rich chemistry of graphenic materials. Here, we fabricate a novel device for localized, dynamic doping and functionalization of graphene that is compatible with CMOS processing. The device is enabled by a top-gated, solid electrochemical cell designed with calcium fluoride (CaF$_2$) substituting the oxide of a traditional MOSFET. When the CaF$_2$ is gated, F flows from cathode to anode, segregating Ca and F. In this work, one electrode is graphene. When saturated with fluorine, graphene undergoes covalent modification, becoming a wide-bandgap semiconductor. In contrast, when functionalized with calcium or dilute fluorine, graphene is electron or hole doped, respectively. With transport, Raman, and XPS, we demonstrate this lithographically localized graphene sheets encapsulated by various thicknesses of boron nitride. We discuss the implications of our work for future electrolyte gating studies of materials protected by boron nitride.

We gratefully acknowledge support from the National Science Foundation under ECCS-1232018 and DMR-1156737.

On-Chip Electrolytic Chemistry for the Tuning of Graphene Devices

Astronomy — Solid-state nanopores act as single-molecule sensors whereby passage of an individual molecule in aqueous electrolyte through a nanopore is modulated of the Fermi level on the carbon side of the junction or tunneling through the barrier due to its gate field induced thinning. Devices fabricated with a continuous layer of graphene probed principally the barrier height lowering mechanism (responsible for 2 1/2 order of magnitude current modulation) while devices fabricated with graphene into which random, micron scale holes had been created probed tunneling as well (resulting in 6 orders of magnitude current modulation). The random hole density in the latter case was limited to 20% of the graphene surface area. Here we describe the performance of devices in which ordered hole arrays permit the exploration of higher hole density G-VFETs.

DNA translocation through these nanopores, where access resistance becomes comparable to the resistance through the nanopore itself.

Thursday, March 5, 2015 11:15AM - 2:15PM — Session T16 DMP: Focus Session: Graphene Electronic Devices

11:15AM T16.00001 Electrolyte gating of graphene protected by boron nitride, KEVIN THARRATT, PATRICK GALLAGHER, MENYOUNG LEE, Department of Physics, Stanford University, Stanford, California 94305, USA, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan, DAVID GOLDHABER-GORDON, Department of Physics, Stanford University, Stanford, California 94305, USA — Electrolyte gating is a technique used to induce a high carrier density at a sample surface. We have recently shown that for strontium titanate surfaces protected by boron nitride, electrolyte gating can induce high carrier densities while maintaining high electron mobility and limiting electrochemical reactions at the sample. In this talk, we describe electrolyte-gating experiments on single-layer graphene sheets encapsulated by various thicknesses of boron nitride. We discuss the implications of our work for future electrolyte gating studies of materials protected by boron nitride.


11:39AM T16.00003 On-Chip Electrolytic Chemistry for the Tuning of Graphene Devices

11:51AM T16.00004 Ab initio quantum transport in N-doped graphene

12:03PM T16.00005 Hofstadter’s Butterfly in the strongly interacting regime

12:39PM T16.00006 ABSTRACT WITHDRAWN
12:51PM T16.00007 Equilibration of Edge States at the Graphene P-N Junction Interface
SON LE, NIKOLAI KLIMOV, DAVID NEWELL, CURT RICHTER, NIST - Natl Inst of Stds & Tech, JUN YAN, Department of Physics, University of Massachusetts, Amherst, PRATIK AGNIOHOTRI, EVERETT COMFORT, JIUNG LEE, College of Nanoscale Science and Engineering, SUNY Pi, NY — The interaction of chiral quantized edge states at the graphene pn-junction (pnJ) interface at low temperature and high magnetic fields is topic of intense research recently [1]. It has been presumed that electron and hole edge states completely equilibrate with each other at the pnJ interface, creating an unique set of quantized longitudinal resistance values depending on the number of edge states that present in the device [2]. Experimentally, we have used a unique buried-split gate structure to electrostatically form a graphene pnJ with independent control of the number of edge state in the n- and p-regions of the device's channel. Measurement of both longitudinal and pseudo-Hall resistance shows quantized values that cannot be explained by using the complete equilibration model. We present a new “non-equilibration” model, in only the lowest Landau level’s (LLs) edge states equilibrate at the pnJ interface, while edge states arising from higher filling factor LLs propagate along the interface without equilibration. Our new model agrees with both the longitudinal and pseudo-Hall resistance results.


1:03PM T16.00008 Graphene/Lead (Pb)-based Cooper-pair splitter, IVAN BORZENETS, YUYA SHIMAZAKI, University of Tokyo, GARETH JONES, SAVERIO RUSSO, University of Exeter, MICHISHICA YAMAMOTO, SEIGO TARUCHA, University of Tokyo — We have fabricated a topological split gate structure based on a superconductor- two normal leads. (Compared to nonwire-appearing devices, the two dimensional nature of graphene allows for the normal leads to be placed arbitrarily close together and in a non-parallel arrangement.) The superconducting lead is created by contacting graphene with lead (Pb), thus inducing a supercurrent via the proximity effect. The normal metal leads are patterned into quantum dots by etching nano-constrictions with self-aligned side gates. Quantum dots strongly suppress two electron processes, allowing only one electron to pass at a time. Thus, the Cooper-pair splitting efficiency is enhanced as the split electrons must necessarily tunnel through different quantum dots. Therefore, we measure the longitudinal and transverse resistance of our graphene-based split gates, as well as the effect of graphene on the time evolution of the effect and its dependence on the number of edge state in the n- and p-regions of the device's channel.

HINNEFELD, Univ of Illinois - Urbana, RUIJUAN XU, University of California - Berkeley, STEVEN ROGERS, MOONSUB SHIM, Univ of Illinois - Urbana, LANE MARTIN, University of California - Berkeley, NADYA MASON, Univ of Illinois - Urbana — Graphene’s linear dispersion relation and the attendant implications for bipolar electronic applications have motivated a range of experimental efforts aimed at producing p-n junctions in graphene. Recent experimental results indicate that the electrical polarization in ferroelectric substrates can modify the local doping in graphene, via a hysteretic gating effect. Here, we exploit this effect to create variably doped local regions in a graphene device having a single, universal back-gate. By patterning devices on a partially shielded ferroelectric substrate, we show through electrical transport measurements that p- and n-doped regions can be induced in the system. We explore the competing effects of substrate polarization and interfacial charge-trap processes that contribute to this behavior, along with the time evolution of the effect and its dependence on the measurement conditions and device parameters.

1:15PM T16.00009 Electromechanically generating electricity with a gapped-graphene electric generator, DONALD DRESSEN, JENE GOLOVCHENKO, Harvard University — We demonstrate the fabrication and operation of a gapped-graphene electric generator (G-GE). The G-GE generates electricity from the mechanical oscillation of droplets of electrolytes and ionic liquids. The spontaneous adsorption of ionic species on graphene charges opposing electric double-layer capacitors (EDLCs) on each half of the device. Modulating the area of contact between the droplet and graphene leads to adsorption/desorption of ions, effectively charging/discharging each EDLC and generating a current. The flow of current supports a potential difference across the G-GE due to the device’s internal impedance. Both the magnitude and polarity of the induced current and voltage show a strong dependence on the type of ionic species used, suggesting that certain ions interact more strongly with graphene than others. We find that a simple model circuit consisting of an AC current source in series with a resistor and a time-varying capacitor accurately predicts the device’s dynamic behavior. Additionally, we discuss the effect of graphene’s intrinsic quantum capacitance on the G-GE’s performance and speculate on the utility of the device in the context of energy harvesting.

1:27PM T16.00010 Transport measurements of negative refractive behavior in ballistic graphene hetero junctions, GIL-HO LEE, GEON-HYOUNG PARK, MINSOO KIM, JAE HYEONG LEE, HU-JONG LEE, Pohang University of Science and Technology — We investigated the electronic current refraction at p-n junctions (PNJs) in ballistic monolayer graphene. Given a peculiar band structure of the graphene, the transmission of electrons through a PNJ is predicted to be similar to the optical refraction at the boundary of metamaterials with negative refractive index. In consequence, electrons waves injected at a point in one side of a junction can be refocused into a single point in the other side of the junction, which demonstrates Veselago lensing for the electrons. By adopting high-yield dry-transfer technique, we fabricated fully ballistic gapped graphene devices encapsulated by hexagonal boron nitrides with a local top gate. We will present the signatures of negative refractive transport behavior of electrons in PNJs and also discuss about the electronic current focusing in p-n heterojunctions in terms of Veselago lensing.

1:39PM T16.00011 A ballistic gate-tunable contact junction in graphene, QUENTIN WILMART, MICHAEL ROSTICHER, MOHAMED BOUKHICHA, ANDREAS INHOFER, PASCAL MORFIN, GWENDAL FEVE, JEAN-MARC BERROIR, BERNARD PLACAI, Laboratoire Pierre Aigrain, Ecole Normale Supérieure-PSL Research University, CNRS, EQUIPE DE PHYSIQUE MÉSOSCOPIQUE TEAM — Field-effect control of carrier is very efficient in graphene and allows controlling the doping profile with a great accuracy and high spatial resolution. This is needed if one wants to implement Dirac fermion optics experiments or simply to improve the performance of graphene devices. In this work we realize graphene transistors equipped with a set of local back-gates that provide control of local electric fields in the $10^{17}/\text{m}$ range at the 10 nanometer scale. In particular we demonstrate ballistic contact junctions using transistors with independent channel and contact back-gates. We will discuss the possibilities offered by this technology for ballistic electronic and opto-electronic applications.

1:51PM T16.00012 Enhanced OFF state resistance in reconfigurable graphene p-n junction, PRATIK AGNIOHOTRI, SURAJIT SUTAR, EVERETT COMFORT, State Univ of NY - Albany, JAMES HONE, Columbia University, PHILIP KIM, Harvard University, JI UNG LEE, State Univ of NY - Albany — Graphene, since its discovery, has proved to be a promising candidate to meet the challenges facing CMOS-based logic devices. Normal conduction modes which are perpendicular to the junction are blocked geometrically by rotating the channel with respect to the junction. "Y" shaped junction with graphene as the base material. (Compared to nonwire-appearing devices, the two dimensional nature of graphene allows for the normal leads to be placed arbitrarily close together and in a non-parallel arrangement.) The superconducting lead is created by contacting graphene with lead (Pb), thus inducing a supercurrent via the proximity effect. The normal metal leads are patterned into quantum dots by etching nano-constrictions with self-aligned side gates. Quantum dots strongly suppress two electron processes, allowing only one electron to pass at a time. Thus, the Cooper-pair splitting efficiency is enhanced as the split electrons must necessarily tunnel through different quantum dots. Therefore, we measure the longitudinal and transverse resistance of our graphene-based split gates, as well as the effect of graphene on the time evolution of the effect and its dependence on the number of edge state in the n- and p-regions of the device's channel.

The interaction of chiral quantized edge states at the graphene pn-junction (pnJ) interface at low temperature and high magnetic fields is topic of intense research recently [1]. It has been presumed that electron and hole edge states completely equilibrate with each other at the pnJ interface, creating an unique set of quantized longitudinal resistance values depending on the number of edge states that present in the device [2]. Experimentally, we have used a unique buried-split gate structure to electrostatically form a graphene pnJ with independent control of the number of edge state in the n- and p-regions of the device’s channel. Measurement of both longitudinal and pseudo-Hall resistance shows quantized values that cannot be explained by using the complete equilibration model. We present a new “non-equilibration” model, in only the lowest Landau level’s (LLs) edge states equilibrate at the pnJ interface, while edge states arising from higher filling factor LLs propagate along the interface without equilibration. Our new model agrees with both the longitudinal and pseudo-Hall resistance results.


2:03PM T16.00013 Controllable P-N Junctions in Graphene-Ferroelectric Devices, J. HENRY HINNEFELD, Univ of Illinois - Urbana, RUJUAN XU, University of California - Berkeley, STEVEN ROGERS, MOONSUB SHIM, Univ of Illinois - Urbana, LANE MARTIN, University of California - Berkeley, NADYA MASON, Univ of Illinois - Urbana — Graphene’s linear dispersion relation and the attendant implications for bipolar electronic applications have motivated a range of experimental efforts aimed at producing p-n junctions in graphene. Recent experimental results indicate that the electrical polarization in ferroelectric substrates can modify the local doping in graphene, via a hysteretic gating effect. Here, we exploit this effect to create variably doped local regions in a graphene device having a single, universal back-gate. By patterning devices on a partially shielded ferroelectric substrate, we show through electrical transport measurements that p- and n-doped regions can be induced in the system. We explore the competing effects of substrate polarization and interfacial charge-trap processes that contribute to this behavior, along with the time evolution of the effect and its dependence on the measurement conditions and device parameters.
11:15AM T17.00001 In-plane electric polarization of bilayer graphene nanoribbon by interlayer bias voltage. RYO OKUGAWA, JUNYA TANAKA, Tokyo Institute of Technology, TAKASHI KORETSUNE, RIKEN Center for Emergent Matter Science, SUSUMU SAITO, SHUICHI MURAKAMI, TIES, Tokyo Institute of Technology — Bilayer graphene nanoribbons are known to show various energy bands depending on the shapes of the edges and the width of the nanoribbons. In particular, the energy bands of the graphene nanoribbons with armchair edges become gapless or gapped when the width changes. We theoretically study a polarization along the ribbon direction induced by an external interlayer bias voltage by using a tight-binding model, when the nanoribbon is insulating. We find that a polarization is induced for armchair-edges but not for zigzag-edges. The polarization shows different behavior depending on the width as well as the bias voltage. When the interlayer bias voltage is weak, the polarization has opposite signs depending on the width modulo three. This difference can be understood by an effective two-band model from the tight-binding model. Furthermore, our ab initio calculations also agree with the results. On the other hand, under a strong bias voltage, we find that the polarization takes one-third or zero depending on the width modulo three.

11:27AM T17.00002 Characterization of graphene/metal interface and its modification by insertion of thin nano-carbon layer. AKINOBU KANDA, KENTA KATAKURA, YU ITO. Faculty of Pure and Applied Sciences and TIMS, University of Tsukuba, YOUTI OOTUKA, Faculty of Pure and Applied Sciences, University of Tsukuba — Due to high mobility and atomic thickness, graphene is a promising candidate for the next-generation electronic material. While considerable effort has been devoted to achieve higher mobility in graphene films, relatively little attention has been paid to the effect of making contact between graphene and metals, which is indispensable to the electric devices. In general, at a graphene/metal interface, mainly due to the difference in work functions, carriers are injected from the metal to graphene. The resulting shift of Dirac point is not limited at the graphene/metal interface but extends by ~1 μm into the graphene channel, which affects more significantly the performance of graphene field effect devices with shorter channel. Here, we experimentally investigate the channel length dependence of graphene transport properties and extract the effect of metal contact (i.e., strength of carrier doping). Several metal species are investigated and results are compared with numerical models. Furthermore, we try to reduce the influence of metal contact by inserting a thin nano-carbon film at the interface.

11:39AM T17.00003 Ordered Self-assembled Alkane Monolayer on Graphite and Graphene Surface. YUDAN SU, Department of Physics, Fudan University, HUILING HAN, FENG WANG, Department of Physics, University of California at Berkeley, QUN CAI, CHUANSHAN TIAN, Department of Physics, Fudan University, Y.R. SHEN, Department of Physics, University of California at Berkeley — The 2D self-assembly of long chain alkane molecule on graphite and graphene had been studied with phase-sensitive sum-frequency vibrational spectroscopy (PS-SFVS) and scanning tunneling microscopy (STM). The spectrum of Im(χ(2)) which directly characterizes the surface resonances, shows 10 cm~−1 red-shift of the symmetric-stretch frequency of the CH2 groups pointing towards graphite (or graphene) surface indicating Van der Waals interaction in between. The Gibbs adsorption energy of polyethylene (PE, n ~ 140) on graphite from chloroform solution was determined to be -42kJ/mol per molecule or -0.6 kJ/mol per CH2 unit. This large adsorption energy drives the long alkane chain to form an ordered self-assembled monolayer on graphite (or graphene). The sum frequency spectra suggest the orientation of carbon skeleton plane of alkane is predominately perpendicular to the graphite/graphene surface. Our STM result also provides clear evidence for the proposed molecular adsorption model. These results explain the large amount residual of long chain alkane on polystyrene (PS) or poly(methyl methacrylate) (PMMA) transferred graphene, and facilitate a better way to fabricate cleaner large-size graphene.

11:51AM T17.00004 Thin films of bottom-up synthesized graphene nanoribbons. MIKHAIL SHEKHIREV, ALEXEY LIPATOV, TIMOTHY VO, MOHAMMAD MEHDI POUR, ALEXANDER SINITSKII, Univ of Nebraska - Lincoln — Bottom-up solution synthetic approaches for graphene nanoribbons (GNRs) receive a great deal of attention, because they yield large quantities of atomically precise GNRs with intriguing electronic and optical properties. However, poor solubility of these GNRs in conventional solvents remains a great challenge and limits their processability for applications in nanoelectronics, photovoltaics and complementary organic electronics. We developed a protocol for thin film fabrication that could be applied for different types of bottom-up synthesized GNRs in chlorosulfonic acid and developed a protocol for thin film fabrication that could be applied for different types of bottom-up synthesized GNRs. The developed procedure also provides control over the thickness of films that can be made as thin as one GNR thick. Reactivity of the GNRs with chlorosulfonic acid and electrical properties of fabricated films will also be discussed.

12:03PM T17.00005 Electropolymerization of low-k polymer on graphene for top-gated FETs. ALEXEY LIPATOV, BENJAMIN B. WYMORE, ALEXANDRA FURSINA, TIMOTHY H. VO, ALEXANDER SINITSKII, JODY G. REDEPENNING, Univ of Nebraska - Lincoln — The most crucial step for field effect transistor (FET) fabrication is forming a thin and uniform layer of insulator on the surface of a body material to separate it from top-gate electrode. Due to hydrophobic and inert nature of graphene it has quickly become a challenge to deposit a uniform dielectric layer with atomic layer deposition (ALD). One promising method to overcome the problems associated with coating graphene is to incorporate a low dielectric constant (low-k) polymer buffer layer or an organic seed layer. This low-k dielectric layer on top of graphene provides the functional groups necessary for the ALD precursors to adhere. In our work we for the first time demonstrate electrodeposition of pinhole free thin (3-4 nm) layers of low-k polymer on monolayer graphene samples. Advantages of the technique include selectivity and scalability. It is possible to deposit the films selectively on a single graphene flake/device, and on a large number of devices simultaneously. The performance of top-gated FET devices demonstrates the utility of electrophotodeposited polymer films as a dielectric material between graphene and top-gate electrode.

12:15PM T17.00006 Processing of pristine graphene dispersions, gels, and composites. FAHMIDA IRIN, SRIYA DAS, Texas Tech University, DORSA PARVIZ, MICAH GREEN, Texas A&M University — This work focuses on the central concept of producing graphene from graphite without covalently functionalizing the graphene basal plane; such graphene may be stabilized, dispersed, and processed for use in a range of high-performance materials. In particular, we show that various dispersants such as triphenylene derivatives, polymers (polyvinylpyrrolidone), pyrene derivatives etc. can naturally adsorb to the graphene surface, create repulsive (steric and electrostatic) forces, and prevent aggregation. This allows for graphene dispersion in a wide range of organic solvents and composite precursors without compromising graphene structure. Such dispersions are stable against aggregation even when subjected to extreme temperature changes, pH changes, and freeze drying. The applications of these dispersions include the production of graphene/polymer nanocomposites, synthesis of self-healing aerogels, and electrically conductive aerogels. We fabricate graphene loaded polyvinyl alcohol (PVA) films which show enhanced modulus, strength, and electrical conductivity. We also demonstrate novel results in the area of creating graphene loaded self-healing aerogels. The hydrogels can be converted into electrically conductive aerogels that can be utilized as a template for doubly-percolated polymer composites.
12:27PM T17.00007 Facile preparation of reduced graphene oxide - ruthenium oxide nanocomposite electrodes for high-performance supercapacitors, FATIMA AMIR, Winthrop University, VIET PHAM, JAMES DICKERSON, Brookhaven National Laboratory, WINTHROP UNIVERSITY TEAM, CFN-BROOKHAVEN NATIONAL LAB TEAM. Here we report a facile approach of synthesis of graphene oxide (GO) sheets modified with ruthenium oxide (RuO₂) nanoparticles, followed by a reduction of graphene oxide in an alkaline medium. The as-prepared reduced graphene oxide (rGO)/ruthenium oxide (RuO₂) nanocomposite was used for the fabrication of a symmetric supercapacitor. The specific capacitance and charge-discharge periods of the supercapacitor were found to be dependent on both the structural and morphological properties, and the electrolytes used. Surface morphology analysis using scanning electron microscopy (SEM) shows the RuO₂ nanoparticles decorating rGO sheets, comprising a highly porous surface. Structural analysis obtained by x-ray diffraction (XRD) revealed an amorphous structure that is necessary to achieve a high cycling rate capability. The electrochemical properties of rGO/RuO₂ were measured in a two electrodes system, using two different electrolytes: H₂SO₄ and Na₂SO₄. The specific capacitance of rGO/RuO₂ in H₂SO₄ was found to be 318 F/g, and is much higher than that of Na₂SO₄ (184 F/g).

12:39PM T17.00008 Enhanced hydrogen storage from nanostructured graphene and nickel hybrids based on spiller mechanism, LIN WEI, YUANBING MAO, The University of Texas-Pan American — As a fascinating 2-dimensional carbon material, graphene has been decorated with metal nanoparticles to enhance its hydrogen storage performance based on the spiller mechanism. In this work, Ni and Ni alloys have been used to decorate the surface of graphene. Graphene oxide was fabricated from graphite by improved Hummer method. To form Ni/graphene and Ni/Pd/graphene hybrids, the graphene oxide water dispersion was mixed with nickel chloride (and palladium chloride). Ni(OH)₂/graphene and Ni(OH)₂/Pd(OH)₂/graphene hybrids were synthesized through hydrothermal treatment, using water as a solvent and HMT as a capping agent. After heat treatment and in situ reduction with hydrogen flow, the nanostructured Ni/graphene and Ni/Pd graphene hybrids were obtained. The nanostructured Ni/Pd/Ag/graphene hybrid was synthesized from graphene oxide in the ethylene glycol solution and metal nitrates using similar reactions. XRD, Raman, SEM, AFM were used to characterize these products. ASAP 2020 was used to test the hydrogen adsorption and desorption capacities.

12:51PM T17.00009 Tailored crumpling and unfolding of spray-dried pristine graphene and graphene oxide nanosheets, DORSA PARVIZ, Texas A&M Univ, SRiya DAS, FAHMIDA IRIN, Texas Tech Univ, MICAH GREEN, Texas A&M Univ — 3D Crumpled graphene was directly obtained from aqueous dispersions of pristine graphene using an industrially scalable spray drying technique. Capillary forces during the water evaporation induced the crumpling of nanosheets to multi-faced dimpled morphology. For the first time, the transition of 2D graphene nanosheets to a 3D crumpled morphology was directly observed inside the spray dryer. Graphene oxide (GO) was spray dried using the same procedure; however, their highly wrinkled final morphology was different than the crumpled pristine graphene nanosheets. The degree of crumpling of the nanosheets was controlled by changing the dimensionless ratio of evaporation rate to diffusion rate. Crumpled particles were dispersed into various solvents to evaluate their morphological changes as a response to rewetting. Crumpled GO nanosheets remained crumpled as a response to hydration, while the pristine graphene nanosheets unfolding behavior was solvent-dependent. This study holds significance for both fundamental understanding of the origins of nanosheets crumpling and also for the use of crumpled nanosheets for further material processing.

1:03PM T17.00010 Local field enhanced photoluminescence and Raman effect in Reduced Graphene Oxide Nanoclusters, SANJAY KARNA, TAE-YOUL CHOI, RAKESH SHAH, MEG MAHAT, ARUP NEOGI, Univ of North Texas — The increase in local field due to metal nanoparticles can influence the radiative emission and phonon interaction in semiconductors. Graphene oxide can be reduced to modify its bandgap and tune its emission energy from the red to the ultraviolet wavelength range. Reduced graphene oxide (rGO) with Ag nanoparticles has been synthesized and studied to enhance the effect of resonant surface plasmon interaction on the light emission from rGO. Comparative study of sp² cluster size, defect density and electrical conductivity has been performed. Preliminary results show that the maximum decrease in the defects density in rGO structure as treated with Ag NPs and also in the same way the inter-defect distance increase as density of defects decrease and sp² cluster size increase rapidly. The increase in size of sp² cluster and decrease in defect density due to localized electric field due to Ag NPs is responsible for the increase in electrical conductivity and in PL emission. The localized electric field increases the electrical conductivity due to the decrease in sp² clusters compared to an (defects oxides functional in GO)? increase in sp² in the rGO clusters. The increase in electric field due to localized plasmon due to Ag NP resonant to the emission from rGO results in an increase in enhancement from emission from rGO. By controlling the localized surface plasmon density, the enhancement efficiency from rGO can be enhanced.

1:15PM T17.00011 Gas Barrier and Separation Behavior of Graphene Oxide Nanobrick Wall Thin Films, JAIME GRUNLAN, Texas A&M University — In many cases, electronics packaging requires electrical conductivity and barrier to oxygen, even under humid conditions. These two properties have simultaneously been realized through the use of surfactant-free aqueous layer-by-layer (LbL) processing, in the form of a polymeric composite nanocoating. By layering graphene oxide (GO) with polyethyleneimine (PEI), a “nano brick wall” structure has been created, imparting gas barrier properties to the film. Reducing the graphene oxide with a thermal treatment further produces high oxygen barrier in humid conditions (≥ 1750 S/m). These thin films (<400 nm) are flexible relative traditional conductive thin films (e.g. ITO), and processing occurs under ambient conditions with water as the only solvent. Additionally, these PEI/GO thick films exhibit H₂/CO₂ selectivity (>300), making them interesting for gas purification membranes. The flexible nature of the aforementioned thin films, along with their excellent combination of transport properties, make them ideal candidates for use in a broad range of electronics and other packaging applications.

1:27PM T17.00012 Near-Field Radiation Between Graphene-Covered Carbon Nanotube Arrays, RICHARD ZHANG, XIANGLIE LIU, ZHUOMIN ZHANG, Georgia Institute of Technology, NANOSCALE THERMAL RADIATION LABORATORY TEAM — It has been shown that at nanometer gap distances, or the near-field, thermal radiation is enhanced over blackbody by hyperbolic metamaterials. It was shown that vertically aligned carbon nanotube (VACNT) arrays in the near-field demonstrate exceptional enhancement. In this study, graphene is covered on the surfaces of two semi-infinite VACNT arrays separated by a sub-micron vacuum gap. Doped graphene (μ ≥ 0.3 eV) is found to improve photon tunneling in a broad hyperbolic frequency range, due to the interaction with graphene grapheme surface plasmons. Increasing doping that shifts the peak spectral heat flux toward higher frequencies attests to the tunable bandgap of graphene. Although graphene covering of VACNT does not offer many magnitudes of near-field heat flux enhancement over uncovered VACNT, this study identifies conditions (i.e. gap distance and doping) that best augments heat transfer to that of VACNT arrays. In addition, this study demonstrates the near-field Poynting vector to determine the energy absorption due to graphene. It is found that graphene, in low frequencies and high chemical potentials, attenuates large penetration depths of hyperbolic modes, thereby increasing the contribution of graphene-graphene surface plasmons. This study has an impact toward designing carbon-based emitters and thermal junctions.
Electronic and Optical Properties of Atomically Precise Graphene Nanoribbons and Heterojunctions. CARLO ANTONIO PIGNEDOLI, Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland — Among graphene related materials, nanoribbons (GNRs) — narrow stripes of graphene — have emerged as promising building blocks for nanoelectronic devices. The lateral confinement in GNRs opens a bandgap that sensitively depends on the ribbon width, allowing in principle for the design of GNR-based structures with tunable properties. However, structuring with atomic precision is required to avoid detrimental effects induced by edge defects. Recently, we have introduced a versatile route for the bottom-up fabrication of GNRs [1], allowing for the atomically precise synthesis of ribbons with different shapes as well as heterojunctions between doped and undoped ribbon segments [2,3]. Here, we report on detailed experimental and computational investigations of the structural, electronic and optical properties of selected GNRs and heterojunctions [1-3]. For the case of armchair GNRs of width \( N = 7 \), the electronic band gap and band dispersions have been determined with high precision [4,5]. Optical characterization has revealed important excitonic effects [6], which are in good agreement with ab initio calculations including many-body effects. For the case of heterojunctions, consisting of seamlessly assembled segments of pristine (undoped) graphene nanoribbons and deterministically nitrogen-doped graphene nanoribbons, we find a behavior similar to traditional p–n junctions. With a band shift of 0.5 eV and an electric field of \( 2 \times 10^8 \) V m\(^{-1} \) at the heterojunction, these materials bear a high potential for applications in photovoltaics and electronics. Finally, we will discuss the potential of the bottom-up approach with regard to the fabrication of GNRs exhibiting zigzag edges, which are predicted to exhibit spin-polarized edge states.

Thursday, March 5, 2015 11:15AM - 1:45PM –
Session T19 FIAP: Invited Session: FIAP Prize Session and the Forum on Entrepreneurship in Physics  Mission Room 103B - John Rumble, R&R Data Services

11:15AM T19.00001 Prize for Industrial Applications of Physics: Materials science, microelectronics scaling, and beyond the silicon transistor, SUPRATIK GUHA, IBM — Conventional density and performance scaling of the silicon microprocessor will reach an end within about a decade. In anticipation of this, there has been extensive interest in examining materials and devices that will replace silicon transistors. There is also the far reaching interest in going beyond conventional computing and exploring non-Boolean forms of logic, and the devices and materials that will go with it. I will describe some of the research at IBM in these areas, including our work in developing carbon nanotube transistors as a drop in replacement for the silicon MOSFET.

11:51AM T19.00002 George E. Pake Prize Lecture: Physical Sciences Research at IBM: Still at the Cutting Edge, THOMAS THEIS1, IBM Research — The information technology revolution is in its “build out” phase. The foundational scientific insights and hardware advances are now many decades old. The microelectronics industry is maturing. An increasing fraction of the total research investment is in software and services. As applications of information technology transform every business and every sector of the public and private economy. Yet IBM Research continues to make substantial investments in hardware technology and the underlying physical sciences. While some of this investment is aimed at extending the established transistor technology, an increasing fraction is aimed at longer-term and possibly disruptive research — new devices for computing, such as tunneling field-effect transistors and nanophotonic circuits, and new architectures, such as neurosynaptic systems and quantum computing. This research investment is a bet that the old foundations of information technology are ripe for reinvention. After all, today’s information technology devices and systems operate far from any fundamental limits on speed and energy efficiency. But how can IBM make risky long-term research investments in an era of global competition, with financial markets focused on the short term? One important answer is partnerships. Since its early days, IBM Research has pursued innovation in information technology and innovation in the ways it conducts the business of research. By continuously evolving new models for research and development partnerships, it has extended its global reach, increased its impact on IBM’s customers, and expanded the breadth and depth of its research project portfolio. Research in the physical sciences has often led the way.

1 currently on assignment to the Semiconductor Research Corporation

12:27PM T19.00003 Distinguished Lectureship Award on the Applications of Physics: Illuminating My Career From Flash Gordon to Laser Surgery, JAMES WYNE, IBM T J Watson Res Ctr — As a child, I was fascinated by television programs about Flash Gordon. His partner in conquering the universe was Dr. Alexis Zarkov, a physicist, who had invented, among other things, a death ray gun. My personal “death ray” was a magnifying glass, focusing sunlight on unsuspecting insects, like crawling ants. I also practiced sneaking up on resting, flying, stinging insects and burning their wings before they could take off and attack me. So I understood something about the power of sunlight. In my senior year of high school, I had a fabulous physics teacher, Lewis E. Love, and I knew after one week that I wanted to be a physicist, not a medical doctor, which is the career my parents wanted me to pursue. It turns out that the first laser functioned on May 16, 1960, just one month before I graduated from high school, and it was inevitable that I would pursue a career working with lasers. My first job as a physicist, during the summer of 1963, was working with lasers at TRG, Inc. a small company whose guru was Gordon Gould, now recognized as the inventor of the laser. After three summers at TRG, I spent three years working on nonlinear optics for my PhD thesis, under the guidance of Prof. Nicolaas Bloembergen, who later won the Nobel Prize in Physics for his pioneering work in nonlinear optics. Following completion of my PhD research in 1969, I joined IBM Research, where I have worked ever since. Upon joining the Quantum Electronics group in the Physical Sciences Dept. of the T.J. Watson Research Center, my management told me to “do something great” with lasers. After working on atomic spectroscopy with dye lasers through the 1970s, I had the inspiration to acquire an excimer laser for the Laser Physics and Chemistry group. Using this laser, my colleagues and I discovered excimer laser surgery, capable of removing human and animal tissue with great precision, while leaving the undermined and adjacent tissue free of collateral damage. This discovery laid the foundation for the laser refractive surgical procedures of PRK and LASIK, which have been used to improve the visual acuity of nearly 30 million people. Today, I am working on validating my concept that the argon fluoride excimer laser can serve as a “smart scalpel,” capable of debriding necrotic lesions of the skin without damaging the underlying and adjacent viable tissue, leading to faster healing, reduced pain, reduced probability of infection, and minimal scarring. To quote Louis Pasteur, “Chance favors the prepared mind!”

1:03PM T19.00004 FIAP Forum on Entrepreneurship in Physics — With the changes in science as globalization has taken root, the future role of physicists becoming a part of the industrial physics community is more imperative. When 80% of graduating physicists will not be employed in academic positions, and 50% of all jobs for these physicists will be industrial sector, the importance of bringing our next generation of scientists up to speed on industrial applications is becoming much more important with the rapid, world-wide development of technology. FIAP is initiating a forum on entrepreneurship as a major role for the next generation of scientists. As physicists are problem solvers and the entrepreneurial experience is all about problem solving: whether involving technology, building a team, or financing a business. This forum seeks to link successful entrepreneurial physicists with the upcoming generation, through the dissemination of their global expertise and experience. Speakers will include Dr. Leo Showalter (Crystal IS), Dr. Cha Mei Tang (MicroTech), Mr. Aaron Weiss (Google), Dr. Sefan Murry (Applied Optoelectronics), Mr. Blaine Johns (Film-Sense), and Dr. Maximilian Biberger (SDC Materials).
Thursday, March 5, 2015 11:15AM - 2:15PM
Session T20 GQI DAMOP: Invited Session: Recent Frontiers of Quantum Thermodynamics: From Theory to Experiment  Ballroom B - Akimasa Miyake, University of New Mexico

11:15AM T20.00001 Quantum Quantum-Thermodynamics, TERENCE RUDOLPH, Imperial College London — The thermodynamic implications of quantization of energy were realized before the full quantum theory was developed, and today its effects are very well (though perhaps not completely) understood. By contrast the thermodynamic implications of quantum coherence, in the myriad guises it can arise, are still encountered in a somewhat piecemeal fashion and are lacking a (coherent!) unified and completely general framework. I will discuss some attempts to provide such a framework using tools of quantum information theory and to explain how thermodynamical constraints on the manipulation of quantum coherence arise.

11:51AM T20.00002 Quantum thermalization and the dynamics of entanglement, DAVID HUSE, Princeton University — I will address some aspects of how conventional thermodynamics emerges from quantum many-body physics, and also discuss one generic example where it fails to emerge, namely many-body Anderson localization. One aspect of this is the Eigenstate Thermalization Hypothesis (ETH), which suggests alternative statistical-mechanical ensembles that consist of only a single eigenstate of the many-body Hamiltonian. These ensembles, unlike the standard statistical mechanical ensembles, can detect many-body localization and the dynamical phases and quantum phase transitions within the localized phase. I will also discuss the dynamics of many-body quantum entanglement.

12:27PM T20.00003 Single ion heat engine, KILIAN SINGER, University of Mainz — An experimental realization of a heat engine with a single ion is presented, which will allow for work extraction even with non-classical thermal reservoirs. To this goal a custom designed linear Paul trap with a single ion performing an Otto cycle is presented. The radial state of the ion is used as the working gas analogous to the gas in a conventional heat engine. The conventional piston is realized by the axial degrees of freedom and the axial motional excitation stores the generated work, just like a conventional fly-wheel. The heat baths can be realized by tailored laser radiation. Alternatively electrical noise can be used to control the state of the ion. The presented system possesses advantageous properties, as the working parameters can be tuned over a broad range and the motional degrees of freedom of the ion can be accurately determined. Dark resonances allow for fast stroboscopic thermometry during the entire working cycle. Monte Carlo simulations are performed to predict the efficiency and the gained work of the working cycle [1]. We have also shown how the equations for the Carnot limit have to be modified if a squeezed thermal reservoir is employed [2]. Furthermore structural phase transitions with laser cooled linear ion crystals are induced verifying the Kibble-Zurek mechanism [3].


1:03PM T20.00004 Cavity Cooling for Ensemble Spin Systems, DAVID CORY, University of Waterloo — Recently there has been a surge of interest in exploring thermodynamics in quantum systems where dissipative effects can be exploited to perform useful work. One such example is quantum state engineering where a quantum state of high purity may be prepared by dissipative coupling through a cold thermal bath. This has been used to great effect in many quantum systems where cavity cooling has been used to cool mechanical modes to their quantum ground state through coupling to the resolved sidebands of a high-Q resonator. In this talk we explore how these techniques may be applied to an ensemble spin system. This is an attractive process as it potentially allows for parallel remove of entropy from a large number of quantum systems, enabling an ensemble to achieve a polarization greater than thermal equilibrium, and potentially on a time scale much shorter than thermal relaxation processes. This is achieved by the coupled angular momentum subspaces of the ensemble behaving as larger effective spins, overcoming the weak individual coupling of individual spins to a microwave resonator. Cavity cooling is shown to cool each of these subspaces to their respective ground state, however an additional algorithmic step or dissipative process is required to couple between these subspaces and enable cooling to the full ground state of the system.

1:39PM T20.00005 Experimental investigation of Demon-like Algorithmic Quantum Cooling and its Applications1, CHUAN-FENG LI, University of Science and Tech of China — Simulation of the low-temperature properties of many-body systems remains one of the major challenges in theoretical and experimental quantum information science. Firstly we demonstrate experimentally a Demon-like algorithmic cooling method that is applicable to any physical system that can be simulated by a quantum computer. This method allows us to distill and eliminate hot components of quantum states like a quantum Maxwell’s demon. The experimental implementation is realized with a quantum optical network, and the results are in full agreement with theoretical predictions (with fidelity higher than 0.978). Secondly, we use the demon-like algorithmic cooling method to experimentally investigate Majorana zero modes exhibiting a fundamental property of non-Abelian statistics.

1This work was supported by the National Basic Research Program of China (2011CB921200), the CAS, The National Natural Science Foundation of China.

Thursday, March 5, 2015 11:15AM - 1:51PM
Session T21 DCMP: Numerical Methods for Correlated Electrons 201 - Emmanuele Gull, University of Michigan

11:15AM T21.00001 Quantum quenches in 2D via arrays of coupled chains, ANDREW JAMES, London Center Nanotechnology, ROBERT KONIK, Brookhaven National Laboratory — Matrix product state (MPS) methods are extremely powerful when applied to strongly correlated systems in 1D. However they are less efficacious in 2D due to the ‘area law’ growth of entanglement, limiting the system sizes that can be studied. We combine MPS methods with analytical results for integrable chains to build an algorithm that can study large (anisotropic) 2D many body quantum systems, because it reduces the need for a large ‘area’. As an example we describe the application of our method to quantum quenches of the 2+1 dimensional quantum Ising model.

11:27AM T21.00002 Exact transient dynamics of the Anderson impurity, ANDREY ANTIPOV, DONG QIAOYUAN, EMANUEL GULL, Univ of Michigan - Ann Arbor — We study dynamics of a single Anderson impurity model subject to voltage and thermal quenches. We develop a hybridization expansion diagrammatic Monte Carlo algorithm to describe the exact dynamics of the problem. By including the initial correlations into the problem we describe the destruction of the Kondo state and infer the characteristic time scales of the problem. An interplay between different time scales of spin and charge excitations of the strongly correlated setup as visible in the ultra-fast response is in the focus of our study. We compare our results with frequently employed non-crossing and one-crossing approximations.
11:39AM T21.00003 Time Evolution of a Quantum Impurity System following a Sudden Quench and General Pulse at Finite Temperatures - a td-NRG Study. HOA NGHIE, THEODOULOS COSTI, Forschungszentrum Juelich — To study the time evolution of an observable of a quantum impurity system after a sudden quench at an arbitrary temperature, we apply the recently developed time-dependent numerical renormalization group approach (td-NRG) to the Anderson model and resonant level model. In the application to the Anderson model, we quantify the results in the short and long time limits by comparing them to the thermodynamic values in the initial and final states. In the case of the resonant level model, we compare the time evolution of the local occupancy calculated by td-NRG to the exact analytic result. We also present the time evolution in response to general continuous pulses, acting in a finite time interval, and in response to periodic driving fields. The study is accomplished by a generalization of the single-quench formalism to multiple quenches and by approximating smooth pulses (or periodic trains of pulses) by a sufficient number of smaller quenches.


11:51AM T21.00004 Non-equilibrium Hybridization Expansion Impurity-solver1, QIAOYUAN DONG2, Univ of Michigan - Ann Arbor — The study of non-equilibrium phenomena in strongly correlated systems has developed into one of the most active and exciting branches of condensed matter physics. Meanwhile, quantum impurity models play a prominent role as mathematical representations of quantum dots, single-molecule devices, and effective models for the dynamical mean field theory. We show results for a generalization of the hybridization expansion diagrammatic Monte Carlo technique for the Anderson impurity model. And we perform non-equilibrium calculations on the full Keldysh contour, where a dynamical sign problem vastly increases the complexity of real-time simulation. By further combining this method with a non-crossing approximation, our "bold-line" Monte Carlo can reach substantially longer times out of equilibrium than previously accessible, and provides an accurate description of quench and driven dynamics of correlated systems.

1Sponsored by the Department of Energy
2Colleagues: Andrey Antipov, Emanuel Gull

12:03PM T21.00005 Electric-field-driven resistive switching in dissipative Hubbard model1. JIAJUN LI, State Univ of NY - Buffalo, CAMILLE ARON, Princeton University, GABRIEL KOTLIAR, Rutgers University, JONG HAN, State Univ of NY - Buffalo — Understanding of solids driven out of equilibrium by external fields has been one of the central goals in condensed matter physics for the past century and is relevant to nanotechnology applications such as resistive transitions. We study how strongly correlated electrons on a dissipative lattice evolve from equilibrium when driven by a constant electric field, focusing on the extent of the linear regime and hysteretic non-linear effects at higher fields. We access the non-equilibrium steady state non-perturbatively in both the field and the electronic interactions, by means of a non-equilibrium dynamical mean-field theory in the Coulomb gauge. The linear response regime is limited by Joule heating effects and breaks down at fields orders of magnitude smaller than the quasi-particle energy scale. For large electronic interactions, strong but experimentally accessible electric fields can induce a resistive switching by driving the strongly correlated metal into a Mott insulator. Hysteretic I-V curves suggest that the non-equilibrium current is carried through a spatially inhomogeneous metal-insulator mixed state.

1Supported by NSF DMR-0907150, NSF DMR-1308141
2J. E. Han and Jiajun Li, Phys. Rev. B 88, 075113 (2013)

12:15PM T21.00006 The Actinide Transition Revisited by Gutzwiller Approximation. WENHUI XU, Brookhaven Natl Lab, NICOLA LANATA, Rutgers University, YONGXIN YAO, Ames Laboratory, GABRIEL KOTLIAR, Rutgers University — We revisit the problem of the actinide transition using the Gutzwiller approximation (GA) in combination with the local density approximation (LDA). In particular, we compute the equilibrium volumes of the actinide series and reproduce the abrupt change of density found experimentally near plutonium as a function of the atomic number. We discuss how this behavior relates with the electron correlations in the 5f states, the lattice structure, and the spin-orbit interaction. Our results are in good agreement with the experiments.

12:27PM T21.00007 Magnetic formfactor and dynamic magnetic susceptibility within DMFT for α − γ transition in Cerium and δ-Plutonium . BISMAYAN CHAKRABARTI, Rutgers University, MARIA PEZZOLI, None, GIOVANNI SORDI, Royal Holloway, University of London, KRISTJAN HAULE, GABRIEL KOTLIAR, Rutgers University — Using LDA+DMFT we study the magnetic properties of the isostuctural volume collapse transition between α and γ Cerium. We compute the magnetic formfactor F(q,ω) and show that it is very close to free ion behavior in both the local moment γ phase as well as the more itinerant α phase, in excellent agreement with neutron scattering experiments. In sharp contrast, the dynamic local magnetic susceptibility χloc(ω) of the two phases is strikingly different. In the γ phase, the spectra is dominated by the sharp low energy peak due to local moment formation, whereas in the α phase we see two broad peaks, the first due to Kondo screening and the second due to Hund’s coupling. We also calculate the magnetic spectral function S(q,ω) where we achieve excellent agreement with experiment. This shows that hybridization plays a central role in the α − γ transition in cerium, and that the 4f electrons are strongly correlated in both phases. We also study the magnetic properties of δ-Plutonium where our results give us important clues about the magnetic excitations of the system.

12:39PM T21.00008 Geometry Dependence of the Sign Problem. VLADIMIR IGLOVIKOV, Physics Department, University of California, Davis, California 95616, USA, EHSAN KHATAMI, Department of Physics and Astronomy, San Jose State University, San Jose, CA 95192, USA, RICHARD FYE, RICHARD SCALETTR, Physics Department, University of California, Davis, California 95616, USA — The sign problem is a fundamental limitation to Quantum Monte Carlo (QMC) simulations of the statistical mechanics of interacting fermions and frustrated quantum spins. We produced a comprehensive dataset on the geometry dependence of the sign problem for different densities, interaction strengths, inverse temperatures and spatial lattice sizes. We supplement this data with several observations concerning general patterns/trends in the data, including the dependence on spatial volume and how this can be probed by examining decoupled clusters, the scaling of the sign in the vicinity of a particle-hole symmetric point, and the correlation between the total sign and the signs of the individual spin up and spin down components.

12:51PM T21.00009 ABSTRACT WITHDRAWN
β-enhanced impurity solver for single-site DMFT [1]. The novel algorithm is based on a multigrid version of BSS-QMC [2,3], which yields Green functions free of significant Trotter errors, and scales linearly with the inverse temperature $\beta = 1/T$ and cubically in the cluster size $N$. We use the superior scaling to explore ultra-low temperature regimes at moderate cluster sizes, not reachable with state-of-the-art continuous time QMC impurity solvers that scale cubically in $\beta$. Benchmark results for the two-dimensional (2d) Hubbard model, compared with complementary methods (unbiased lattice QMC, dynamical vertex approximation (DVA) [4]), are presented as well as a study of the 2d doped Kondo lattice model.


1:15PM T21.00011 The density matrix renormalization group as a solver for cluster perturbation theory, CHUN YANG, ADRIAN FEIGUIN, Northeastern Univ — Cluster Perturbation Theory (CPT) provides an approximation for the single particle Green’s function of strongly correlated models in the thermodynamic limit by coupling clusters of small size using a variation of strong coupling perturbation theory. The method itself cannot account for the effects of symmetry breaking, such as in the presence of antiferromagnetic long range order, since it relies on the exact solution of clusters that are too small. The DMRG method provides a path toward a more reliable application of the CPT in the presence of long range order since it is able to calculate the single particle Green’s function of an infinite (very large) one dimensional chain, or ladder. By coupling these chains and ladders in the perpendicular direction using CPT we recover the spectral functions of the 2D lattice in the thermodynamic limit. A remarkable advantage of this approach is that unlike small clusters, the one-dimensional systems are already “(it) infinite”. We can study the effects of the onset of long range order and its spectral signatures by extending our study to multi-leg ladders.

1:27PM T21.00012 Typical medium dynamical cluster approximation applied to Migdal-Eliashberg theory 1, ZHOU LI, Department of Physics & Astronomy and Center for Computation and Technology, Louisiana State University, HANNA TERLETSKA, Department of Physics & Astronomy and Center for Computation and Technology, Louisiana State University, currently at Ames lab, ELISHA SIDDIQI, JUANA MORENO, MARK JARRELL, Department of Physics & Astronomy and Center for Computation and Technology, Louisiana State University — We use the recently developed typical medium dynamical cluster approximation (TMDCA) to study Anderson localization and the superconductor-insulator transition. In our analysis both phonons and disorder are treated on equal footing. For phonons we use the Holstein model Hamiltonian and perform analysis for different types of disorder distributions, i.e. binary or box distribution. It is of interest to see how phonons and disorder compete in fine-tuning of this phase transition by re-normalizing the gap parameter. For weak disorder we find that the size of the gap depends on the phonon frequency. Since for large phonon frequencies the Holstein model maps onto an attractive Hubbard model, we focus on the region where the phonon frequency is small and intermediate for both weak and strong disorders.

1:30PM T21.00013 Correlations in lacunar spinels: dynamical mean-field study with configuration interaction based impurity solver1, ARA GO, Department of Physics, Columbia University, HEUNG-SIK KIM, Department of Physics, University of Toronto, HOSUB JIN, Center for Correlated Electron Systems, Institute for Basic Science / Department of Physics and Astronomy, Seoul National University, ANDREW MILLIS, Department of Physics, Columbia University — Density functional plus dynamical mean field methods are used to study the role of correlations in lacunar spinel compounds GaM$_4$X$_8$ ($M$=Nb, Mo, Ta and and $X$=S, Se and Te) to investigate the interplay of correlations and topology in materials with strong spin-orbit coupling. A novel configuration-interaction exact diagonalization solver enables inclusion of more bath orbitals, enabling a better treatment of spectral functions and more accurate computations of phase boundaries. Focussing on GaTa$_4$Se$_8$, we discuss how the correlation induces metal-insulator transition in presence of the spin-orbit coupling, based on spectral functions and optical conductivities.

1 This work was supported by the US Department of Energy under Grants No. DOEFG02-04ER46169 and DE-SC0006613.


11:15AM T22.00001 Many-body localization as percolation in $d>1$, ANUSHYA CHANDRAN, Perimeter Institute, CHRISS LAUMAN, University of Washington, DANIEL GOTTESMAN, Perimeter Institute — Statistical mechanics is the framework that connects thermodynamics to the microscopic world. It hinges on the assumption of equilibration. Isolated quantum systems need not equilibrate; this is the phenomenon of many-body localization (MBL). While a detailed understanding of MBL and the associated delocalization transition is beginning to emerge in one dimension, relatively little is known about higher dimensions. In this work, we present a minimal tractable model for MBL in all spatial dimensions. Specifically, we analyze a disordered Floquet circuit composed of Clifford gates. In one dimension, the system is always localized, while in higher dimensions, it exhibits both delocalized and localized phases. The localized phase consists of well-defined metallic puddles embedded in an insulating matrix. When the puddles percolate, the system delocalizes; this maps the dynamical transition to critical percolation. We also comment on the stability of the phases to generic perturbations away from the Clifford class.

11:27AM T22.00002 Quasi Many-Body Localization in Translation Invariant Systems, NORMAN YAO, University of California Berkeley, CHRISS LAUMANN, University of Washington, J. IGNACIO CIRAC, Max Planck Institute for Quantum Optics, MIKHAIL LUKIN, Harvard University, JOEL MOORE, University of California Berkeley — We examine localization phenomena associated with generic, high entropy, states of a translation invariant, one-dimensional spin ladder. At intermediate time scales, we find slow growth of entanglement entropy consistent with the known phenomenology of many-body localization in disordered, interacting systems. At longer times, however, anomalous diffusion sets in, leading to full spin polarization decay on a time-scale exponential in system size. We identify a single length scale which parametrically controls both the eventual spin transport times and the divergence of the susceptibility to spin glass ordering. We dub this pre-thermal dynamical behavior, quasi many-body localization.
we introduce a parameter \( V \)

Physics — We propose the statistics of matrix elements of local operators as a new probe of the many-body localized (MBL) phase. Matrix elements of a given localized systems.

provides a quantitative, experimentally observable alternative to entanglement growth as a measure of the "non-ergodic but dephasing" nature of many-body

of dephasing. In contrast, the ergodic phase acts as a bath for the qubit, with no revivals visible on the time scales studied. The suppression of quantum revivals

localization, the magnetization exhibits periodic revivals, whose rate is strongly suppressed upon adding interactions after a time scale corresponding to the onset

dynamics of a single "qubit" spin weakly coupled to an otherwise isolated disordered spin chain and first demonstrate that in the localized regime the spin

chain is unable to act as a source of dissipation for the qubit, which therefore retains an imprint of its initial magnetization at infinite time. For Anderson

localization, the magnetization exhibits periodic revivals, whose rate is strongly suppressed upon adding interactions after a time scale corresponding to the onset of dephasing. In contrast, the ergodic phase acts as a bath for the qubit, with no revivals visible on the time scales studied. The suppression of quantum revivals provides a quantitative, experimentally observable alternative to entanglement growth as a measure of the "non-ergodic but dephasing" nature of many-body localized systems.

and dynamics of the system. The distribution of matrix elements of a local operator between system's eigenstates exhibits qualitatively different behavior in the

and ergodic phases, allowing for an accurate determination of the two phases. To characterize this distribution, for a given system size \( L \), we introduce a parameter \( g(L) = (\log \frac{\langle \Delta \rangle}{\Delta}) \), which is a disorder-averaged ratio of the matrix element of operator \( Y' \) between adjacent eigenstates, and \( \Delta \) is the level spacing. We find that \( g(L) \) decreases with \( L \) in the MBL phase, and grows in the ergodic phase. We propose that at the MBL-delocalization transition \( g(L) \) is independent of system size, \( g(L) = g_\infty \sim 1 \), and use this criterion to map out the phase diagram of a disordered 1D XXZ spin-1/2 chain. By studying the scaling of \( g(L) \) as a function of energy density, we locate the many-body mobility edge. We discuss implications for delocalization phase transition.

Strong-randomness phenomena in quantum Ashkin-Teller models. THOMAS VOJTA, HATEM BARGHATHI, FAWAZ HRAHSHEH, Missouri Univ of Sci & Tech, JOSE HOYOS, Instituto de Fisica de Sao Carlos, Universidade de Sao Paulo, RAJ NARAYANAN, Indian Institute of Technology Madras \( \longrightarrow \) N-color quantum Ashkin-Teller spin chain is a prototypical model for the study of strong-randomness phenomena at first-order and continuous quantum phase transitions. This talk discusses strong-disorder renormalization group approaches to this system in the weak-coupling as well as the strong-coupling regimes. Specifically, we introduce a novel general variable transformation that unifies the treatment of the strong-coupling regime. This allows us to determine the phase diagram for all color numbers \( N \), and the critical behavior for all \( N \neq 4 \). In the case of two colors, \( N = 2 \), a partially ordered product phase separates the paramagnetic and ferromagnetic phases in the strong-coupling regime. This phase is absent for all \( N > 2 \), i.e., there is a direct phase boundary between the paramagnetic and ferromagnetic phases. In agreement with the quantum version of the Aizenman-Wehr theorem, all phase transitions are continuous, even if their clean counterparts are of first order. We also discuss the various critical and multicritical points. They are all of infinite-randomness type, but depending on the coupling strength, they belong to different universality classes.

1We are grateful for the support from NSF under Grant Nos. DMR-1205803 and PHYS-1066293, from Simons Foundation, from FAPESP under Grant No. 2013/09850-7, and from CNPq under Grant Nos. 590093/2011-8 and 305261/2012-6.

Electronic glasses, regardless of disorder.

Our study suggests universal characteristics of all electron glasses, regardless of disorder.
**12:51PM T22.00009 Many-body mobility edge due to symmetry-constrained dynamics and strong interactions**, JAN MONDRAGON-SHEM, Univ of Illinois - Urbana, ARUJEET PAL, Harvard University, CHRIS LAUMANN, University of Washington, TAYLOR HUGHES, Univ of Illinois - Urbana — Many-body localization at a finite energy density inhibits thermalization and opens the possibility to study macroscopic quantum phenomena in highly excited states. The system transitions from an ergodic to a nonergodic phase at a critical energy density defined to be the many-body mobility edge. We present a mechanism for the formation of a many-body mobility edge in disordered systems with strong interactions, that satisfy conservation laws. The strong interaction spectrally differentiates eigenstates at positive temperature from those at negative temperature based on correlations, whose quantum dynamics differ dramatically due to the conservation laws. Upon introducing disorder, this difference in the dynamics can lead to an energy-dependent onset of many-body localization, thus leading to the formation of a many-body mobility edge. We exemplify this mechanism in the strongly anisotropic spin-1/2 XXZ model in a random field, whose dynamics is constrained by the conservation of total spin projection. We compute a set of diagnostic quantities that verify the presence of a mobility edge in this model. Furthermore, we discuss how introducing correlated disorder in the model can enhance this effect and stabilize the mobility edge itself.

**1:03PM T22.00010 Lattice aspect ratio effects on transport in two-dimensional quantum percolation**, BRIANNA DILLON, HISAO NAKANISHI, Purdue Univ — In a previous work [Dillon and Nakanishi, E.Phys.J.B, to be published (2014)], we calculated the transmission coefficient of the two-dimensional quantum percolation problem and concluded that there are three regimes, namely, exponentially localized, power-law localized, and delocalized. However, this remains a controversial problem and works by many others fall either in a group claiming that quantum percolation in 2D is always exponentially localized (as one-parameter scaling would suggest) or in one claiming that there is a transition to a less localized (perhaps power-law localized or delocalized) state. Among the many different types of calculations, it stood out that most works based on two-dimensional strips of highly anisotropic aspect ratios fall in the first group, whereas our previous calculations and most others in the second group were based on isotropic square geometry. In order to understand the deviations between our results and those based on strip geometry, we applied our direct calculation of the transmission coefficient to strips of a wide range of aspect ratios, and report on how aspect ratio influences transmission and localization length.

**1:15PM T22.00011 Heat diffusion in the disordered Fermi and electron liquids: the role of inelastic processes**, GEORG SCHWIETE, Johannes Gutenberg University Mainz, ALEXANDER FINKEL’SSTEIN, Texas A&M University — We study transport thermal in the disordered Fermi and electron liquids at low temperatures. Gravitational potentials are used as sources for finding the heat density and its correlation function. For a comprehensive study, we extend the renormalization group (RG) analysis developed for electric transport by including the gravitational potentials into the RG scheme. The analysis reveals that for the disordered Fermi liquid the Wiedemann-Franz law remains valid even in the presence of quantum corrections caused by the interplay of diffusion modes and the electron-electron interaction. In the present scheme this fundamental relation is closely connected with a fixed point in the multi-parametric RG flow of the gravitational potentials. While the disordered electron liquid we additionally analyze inelastic processes induced by the Coulomb interaction at sub-temperature energies. While the general form of the correlation function has to be compatible with energy conservation, these inelastic processes are at the origin of logarithmic corrections violating the Wiedemann-Franz law. The interplay of various terms in the heat density-heat density correlation function therefore differs from that for densities of other conserved quantities, such as total number of particles or spin.

**1:27PM T22.00012 Effect of impurities on strongly-correlated superconductivity with inhomogeneous cluster dynamical mean field theory**, ALEXANDRE FOLEY, SIMON VERRET, Université de Sherbrooke and RQMP, Sherbrooke, Canada, JYOTIRMROY ROY, TIFR, Mumbai, India, ANDRÉ-MARIE TREMBLAY, DAVID SÉNECHAL, Université de Sherbrooke and RQMP, Sherbrooke, Canada — We study the problem of an out-of-plane impurity in the square-lattice Hubbard model using inhomogeneous cluster dynamical mean field theory (1-CDMFT). This problem simulates the effect of impurities in superconducting cuprates. The impurity is located at the center of a 2x2 quasiparticle, surrounded by 8 or 24 other plaquettes without impurities. This system constitutes the repeated unit treated with cluster dynamical mean field theory. We find that the impurity shifts the onset of superconductivity towards higher doping. We study the effect of the impurity on the pseudogap as it appears in the local density of states. We also discuss its effect on the extent of the antiferromagnetic phase.

**1:39PM T22.00013 Disorder Driven Quantum Criticality in Three Dimensional Dirac Semimetals**, JEDEDIAH PIXLEY, PALLAB GOSWAMI, Condensed Matter Theory Center, University of Maryland, College Park — We study the nature of the quantum phase transition between a three dimensional Dirac semi-metal and a disorder controlled diffusive metal. We analyze a lattice model using numerical and field theoretical methods to explore the phase diagram and quantum critical behavior. We determine the scaling properties of the density of states and various thermodynamic observables for sufficiently large system sizes and extract the relevant critical exponents. As a result, we show the scaling functions obey energy over temperature scaling and the quantum critical point is an interacting fixed point.

**1:51PM T22.00014 Microscopic driving force in electronic smectic-nematic transition in La1/3Ca2/3MnO3**, JING TAO, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, K. SUN, Department of Physics, University of Michigan, W.G. YIN, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, S.J. PENNYCOOK, Department of Materials Science and Engineering, University of Tennessee, J.M. TRANQUADA, Y. ZHU, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory — Electronic liquid crystal (ELC) phases provide unique descriptions to characterize the electronic structures and elucidate the underlying physics in correlated materials from symmetry perspective. Although ELC phases have been proposed to play a key role in interpreting the structure-property relationship in a wide range of correlated materials, the experimental manifestations of the nature of the transition between such phases have been waiting to be explored. Using transmission electron microscopic tools with recently developed techniques, we studied the electronic smectic-nematic phase transition in La1/3Ca2/3MnO3 by monitoring the evolution of charge ordering and orbital ordering superstructures as a function of temperature. We observed that the transition is driven by the formation of defects and electronic phase separation. In addition, we found that charge inhomogeneity is responsible for the electronic smectic-nematic phase transition in this material.

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**Thursday, March 5, 2015 11:15AM - 2:15PM – Session T23 DCOMP DMP: Multiscale Modeling**

202B - Richard Lombardini, St. Mary’s University
11:15AM T23.00001 Time Domain Propagation of Quantum and Classical Systems using a Wavelet Basis Set Method, RICHARD LOMBARDINI, EWAN NOWARA, St. Mary's University (San Antonio, TX), BRUCE JOHNSON, Rice University — The use of an orthogonal wavelet basis set (Optimized Maximum-N Generalized Colleffts) to effectively model physical systems in the time domain, in particular the electromagnetic (EM) pulse and quantum mechanical (QM) wavefunction, is examined in this work. Although past research has demonstrated the benefits of wavelet basis sets to handle computationally expensive problems due to their multisresolution properties, the overlapping supports of neighboring wavelet basis functions poses problems when dealing with boundary conditions, especially with material interfaces in the EM case. Specifically, this talk addresses this issue using the idea of derivative matching creating fictitious grid points (T.A. Driscoll and B. Fornberg), but replaces the latter element with fictitious source functions in conjunction with wavelet reconstruction filters. Two-dimensional (2D) systems are analyzed, EM pulse incident on silver cylinders and the QM electron wave packet circling the proton in a hydrogen atom system (reduced to 2D, and the new wavelet method is compared to the popular finite-difference time-domain technique.

11:27AM T23.00002 A Hamiltonian theory of adaptive resolution simulations of classical and quantum models of nuclei, KARSTEN KREIS, DAVIDE DONADIO, KURT KREMER, RAFFAELLO POTESTIO, Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — Quantum delocalization of atomic nuclei strongly affects the physical properties of low temperature systems, such as superfluid helium. However, also at room temperature nuclear quantum effects can play an important role for molecules composed by light atoms. An accurate modeling of these effects is possible making use of the Path Integral formulation of Quantum Mechanics. In simulations, this numerically expensive description can be restricted to a small region of space, while modeling the remaining atoms as classical particles. In this way the computational resources required can be significantly reduced. In the present talk we demonstrate the derivation of a Hamiltonian formulation for a bottom-up, theoretically solid coupling between a classical model and a Path Integral description of the same system. The coupling between the two models is established with the so-called Hamiltonian Adaptive Resolution Scheme, resulting in a fully adaptive setup in which molecules can freely diffuse across the classical and the Path Integral regions by smoothly switching their description on the fly. Finally, we show the validation of the approach by means of adaptive resolution simulations of low temperature parahydrogen.

11:39AM T23.00003 Simulating long time behavior of materials: a case study of sintering of nanoparticles, AMIT SAMANTA, SELIM ELHADJ, JEFF BUDE, TAMMY OLSON, JON LEE, JAE HYUCK YOO, Lawrence Livermore National Laboratory — Physical processes in nature exhibit disparate time-scales, for example time scales associated with processes like phase transitions, various manifestations of creep, sintering of particles etc. are often much higher than time the system spends in the metastable states. The transition times associated with such events are also orders of magnitude higher than time scales associated with vibration of atoms. Thus, atomistic simulations of such transition events is a challenging task. In this talk, I will present a method to overcome the time-scale problem and efficiently explore the free energy surface of a complex system. I will discuss how this method can be used to gain quantitative atomic-scale insights into the sintering of nanoparticles. The simulations suggest that processes like interfacial and bulk diffusion along with grain rotation play an important role during sintering. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. LLNL-ABS-664253.

11:51AM T23.00004 Time-dependent potential-functional embedding theory, CHEN HUANG, Department of Scientific Computing, Florida State University, USA, FLORIAN LIBISCH, Institute for Theoretical Physics, Vienna University of Technology, Austria, QING PENG, Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic Institute, USA, EMILY CARTER, Department of Mechanical and Aerospace Engineering, Princeton University, USA — We introduce a time-dependent potential-functional embedding theory (TD-PFET), in which atoms are grouped into subsystems. In TD-PFET, subsystems can be propagated by different suitable time-dependent quantum mechanical methods and their interactions can be treated in a seamless, first-principles manner. TD-PFET is formulated based on the time-dependent quantum mechanics variational principle. The action of the total quantum system is written as a functional of the time-dependent embedding potential, i.e., a potential-functional formulation. We derive the integral equation that such an embedding potential needs to satisfy. As proof-of-principle, we demonstrate TD-PFET for a Na4 cluster, in which each Na atom is treated as one subsystem and propagated by time-dependent Kohn-Sham density functional theory (TDDFT) using the adiabatic local density approximation (ALDA). Our results agree well with a direct TDDFT calculation on the whole Na4 cluster using ALDA. We envision that TD-PFET will ultimately be useful for studying ultrafast quantum dynamics in condensed matter, where key regions are solved by highly accurate time-dependent quantum mechanics methods, and unimportant regions are solved by faster, less accurate methods.

12:03PM T23.00005 Coupled molecular-dynamics and first-principle transport calculations of metal/oxyde/metal heterostructures, PETER ZAPOL, Argonne Natl Lab, DMITRY KARPEYEV, University of Chicago, KETAN MAHESHWARI, XIANGLIANG ZHONG, BADRI NARAYANAN, SUBRAMANIAN SANKARANARAYANAN, MICHAEL WILDE, OLLE HEINONEN, Argonne Natl Lab, IVAN RUNDGER, Trinity College — The electronic conduction in Hf-oxygen heterostructures for use in, e.g., resistive switching devices, depends sensitively on local oxygen stoichiometry and interactions at interfaces with metal electrodes. In order to model the electronic structure of different disordered configurations near interfaces, we have combined molecular dynamics (MD) simulations with first-principle based non-equilibrium Green’s functions (NEGF) methods, including self-interaction corrections. We have developed an approach to generating automated workflows that combine MD and NEGF computations over many parameter values using the Swift parallel scripting language. A sequence of software tools transforms the result of one calculation into the input of the next allowing for a high-throughput concurrent parameter sweep. MD simulations generate systems with quenched disorder, which are then directly fed to NEGF and on to postprocessing. Different computations can be run on different computer platforms matching the computational load to the hardware resources. We will demonstrate results for metal-HfO2-metal heterostructures obtained using this workflow.

12:15PM T23.00006 Quasi-continuum multiscale theory for confined Lennard-Jones fluid mixture, MOHAMMAD H. MOTEVASSELIAN, SIKANDAR Y. MASHAYKH, NARAYANA R. ALURI, Univ of Illinois - Urbana — A continuum-based approach is developed to predict the structure of confined multicomponent Lennard-Jones fluids at multiple length-scales, ranging from few angstroms to microns. The continuum approach is based on the empirical potential-based quasi-continuum theory (EQT) that incorporates atomistic detail into a continuum framework such as the Nernst-Planck equation. It can also be used to construct a grand potential functional for classical density functional theories (cDFT). EQT and cDFT combination, provide a simple and fast approach to predict the inhomogeneous density, potential profiles and thermodynamic properties of confined fluids. In this work, we demonstrate EQT-cDFT approach by simulating a mixture of methane and hydrogen inside slit-like channels of graphene. We show that the structure of the confined mixture compares well with MD simulation results.
12:27PM T23.00007 Multiscale Investigations of the Oxidation of Stepped Cu Surfaces, QING ZHU, Chemical Engineering, University of Pittsburgh, WISSAM SAIDI, Materials Science, University of Pittsburgh, JUDITH YANG, Chemical Engineering, University of Pittsburgh — Defects on metal surfaces can induce non-canonical oxidation channels that may lead to the formation of novel nanostructures. Cu surfaces have been actively researched in the surface science community due to their wide range of applications in many fields. Recently, in situ TEM experiments showed that the oxidation of stepped surfaces promotes the formation of a flat metal-oxide interface through the Cu adatoms detachment from steps and diffusion across the terraces. In order to better understand these results, and to provide a tight bridge between the experiment and theory, we have investigated the Cu(100) oxidation using a multiscale computational approach that employs density functional theory and reactive force field. Our results demonstrate that the step-edge defects induce markedly different oxidation dynamical behavior compared to the flat surface. Additionally, on the stepped-surfaces, we find that the oxidation of the upper-terrace are more favored than the lower-terrace. We show that this behavior is due to a negative Ehrlich-Schwoebel diffusion barrier for oxygen in the ascending direction. The favoring of the oxidation of the top terrace drives Cu diffusion flux from the upper-terrace to the lower-terrace that explains the recent TEM experiments.

We acknowledge support from the NSF, Alfred P. Sloan Foundation, and KITP.

12:39PM T23.00008 A systematically improvable second-principles method including electron and lattice degrees of freedom, PABLO GARCIA-FERNANDEZ, Departamento CITIMAC, Universidad de Cantabria, Avenida de los Castros s/n, 39005 Santander, Spain, JACEK WOJDELA, JORGE IÑIGUEZ, Institut de Ciencia de Materiales de Barcelona (ICMAB-CSIC), Campus UAB, E-08193 Bellaterra, Spain, JAVIER JUNQUIERA, Departamento CITIMAC, Universidad de Cantabria, Avenida de los Castros s/n, 39005 Santander, Spain — One of the most difficult tasks when trying to expand Density Functional Theory (DFT) calculations to large systems is the scaling of computational time with the number of electrons in the simulation box. However, not all electrons play a relevant role in the determination of the physical magnitude under scrutiny. In this work we present a systematic approach to DFT based on a rigorous separation of these active electrons and holes from those of a reference state. Using a similar expansion to that found in Tight-binding DFT methods we obtain a large term containing the energy of the reference system, and a second, much smaller one, associated to the active part of the electron density. We associate the energy of the reference system to the lattice degrees of freedom and use a well-tested model Hamiltonian to represent them, on the other hand, the active electrons are described using a small but accurate Wannier function basis-set. Combined with an efficient Lanczos-based diagonalization, our method provides a systematically improvable scheme to simulate systems including tens of thousands of atoms under experimental conditions. We provide several examples of its application in the field of transition-metal oxides.

1:03PM T23.00010 The impact of resolution upon the complexity, information, thermodynamics, and transferability of coarse-grained models, THOMAS FOLEY, Pennsylvania State University. M. SCOTT SHELL, University of California, Santa Barbara, WILLIAM NOIID, Pennsylvania State University, NOIID/SHELL TEAM — By eliminating atomic degrees of freedom, coarse-grained (CG) models allow highly efficient simulations of complex phenomena. However, as a consequence of changing the model resolution, the coarse-graining procedure alters the apparent thermodynamic properties and model transferability. The present work analyzes the effects of model resolution upon the exact many-body potential of mean force (PMF), W, and, in particular, its entropic component, S_T. We demonstrate that S_T quantifies the loss of information from the atomistic model and impacts the complexity, thermodynamics, and transferability of the CG model. In order to investigate these formal results, we analytically calculate the exact PMF for the popular Gaussian Network Model of proteins and quantify both the energy-entropy balance as well as the entropic contribution to intramolecular interactions as a function of resolution. Interestingly, seven diverse proteins demonstrate strikingly similar shifts in energy-entropy balance with decreasing model resolution. We expect that these results may provide general insight into both the thermodynamic properties and model transferability. The present work analyzes the effects of model resolution upon the complexity, information, thermodynamics, and transferability of coarse-grained models for soft materials.

1:15PM T23.00011 Calculation of energy relaxation rates of fast particles by phonons in crystals, MICAH PRANGE, LUKE CAMPBELL, DANGXIN WU, SEBASTIEN KERISIT, Pacific Northwest National Laboratory — We present ab initio calculations of the temperature-dependent exchange of energy between a classical charged point-particle and the phonons of a crystalline material. The phonons, which are computed using density functional perturbation theory (DFPT) methods, interact with the moving particle via the Coulomb interaction between the density induced in the material by phonon excitation and the charge of the classical particle. Energy relaxation rates are computed using time-dependent perturbation theory. The method, which is applicable wherever DFPT is, is illustrated with results for several important scintillators whose performance is affected by electron thermalization. We discuss the influence of the form assumed for quasiparticle dispersion on theoretical estimates of electron cooling rates.

We acknowledge support from the NSF, Alfred P. Sloan Foundation, and KITP.

12:51PM T23.00009 Mesoscale modeling of functional properties in core-shell nanoparticles, JOHN MANGERI, Department of Physics, University of Connecticut, Storrs, CT, United States, OLLE HEINONEN, Material Science Division, Argonne National Laboratory, Lemont, IL, United States, DMITRY KARPEEV, University of Chicago, Chicago, IL, United States, SERGE NAKHMANSON, Institute of Materials Science, University of Connecticut, Storrs, CT, United States — Core-shell nanoparticle systems of Zn-ZnO and ZrO-TiO_2 are studied computationally using the highly scalable MOOSE finite-element framework, developed at Idaho National Lab. The elastic anisotropic mismatch of the core and shell create an imprinting effect within the shell that produces a wide variation of strains. Due to this diversity of strains, the sharp band gap edges of the bulk semiconductor are observed to be “thinned-out” much like amorphous silicon. We show that a variety of factors, such as particle size, core-to-shell volume ratio, applied hydrostatic pressure, shell microstructure, as well as the effect of surface elasticity, can influence the distribution of optical band-gap values within the particle, which may prove useful within the field of photovoltaics.

1Part of the work by O.H. was supported by award 70NANB14H012 from U.S. Department of Commerce, National Institute of Standards and Technology as part of the Center for Hierarchical Material Design.

2Northwestern-Argonne Institute of Science and Engineering, Northwestern University, Evanston, IL, United States
The limitations and possible modifications of the stress theorem are discussed. Strained orbitals minimize the non-interacting kinetic energy. The first assumption is correct. I find that the second assumption applies only in special cases.

The non-interacting kinetic energy depends on two assumptions: 1) the modulus squared of the strained orbitals equals the strained electron density, and 2) the density at zero strain; it does. The algebraic derivatives of the Hartree and exchange energies are straightforward. The derivative with respect to strain of the lattice of ions can be obtained by evaluating the algebraic derivative of the DFT energy (in practice a local or other approximation) of an electron density.

Within the scheme, non-equilibrium situation and quantum transport within the open-boundary condition are described by the region-dependent ∆ of Science and Technology — We report on the development of a novel first-principles method for the calculation of non-equilibrium quantum transport process. Within the scheme, the non-equilibrium situation and quantum transport within the open-boundary condition are described by the region-dependent. ∆ self-consistent field method and matrix Green’s function theory, respectively. We will discuss our solutions to the technical difficulties in describing bias-dependent electron transport at complicated nanointerfaces and present several application examples.

1:27PM T23.00012 Using the IRC n-Tiered model to generate exact numeric solutions for possible leptons. ARAN STUBBBS, Inframatter Research Center — Our model has 3 tiers below leptons and quarks: proto-matter, mezzo-matter, and infra-matter. Each has characteristic tachyons binding together the lower level structures to produce the higher level. Each class of tachyon generates its own granularity constant. The proto-matter is bound by gravitons to form the leptons and quarks. The mezzo-matter is bound by mezzo-tachyons to form the proto-matter. The infra-matter is bound by infra-tachyons to form the mezzo-matter. 2 types of mezzo tachyons bind the mezzo-matter structures: a charge tachyon binding s mezzo-matter (with l =0), and a color tachyon binding structures with l>0. The s structure has 1 infra-tachyon and 1 infra-photon, in 1s orbits. The p structure has 7 of each: among 4 s sub-shells and 1 p. The d structure has 11 s sub-shells, 3 p, and 1 d. Etc. Based on the first 2 leptons, a solution for the energy of the s (charge) structure, and the p (color) structure were deduced, from which the other mezzo structures energies were generated. From the mezzo matter energy content, and a pattern of orbits at the proto-matter level, energies for the next few leptons were found (to 3 sig figs): 140 MeV, 827 MeV, 1780 MeV, and 4690 MeV.

1:39PM T23.00013 A variational free-energy functional approach to the Schrödinger-Poisson theory. FRANCISCO J. SOLIS, School of Mathematical and Natural Sciences, Arizona State University, VIKRAM JADHAO, Department of Physics and Astronomy, Johns Hopkins University, KAUSHIK MITRA, None, MONICA OLVERA DE LA CRUZ, Department of Materials Science and Engineering, Northwestern University — In the numerical simulation of model electronic device systems, where electrons are typically under confinement, a key obstacle is the need to iteratively solve the coupled Schrödinger-Poisson equation in order to obtain the electronic potential. We show that it is possible to bypass this obstacle by adopting a variational approach and obtaining the solution of the SP equation by minimizing a functional. We construct the required functional and establish some of its properties. We apply this formulation to the case of narrow channel quantum wells where the local density approximation yields accurate results.

1:51PM T23.00014 Ab initio quantum transport in atomic carbon chains. ANDRÉS R. BOTELLO-MÉNDEZ, JEAN-CHRISTOPHE CHARLIER, University of Louvain, Institute of Condensed Matter and Nanosciences (Belgium), FLORIAN BANHART, Université de Strasbourg, Institut de Physique et Chimie des Matériaux (France), NAPS TEAM, CARBYNE COLLABORATION — Carbyne, the sp-hybridized phase of carbon, is still a missing link in the family of carbon allotropes. Recently, detailed electrical measurements and first-principles electronic transport calculations have been performed on monoatomic carbon chains [1]. When the 1D system is under strain, the current-voltage curves exhibit a semiconducting behavior, which corresponds to the polyyne structure of the atomic chain with alternating single and triple bonds. Conversely, when the chain is unstrained, the ohmic behavior is observed in agreement with the metallic cumulene structure with double bonds, confirming recent theoretical predictions, namely that a metal-insulator transition can be induced by adjusting the strain. The key role of the contacting leads is also scrutinized by ab initio quantum conductance calculations [2], explaining the rectifying behavior measured in monoatomic carbon chains in a non-symmetric contact configuration.


2:03PM T23.00015 Development of a non-equilibrium quantum transport calculation method based on constrained density functional1. HAN SEUL KIM, YONG-HOON KIM, Graduate School of EEWS, Korea Advanced Institute of Science and Technology — We report on the development of a novel first-principles method for the calculation of non-equilibrium quantum transport process. Within the scheme, the non-equilibrium situation and quantum transport within the open-boundary condition are described by the region-dependent ∆ self-consistent field method and matrix Green’s function theory, respectively. We will discuss our solutions to the technical difficulties in describing bias-dependent electron transport at complicated nanointerfaces and present several application examples.

2:17PM T24.00002 A problem with the stress theorem commonly used in DFT codes1. DONALD NICHOLSON, Department of Physics, University of North Carolina Asheville — The change in energy when an affine transformation (strain) is applied to a lattice of ions can be obtained by evaluating the algebraic derivative of the DFT energy (in practice a local or other approximation) of an electron density that has been similarly strained [1]. Because the DFT energy is stationary in the density, it is only required that the strained density reduces to the exact density at zero strain; it does. The algebraic derivatives of the Hartree and exchange energies are straightforward. The derivative with respect to strain of the non-interacting kinetic energy depends on two assumptions: 1) the modulus squared of the strained orbitals equals the strained electron density, and 2) the strained orbitals minimize the non-interacting kinetic energy. The first assumption is correct. I find that the second assumption applies only in special cases. The limitations and possible applications of the stress theorem are discussed.


1Work at the University of North Carolina Asheville and Oak Ridge National Laboratory was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, Materials Science and Engineering Division.
GREGORY MANN, Dept. of Chemistry, UC Berkeley; KIYUHO LEE, Department of Chemical & Biomolecular Engineering, UC Berkeley; MOLECULAR FOUNDRY, Lawrence Berkeley National Lab; MATTEO COCCIONI, Institute of Materials, École polytechnique fédérale de Lausanne, BEREND SMIT, Departments of Chemistry and Chemical & Biomolecular Engineering, UC Berkeley; JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Lab; Dept. of Physics, UC Berkeley — In order to use density functional theory (DFT) to reliably treat small molecule binding at open metal sites in metal-organic frameworks (MOFs), electron correlation effects associated with the localized d-states present at the metal centers must be accounted for. Incorporation of a Hubbard U-like term can be an approximate but computationally efficient means, yielding excellent agreement with experiment provided an appropriate value for the parameter U is chosen. To predict adsorption energetics for as-yet unsynthesized MOFs, we would need to select U using a systematic, physically motivated approach rather than the ad hoc methods typically employed. Here, we use an ab initio linear response approach to calculate U. We show that U values determined with this method reproduce previous results for the binding of carbon dioxide in Co-MOF-74 and Cu-MOF-74, and we discuss the method’s application to other 3d metals in the MOF-74 framework. Our preliminary results suggest that a wide range of U above a critical value will produce accurate binding energies. Finally, we present U values calculated for Co2+ ions in other systems, probing the environment dependence of this parameter. This work supported by DOE, and computational resources provided by NERSC.

11:51AM T24.00004 Density versus spin-density functional in DFT+U and DFT+DMFT
HYOWON PARK, University of Illinois at Chicago; ANDREW MILLIS, CHRIS MARIANETTI, Columbia University — The construction of multi-variable effective action theories such as DFT+U and DFT+DMFT requires the choice of a local subspace of correlated orbitals and an additional variable being either the charge density or spin density. This talk examines the differences between using charge-only and spin-dependent exchange-correlation functionals with the aim of providing guidance for constructing more sophisticated beyond-density functional theories. The widely used spin-dependent approximations to the exchange-correlation functional are found to lead to a large and in some cases unphysical effective exchange coupling within the correlated subspace. Additionally, the differences between Wannier and Projector based definitions of the correlated orbitals are examined, and only small differences are found provided that the orbitals are orthonormal and strongly localized. These results are documented in the context of the rare earth nickelates.

3 This work is supported under the grant DOE-ER-046169 and under the FAME grant, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA.

12:03PM T24.00005 The Hubbard Dimer: A Complete DFT Solution to a Many-Body Problem
JUSTIN SMITH, Univ of California - Irvine; DIEGO CARRASCAL, JAIME FERRER, Universidad de Oviedo; KIERON BURKE, Univ of California - Irvine — In this work we explain the relationship between density functional theory and strongly correlated models using the simplest possible example, the two-site asymmetric Hubbard model. We discuss the connection between the lattice and real-space and how this is a simple model for stretched H2. We can solve this elementary example analytically, and with that we can illuminate the underlying logic and aims of DFT. While the many-body solution is analytic, the density functional is given only implicitly. We overcome this difficulty by creating a highly accurate parameterization of the exact function. We use this parameterization to perform benchmark calculations of correlation kinetic energy, the adiabatic connection, etc. We also test Hartree-Fock and the Bethe Ansatz Local Density Approximation. We also discuss and illustrate the derivative discontinuity in the exchange-correlation energy and the infamous gap problem in DFT.

1 DGE-1321846, DE-FG02-08ER46496

12:15PM T24.00006 Development of a DFT+DMFT method using multi-orbital impurity solver
MANCHEON HAN, HYUNJU OH, CHOONG-KI LEE, HYOUNG JOON CHOI, Department of Physics, IPAP, and Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University — The density functional theory (DFT), often performed with the local density approximation or the generalized gradient approximation, is very successful for ab initio calculations of various materials. However, it has limited accuracy for strongly correlated materials. The dynamical mean field theory (DMFT), which maps a correlated lattice system to an interacting impurity site in a non-interacting bath, may describe local correlation effects. Combination of above methods, DFT+DMFT, can be an adequate approach for investigation of strongly correlated materials. We develop a multi-orbital DFT+DMFT method based on the ab-initio pseudopotential method of the SIESTA code, where electronic wavefunctions are expanded with pseudo-atomic orbitals. An exact diagonalization method is used in our DFT+DMFT method to obtain the local Green function of the impurity site with multiple orbitals. We apply our DFT+DMFT method to the electronic structure of LaFeAsO and compare the results with those from DFT and experiments. This work is supported by the NRF of Korea (Grant No.2011-0018306). Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2013-C3-062).

12:27PM T24.00007 Nonorthogonal generalized hybrid Wannier functions for linear scaling DFT simulations of surfaces and interfaces
ANDREA GRECO, ARASH MOSTOFI, Imperial College London; JOHN FREELAND, Argonne National Laboratory — Semiconductor-based thin-films have applications in microelectronics, where transistors to nano-capacitors. Many of their properties depend on phenomena at multiple length scales, but their complexity makes it difficult to obtain a detailed understanding of their behavior from experiment alone. First-principles simulations based on density-functional theory (DFT) are invaluable for providing insight into materials’ properties including for the study of thin films. In particular, hybrid Wannier functions (WFs), fully extended in the surface plane, but localized along the direction normal to the surface, have been successfully used to explore the properties of systems layered along a given direction. The large length scales associated with structures and processes in more realistic surfaces, however, are beyond the scope of such calculations, because they rely on first performing a traditional cubic-scaling DFT calculation. To overcome this limitation, we extend the concept of hybrid WFs to nonorthogonal orbitals that are directly optimized in situ in the electronic structure calculation. We show that this method, implemented in the ONETEP linear scaling DFT code, enables the study of large-scale surfaces and interfaces with plane-wave accuracy but at reduced computational expense.

12:39PM T24.00008 Performance and Accuracy of Recursive Subspace Bisection for Hybrid DFT Calculations
WILLIAM DAWSON, FRANCOIS GYGI, Univ of California - Davis — The high cost of computing the Hartree-Fock exchange has resulted in limited use of Hybrid Functionals in DFT calculations. Approximations based on transformation to localized orbitals provide one way to reduce this cost. One such method is the recursive subspace bisection method (RSB)[1]. Such localization methods involve truncation of localized orbitals, which introduces an additional approximation. We take advantage of our ability to systematically reduce the error in RSB calculations through a single parameter to study this approximation. We present the errors in ground state energy, forces, and relative energy differences between configurations for a variety of systems, including tungsten oxide, a silicon-water interface, and liquid water including the calculation of empty states.


1 Supported by DOE/BES grant DE-SC0008938
12:51PM T24.00009 Speeding up DFT: A faster method for integrating band energy in SCF cycles

MATTHEW M. BURBIDGE, JEREMY J. JORGENSEN, CONRAD W. ROSENBROCK, Brigham Young University, DEREK C. THOMAS, University of Texas at Austin, BRENT C. HESS, ROYDIE W. FORCADE, Brigham Young University, STEFANO CURTAROLO, Duke University, Center for Materials Genomics, GUS L. W. HART, Brigham Young University — Typically in SCF cycles, a “rectangle rule” is used on uniformly spaced points (Monk Pack meshes) to integrate the band energy. The use of rectangles is motivated by their fast convergence when used on the fully occupied bands of semiconductors. Unfortunately integration with rectangles is extremely inefficient for metals. This motivates the use of gauss quadrature (or other higher order methods) for integrating the band energy. As we show, however, even in the case of semiconductors where the rectangle convergence is extremely efficient, higher order methods are still more efficient. The savings in semiconductors alone are sufficient to motivate the implementation of a higher order method in current DFT codes. Even though higher order quadrature methods were discussed immediately following the original Monkhorst and Pack paper, we revisit the issue in light of modern DFT calculations. [1] H. J. Monkhorst and J. D. Pack, Phys. Rev. B 13, 5188 (1976).

1:03PM T24.00010 Efficient parameter-free calculation of absorption spectra for insulators, semiconductors and metals from time-dependent current DFT

ARJAN BERGER, LCPQ - IRSAMC, Université de Toulouse III - Paul Sabatier, CNRS, Toulouse, France and European Theoretical Spectroscopy Facility — In this work we show that with a simple dynamical kernel we can obtain good absorption spectra from time-dependent current-density functional theory (TDDCFT) for insulators, semiconductors and metals. Our approach is fully parameter free since no artificial broadening parameter is used to match calculated and measured spectra. The cost of a calculation is equal to an RPA calculation. Moreover, our TDDCFT approach scales better with system size than standard TD-DFT implementations.

1:15PM T24.00011 Gauge invariant calculation of magnetic properties from time-dependent current DFT

NATHANIEL RAIMBAULT, Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université Toulouse III - Paul Sabatier, CNRS & European Theoretical Spectroscopy Facility, PAUL L. DE BOEIJ, Scientific Computing & Modeling NV, Vrije Universiteit, Theoretical Chemistry, PINA ROMANIENLO, Laboratoire de Physique Théorique, CNRS, IRSAMC, Université Toulouse III - Paul Sabatier & European Theoretical Spectroscopy Facility, ARJAN BERGER, Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université Toulouse III - Paul Sabatier, CNRS & European Theoretical Spectroscopy Facility — We present a method to calculate magnetic properties from the current density that does not depend on the gauge choice for the vector potential when a finite basis set is used [1]. To obtain this we put paramagnetic and diamagnetic contributions to the current on equal footing by making use of a sum rule [1]. Our method is general. Here we use it to calculate static and dynamical magnetizabilities of molecules within Time-Dependent Current-Density-Functional Theory.

1:27PM T24.00012 Accurate Energies and Orbital Description in Semi-Local Kohn-Sham DFT

ALEXANDER LINDMAA, Linkoping University, STEPHAN KUEMMEL, University of Bayreuth, RICKARD ARMIENTO, Linkoping University — We present our progress on a scheme in semi-local Kohn-Sham density-functional theory (KS-DFT) for improving the orbital description while still retaining the level of accuracy of the usual semi-local exchange-correlation (xc) functionals. DFT is a widely used tool for first-principles calculations of properties of materials. A given task normally requires a balance of accuracy and computational cost, which is well achieved with semi-local DFT. However, commonly used semi-local xc functionals have important shortcomings which often can be attributed to features of the corresponding xc potential. One shortcoming is an overly delocalized representation of localized orbitals. Recently a semi-local GGA-type xc functional was constructed to address these issues [1], however, it has the trade-off of lower accuracy of the total energy. We discuss the source of this error in terms of a surplus energy contribution in the functional that needs to be accounted for, and offer a remedy for this issue which formally stays within KS-DFT, and, which does not harshly increase the computational effort. The end result is a scheme that combines accurate total energies (e.g., relaxed geometries) with an improved orbital description (e.g., improved band structure). [1] PRL 111, 036402 (2013)

1:39PM T24.00013 Understanding Density Functional Theory (DFT) and Completing it in Practice

DIOLA BAGAYOKO, Southern Univ & A&M Coll — A brief review of the seminal article by Hohenberg and Kohn leads to two conditions that have to be met by electronic structure calculations in order for their results to represent the physics content of DFT. One of these conditions is often the verifiable attainment of the absolute minima of the occupied energies. Using the second Hohenberg Kohn theorem, we show that results of calculations that do not meet this condition, when they applies, do not necessarily represent DFT findings. We illustrate this fact with over 100 calculated band gaps that are much smaller than corresponding, measured ones; in contrast, we list calculations that strictly adhered to the aforementioned conditions and whose results are in excellent agreement with experiment. We describe two crucial steps in the latter calculations that add to or complete DFT in practice. Some implications of our findings for academia, industry, and program package developers will be discussed. Acknowledgments: This work was funded in part by the National Science Foundation (NSF) and the Louisiana Board of Regents, through LASIGMA [Award Nos. EPS-1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, the US Department of Energy – National, Nuclear Security Administration (NNSA) (Award Nos. DE-NA0001861 and DE-NA0002630), LaSPACE, and LONI-SUBR.

1:51PM T24.00014 Elimination of the fractional dissociation problem in Kohn-Sham DFT using the ensemble-generalization approach

ELI KRAISLER, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, Israel — Many approximations within density-functional theory (DFT) spuriously predict that a many-electron system can dissociate into fractionally charged fragments. Here, we revisit the case of infinitely separated diatomic molecules, known to exhibit this problem when studied within standard approximations, including the local spin-density approximation (LSDA). We apply the recently suggested ensemble-generalization to LSDA (elSDA) [1,2] and find that fractional dissociation is eliminated in all systems examined. The elSDA Kohn-Sham potential develops a spatial step, associated with the emergence of the derivative discontinuity in the exchange-correlation energy functional. This step, predicted in the past for the exact Kohn-Sham potential and observed in some of its more advanced approximate forms, is a desired feature that prevents any fractional charge transfer between the system’s fragments. Our findings show that, if appropriately generalized for fractional electron densities, even the most simple approximate functionals correctly predict integer dissociation [3].

2:03PM T24.00015 Representability of Bloch states on Projector-augmented-wave (PAW) basis sets
LUIS AGAPITO, Univ of North Texas and Duke Univ, ANDREA FERRETTI, CNR-NANO S3 Center, Istituto Nanoscienze, I-41125, Modena, Italy, STEFANO CURTAROLO, Duke University, MARCO BUONGIORNO NARDELLI, Univ of North Texas — Design of small, yet 'complete', localized basis sets is necessary for an efficient dual representation of Bloch states on both plane-wave and localized basis sets. Such simultaneous dual representation permits the development of faster more accurate (beyond DFT) electronic-structure methods for atomistic materials (e.g. the ACBN0 method) by benefiting from algorithms (real and reciprocal space) and hardware acceleration (e.g. GPUs) used in the quantum-chemistry and solid-state communities. Finding a 'complete' atomic-orbital basis (partial waves) is also a requirement in the generation of robust and transferable PAW pseudopotentials. We have employed the atomic-orbital basis from available PAW data sets, which extends through most of the periodic table, and tested the representability of Bloch states on such basis. Our results show that PAW data sets allow systematic and accurate representability of the PAW Bloch states, better than with traditional quantum-chemistry double-zeta- and double-zeta-polarized-quality basis sets.

1Agapito, Ferretti, Calzolari, Curtarolo and Buongiorno Nardelli, PRB 88, 165127 (2013).
2Agapito, Curtarolo and Buongiorno Nardelli, arXiv:1406.3259 [cond-mat.str-el]

Thursday, March 5, 2015 11:15AM - 1:51PM — Session T25 DMP: Focus Session: Search for New Superconductors II
203B - Jiaqing Yan, University of Tennessee at Knoxville

11:15AM T25.00001 Superconductivity in the vicinity of antiferromagnetic order in CrAs and related materials.
JIANLIN LUO, Institute of Physics, Chinese academy of Sciences, Beijing 100190, China — Transition-metal oxides or pnictides are in rich of novel and intriguing electronic behaviors due to multiple quantum orders and competing phenomena. Among the different electronic states, the emergence of superconductivity in the vicinity of other quantum orders is at the heart of the rich physics. Superconductivity has been observed in a majority of 3d transition-metal compounds except for the Cr- and Mn- based compounds. It is thus of high interest in exploring possible superconductivity in those systems. In this talk, I will present the discovery of superconductivity on the verge of antiferromagnetic order in CrAs via the application of external high pressure. Bulk superconductivity with Tc ≈ 2 K emerges at the critical pressure Pc ≈ 8 kbar, where the first-order antiferromagnetic transition at TN ≈ 265 K under ambient pressure is completely suppressed. In addition, quantum criticality and non-Fermi liquid behavior are observed near Ppc, which we interpret as originating from a second- order magnetic quantum phase transition that is concomitant with a first-order structural transition. The present finding opens a new avenue for searching novel superconductors in the Cr and other 3d transitional-metal based systems. In collaboration with Wei Wu, Jinguang Cheng, Kazuyuki Matsubayashi, Panpan Kong, Fukun Lin, Changqing Jin, Nanlin Wang, Yoshiya Uwatoko, Rong Yi, and Qinmiao Si.

1Work supported by National Basic Research Program of China (No.2011CBA00103) and National Science Foundation of China (No.11190023).

11:51AM T25.00002 Nodal and multi-gap superconductivity in Ta4Pd3Te16 with weakly ferromagnetic normal state
GUANG-HAN CAO, WEN-HE JIAO, CHUN-MU FENG, ZHU-AN XU, Department of Physics, Zhejiang University, INSTITUTE OF CONDENSED MATTER PHYSICS TEAM — We recently discovered bulk superconductivity at Tc ≈ 4.6 K in a transition metal telluride Ta4Pd3Te16 [W. H. Jiao et al., J. Am. Chem. Soc. 136, 1284 (2014)]. This material has a layered structure with one-dimensional PdTe2 chains. Significant electron correlations are indicated by the enhanced Sommerfeld coefficient. Here we report the measurements of magnetoresistance, Hall effect, magnetization and specific heat using high-quality crystals. Our results show that Ta4Pd3Te16 is an anisotropic type-II superconductor. The anisotropy of upper critical fields Hc2(T) is strongly T-dependent, resulted from the multi-band effect. The zero-field electronic specific heat C0(T) far below the Tc is found to be proportional to T3, suggestive of presence of point nodes in at least one of the superconducting gaps, which is further supported by a nonlinear (∝ H1/2) field dependence of Sommerfeld coefficient in the mixed state. Notably, the material shows anisotropic weak-ferromagnetism above Tc, implying that spin-triplet superconductivity is likely in this material.

12:03PM T25.00003 Search for superconductivity in ternary chalcogenides Bi2Rh1S2
UDHARA KALUIRACHCHI, WEIWEI XIE, QISHENG LIN, VALENTIN TAUFOUR, SERGEY BUD'KO, GORDON MILLER, PAUL CANFIELD, Ames Laboratory/ Iowa State University — Recently Sakamoto and co-workers reported[1] that parkerite-type Bi2Rh1S2 is a new superconducting (~0.7 K) compound with the charge density wave (250 K) behavior. In this work we present the physical properties of iso-structural compound[2] Bi2Rh1S2. For the first time we have been able to grow single crystals of Bi2Rh1S2 and separate them from excess melt via high temperature decanting. We will present the detailed characterization of Bi2Rh1S2 and a new, closely related phase by mean of resistivity, magnetization, specific heat and single crystals diffraction measurements.


1This work is supported by the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

12:15PM T25.00004 Superconductivity in non-centrosymmetric BiPd
ANA MALDONADO, University of St Andrews, ZHI-XIANG SUN, MOSTAFA ENAYAT, Max-Planck-Institut fuer Festkoerperforschung, CALUM LITHGOW, University of Edinburgh, ED YELAND, University of St Andrews, DARREN PEETS, Seoul National University, ALEXANDER YARESKO, ANDREAS SCHNYDER, Max-Planck-Institut fuer Festkoerperforschung, PETER WAHL, University of St Andrews — In non-magnetic bulk materials, inversion symmetry protects the spin degeneracy. If the bulk crystal structure lacks a center of inversion, however, Rashba-type spin-orbit interactions lift the spin-degeneracy, leading to a Rashba metal whose Fermi surfaces exhibit a intricate spin texture. In superconducting Rashba metals a pairing wavefunction constructed from these complex spin structures will generally contain both singlet and triplet character. We examine possible triplet components of the order parameter in non-centrosymmetric BiPd, combining macroscopic characterization, atomic-scale ultra-low temperature scanning tunneling spectroscopy and relativistic first-principles calculations. The superconducting state of BiPd appears topologically trivial, consistent with Bardeen-Cooper-Schrieffer theory with an order parameter governed by a single isotropic s-wave gap.
12:27PM T25.00005 Evidence for a superconducting surface state in the half-heusler alloy LuPtBi1, ABHIMANYU BANERJEE, ALAN FANG, CAROLINA ADAMO, PHIL WU, ELI LEVENSEN-FALK, AHARON KAPITULNIK, Stanford University, SHEKHAR CHANDRA, BINGHAI YAN, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids — The half-Heusler alloy LuPtBi is predicted by band structure calculations to be a potential candidate for topological superconductivity. We present experimental evidence for a superconducting surface state at much higher temperatures than the bulk $T_c$ of 0.9K (seen from transport). STM measurements of the 111 surface show a well developed superconducting gap at temperatures below 2.4K, with an IV curve consistent with d-wave superconductivity. The ratio of $\Delta$ to $T_c$ is about 12.0 as opposed to the BCS value of 1.76, implying that the true $T_c$ is about ~7 K. This result is supported by SQUID magnetization measurements as well as theoretical predictions for enhanced surface superconductivity due to a Van-Hove singularity in a Bi-terminated [111] surface. We discuss implications of our measurements and possible future experiments.

1This work was funded by the Department of Energy.

12:39PM T25.00006 Beyond annealing: A revealing story of electron doped cuprate superconductors, YOSHIHARU KROCKENBERGER, MASAFUMI HORIO, HIROSHI IRIE, HIDEKI YAMAMOTO, NTT Basic Research Labs — High superconducting transition temperatures are a unique feature of cuprate superconductors. The standard phase diagram randomly combines cuprates with various Cu coordinations, e.g., octahedral vs. square-planar, thus violates electron-hole symmetry arguments. In contrast to hole-doped cuprates, the concept of doping dependency is disordered on the electron-doped side. Doping alone fails to induce superconductivity and a process commonly referred to as “annealing” is required. We have shown that an elaborate annealing process, i.e. 2-step annealing process, is capable to induce superconductivity into $Pr_{2-x}Ce_xCu_3O_7$ with $x$ as low as $x = 0.00$. Here we show that appropriate synthesis conditions allow for the growth of as-grown superconducting $Pr_{2-x}Ce_xCu_3O_7$ thin films by molecular beam epitaxy. We observe a hole-like Hall coefficient being linear up to high magnetic fields. Hence, high quality thin films of electron doped cuprate superconductors still show a positive Hall coefficient even at optimal doping level. Finally, the transition from a Mott insulator in $T_{La_2Cu_3O_4}$ to a superconducting metal in $T_{La_2Cu_3O_4}$ at $x = 0.00$ is solely associated to the coordination of Cu.

12:51PM T25.00007 Superconductivity in the Tungsten Bronzes, PHILLIP WU, Department of Applied Physics, Stanford University, Stanford, California 94305, USA and Geballe Laboratory for Advanced Materials, Stanford University, SATOSHI ISHII, KENJI TANABE, Department of Applied Electronics, Tokyo University of Science, Katsushika-ku, Tokyo 125-8585, Japan, KO MUNAKATA, ROBERT H. HAMMOND, Department of Applied Physics, Stanford University, Stanford, California 94305, USA and Geballe Laboratory for Advanced Materials, Stanford University, KAZUYASU TOKIWA, Department of Applied Electronics, Tokyo University of Science, Katsushika-ku, Tokyo 125-8585, Japan, THEODORE H. GEBALLE, MALCOLM R. BEASLEY, Department of Applied Physics, Stanford University, Stanford, California 94305, USA and Geballe Laboratory for Advanced Materials, Stanford University — Via pulsed laser deposition and post-annealing, high quality K-doped $WO_3_{-\nu}$ films with reproducible transport properties are obtained. A home built two-coil mutual inductance setup is used to probe the behavior of the films in the superconducting and normal state. The inverse penetration depths and dissipation peaks are measured as a function of temperature and field. Separately, via thin film deposition techniques, we report for the first time stable $Pr_{2-x}Ce_xCu_3O_7$ films by molecular beam epitaxy. We observe a hole-like Hall coefficient being linear up to high magnetic fields. Hence, high quality thin films of electron doped cuprate superconductors still show a positive Hall coefficient even at optimal doping level. Finally, the transition from a Mott insulator in $T_{La_2Cu_3O_4}$ to a superconducting metal in $T_{La_2Cu_3O_4}$ at $x = 0.00$ is solely associated to the coordination of Cu.

1The work was supported by the Natural Science Foundation of China (Grant Nos. 11274335, 91230203, and U1230202).

1:03PM T25.00008 Prediction of Superconductivity in Potassium-Doped Benzene, HAI-QING LIN, Beijing Computational Science Research Center, GUOHUA ZHONG, Center for Photovoltaics and Solar Energy, Shenzhen Institutes of, CHRISTOPHER TIMMS, Univ of Texas - Dallas, ALAN G. MACDIARMID NANOTECH INSTITUTE AT THE UNIVERSITY OF TEXAS AT DALLAS TEAM — To explore underline mechanism for the superconducting phase in recent discovered aromatic hydrocarbons, we carry out the first-principles calculations on benzene, the basic and the simplest unit of the series and examine the structural and phase stability when doped by potassium, K$_2$C$_6$H$_6$, $x = 1.25$. We found that K$_2$C$_6$H$_6$ with the space group of $Pbca$ is the most stable phase with superconducting transition temperature $T_c$ around 6.2K. Moreover, we argue that all existing hydrocarbons should have superconducting phase in the same range, 5K < $T_c$ < 7K, when doped by potassium atoms.

1Sergey Polyakov, Victor Denisov, Vladimir Blank, Ray Baughman, Anvar Zakhidov

2My advisor’s name is Dr. Anvar Zakhidov

1:15PM T25.00009 ESR and Microwave Absorption in Boron Doped Diamond Single Crystals, PHILLIP WU, Department of Applied Physics, Stanford University, Stanford, California 94305, USA and Geballe Laboratory for Advanced Materials, Stanford University, SATOSHI ISHII, KENJI TANABE, Department of Applied Electronics, Tokyo University of Science, Katsushika-ku, Tokyo 125-8585, Japan, KO MUNAKATA, ROBERT H. HAMMOND, Department of Applied Physics, Stanford University, Stanford, California 94305, USA and Geballe Laboratory for Advanced Materials, Stanford University, KAZUYASU TOKIWA, Department of Applied Electronics, Tokyo University of Science, Katsushika-ku, Tokyo 125-8585, Japan, THEODORE H. GEBALLE, MALCOLM R. BEASLEY, Department of Applied Physics, Stanford University, Stanford, California 94305, USA and Geballe Laboratory for Advanced Materials, Stanford University — Via pulsed laser deposition and post-annealing, high quality K-doped $WO_3_{-\nu}$ films with reproducible transport properties are obtained. A home built two-coil mutual inductance setup is used to probe the behavior of the films in the superconducting and normal state. The inverse penetration depths and dissipation peaks are measured as a function of temperature and field. Separately, via thin film deposition techniques, we report for the first time stable $Pr_{2-x}Ce_xCu_3O_7$ films by molecular beam epitaxy. We observe a hole-like Hall coefficient being linear up to high magnetic fields. Hence, high quality thin films of electron doped cuprate superconductors still show a positive Hall coefficient even at optimal doping level. Finally, the transition from a Mott insulator in $T_{La_2Cu_3O_4}$ to a superconducting metal in $T_{La_2Cu_3O_4}$ at $x = 0.00$ is solely associated to the coordination of Cu.

1The work was supported by the Natural Science Foundation of China (Grant Nos. 11274335, 91230203, and U1230202).

1:27PM T25.00010 Detection of pairing in a new high-$T_c$ system: Density of states in nanoclusters, AVIK HALDER, VITALY KRESIN, University of Southern California — A unique property of metal nanocluster particles is the “superatom”-like shell structure of the delocalized electrons. The electronic shell levels are highly degenerate, i.e., present sharp peaks in the density of states, which can enable exceptionally strong electron pairing in certain clusters composed of just tens of hundreds of atoms. This offers the potential of using them as blocking layers in high-$T_c$ materials. But how can one verify the onset of a superconducting transition in a free nanocluster? To answer this question we demonstrate the production of an intense flux of size-resolved nanoclusters with an adjustable internal temperature, and show that an accurate spectroscopic measurement of their photoelectron yield curves reveals the density of states near the Fermi level and strong changes which can occur upon reaching $T_c$. This has enabled our observation of a new family of high-temperature superconductors.

1Research supported by NSF . DMR-1206334
1:39PM T25.00011 High-Tc superconducting state of metal nanoclusters: Experimental observation

VITALY KRESIN, AVIK HALDER, University of Southern California — A spectroscopic investigation of size-resolved aluminum nanoclusters, Aln, has revealed a novel phenomenon: a rapid rise in the near-threshold density of states of several specific clusters with decreasing temperature. The effect is especially prominent in the closed-shell “magic” cluster Al66. The characteristics of this behavior are fully consistent with a pairing transition, implying a high-temperature superconducting state with Tc >∼ 100 K. This value exceeds that of bulk aluminum by two orders of magnitude. This is the first experimental observation of high temperature superconductivity in nanocluster particles. Our results highlight the promise of metal nanoclusters as high-Tc building blocks for materials and networks.

Research supported by NSF DMR-1206334.

Thursday, March 5, 2015 11:15AM - 2:15PM
Session T26 DCP: Computational Applications and Methods I
204A - Bruce Garrett, Pacific Northwest National Laboratory

11:15AM T26.00001 Attenuated second order Møller-Plesset perturbation theory: correcting finite basis set errors and infinite basis set inaccuracies
MATTHEW GOLDEY, Institute for Molecular Engineering, the University of Chicago, MARTIN HEAD-GORDON, Department of Chemistry, University of California, Berkeley — Second order Møller-Plesset perturbation theory (MP2) in finite basis sets describes several classes of noncovalent interactions poorly due to basis set superposition error (BSSE) and underlying inaccurate physics for dispersion interactions. Attenuation of the Coulomb operator provides a direct path toward improving MP2 for noncovalent interactions. In limited basis sets, we demonstrate improvements in accuracy for intermolecular interactions with a three to five-fold reduction in RMS errors. For a range of inter- and intramolecular test cases, attenuated MP2 even outperforms complete basis set estimates of MP2. Finite basis attenuated MP2 is useful for inter- and intramolecular interactions where higher cost approaches are intractable. Extending this approach, recent research pairs attenuated MP2 with long-range correction to describe potential energy landscapes, and further results for large systems with noncovalent interactions are shown.

This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. We acknowledge computational resources obtained under NSF Award CHE-1048789.

11:27AM T26.00002 Vapor liquid equilibria of hydrofluorocarbons via first principles Monte Carlo simulations
NEERAJ RAJ, HIMANSHU GOEL, Mississippi State Univ — The Kohn-Sham density functional theory (DFT) is a popular approach to compute condensed phase properties. In Kohn-Sham DFT, the local or semi local density functionals do not capture van der Waals interactions accurately. An accurate description of van der Waals interactions is essential in determining thermodynamic properties of molecules. The development of fully non local van der Waals density functional adequately describe dispersion interactions. In this work, we present first principles Monte Carlo simulations to obtain vapor liquid coexistence curves for hydrofluorocarbons by using Becke-Lee-Yang-Parr (BLYP) functional, dispersion corrected functionals, and with rVV10 nonlocal van der Waals density functional.

This work is supported by National Science Foundation

11:39AM T26.00003 Optical spectra and quasiparticle energies of molecules using a local basis set
MATHIAS LJUNGBERG, PETER KOVAL, FRANCESCO FERRARI, Donostia International Physics Center, Paseo Manuel de Lardizabal, 4. E-20018 Donostia-San Sebastián, DIETRICH FOERSTER, CPMOH/LOMA, Université de Bordeaux 1, 351 Cours de la Liberation, 33405 Talence, France, DANIEL SÁNCHEZ-PORTAL, Donostia International Physics Center, Paseo Manuel de Lardizabal, 4. E-20018 Donostia-San Sebastián — The Bethe-Salpeter equation (BSE) is the state of the art for computing optical spectra for solids and molecular clusters. Here we present an implementation of BSE for clusters that scales asymptotically like O(N^3) with the number of atoms, achieved by exploiting the locality of the problem in the local basis set representation and by using the Haydock recursion method to compute the spectrum. Using a pseudo-Hermitian Lanczos algorithm we can go beyond the Tamm-Dancoff approximation within our iterative scheme. As a starting point for the BSE we compute quasiparticle energies with our low-scaling GW implementation [1], retaining the frequency dependence of all quantities and thus avoiding the plasmon-pole model or similar schemes. The initial wave functions are taken from a preceding SIESTA calculation. We discuss the influence of self-consistency on the quasiparticle energies [2] and its effect on the BSE spectra. We also investigate the satellite peaks that are present in the GW density of states. Computed GW/BSE spectra are shown for some organic molecules of medium size that are relevant for photovoltaic applications.


11:51AM T26.00004 Computational XPS from Koopmans compliant Functionals
NICOLAS POILVERT, NATHAN KEILBART, ISMAILA DABO, The Pennsylvania State University — X-Ray Photo-emission Spectroscopy (XPS) is one of the most accurate experimental probe when it comes to deciphering the chemical composition of materials like Transition-Metals and Transition-Metal Oxides. Because of the sensitivity of electron binding energies to the local chemistry surrounding an atom, XPS can also help identify atomic oxidation states. Nevertheless, the complexity of XPS signals makes it a challenging task to go from the spectra to a list of chemical species and their respective oxidation states. Electronic structure methods such as Density Functional Theory fall short when it comes to predicting electron binding energies because of large self-interaction errors. The recent introduction of Koopmans-compliant functionals[1] on the other hand has led to the conclusion that UPS spectra can be accurately predicted at the level of Many-Body Perturbation Theory and beyond, while retaining most of the conceptual and computational simplicity of DFT. In this talk, we will more particularly focus our attention on assessing the accuracy of predicted Transition-Metal XPS spectra.

12:03PM T26.00005 Computational studies of the acid catalysts and solvent effects on Diels-Alder cycloaddition and dehydration reactions: Maleic anhydride and 2,5 dimethylfuran, TAHA SALAVATI-FARD, STAVROS CARATZOULAS, DOUGLAS DOREN, University of Delaware — Using DFT calculations, we present a detailed gas-phase mechanism for the conversion of DMF and maleic anhydride to 3,6 dimethyl phthalic anhydride. The conversion includes Diels-Alder cycloaddition followed by dehydration of cycloadduct. In addition, we consider the effects of solvent by making use of the PCM. We provide free energies of uncatalyzed, Lewis acid and Brønsted acid catalyzed reactions in vacuum and in a broad range of solvents. Our calculations show that a Lewis acid catalyzes the reaction through decreasing HOMO-LUMO gap of the addends. Also, a Brønsted acid changes the mechanism of reaction and is able to lower the activation free energy of cycloaddition, effectively. Furthermore, we show that as Lewis acids lower the activation barrier of dehydration reaction which is originally too high, a Brønsted acid changes the mechanism and is extremely effective in catalyzing the dehydration. Also, increasing dielectric constant of solvent decreases the activation barrier of uncatalyzed and Lewis acid catalyzed Diels-Alder reaction. For both the Lewis and Brønsted acid catalyzed Diels-Alder reaction, the dependency of activation free energy to increasing dielectric constant is much stronger when the acid is coordinated to DMF.

12:15PM T26.00006 First-principles Study of the Removal of Boron by Co-precipitation with Hydroxyapatite Using Dolomite as a Starting Material, CHENYANG LI, LAZARO CALDERIN, Pennsylvania State University, KEIKO SASAKI, Kyushu University, ISMAILA DABO, Pennsylvania State University, PENNSYLVANIA STATE UNIVERSITY COLLABORATION, KYUSHU UNIVERSITY COLLABORATION — Boron is a toxic chemical in drinking water and a major health concern worldwide. One method to reduce boron concentration in water consists of co-precipitating boron with hydrated minerals. Nevertheless, little is known about the chemical mechanisms underlying boron reactions with complex minerals. In this work, we have applied first-principles calculations based on density-functional theory (DFT) to characterize boron-bearing hydroxyapatite (HAp) resulting from co-precipitation with hydrated dolomite. DFT calculations have been performed to interpret X-ray diffraction (XRD) and nuclear magnetic resonance (NMR) experiments and to characterize solid residues after boron removal with a focus on determining the absorption sites of B(OH)₃ and B(OH)₄ in the formed minerals. The computed results indicate that the absorption takes place at phosphate (PO₄)3 sites. In addition, changes in the lattice parameters of the co-precipitate of HAp as a function of boron concentration have been calculated and compared with experimental results. Good agreement of the decreasing trend in a-direction and the increasing trend in c-direction has been observed by our calculations. Raman and infrared (IR) spectra have been studied as well to achieve a better understanding the B-HAp structures.

12:27PM T26.00007 Effective Many-Body Interactions in Dipolar Fluids and their Effect on Structure: Can the Dipole-Dipole Interaction be Modelled as a Short-Ranged 3-Body Interaction?, JULIEN SINDT, PHILIP CAMP, University of Edinburgh — In the 1970s, Stell et al. showed that it is possible to map the partition function of a system of particles interacting via anisotropic dipolar pairwise interactions to that of a hypothetical system with isotropic many-body interactions. It follows that “polar and nonpolar fluids have the same critical exponents” irrespective of long-ranged Coulombic interactions. We have calculated the structural properties of a system of soft spheres with the leading-order 2- and 3-body terms of the isotropic many-body potential. We have compared radial distribution functions and structure factors obtained from molecular dynamics simulations of dipolar soft spheres (DSSs) under the same physical conditions. We find that the many-body potential overemphasises chaining when compared to the equivalent DSS system. The chain-inducing component is the three-body Axilrod-Teller potential, and by adjusting its contribution, it is possible to match the structure with that of the DSS fluid, showing that the many-body potential can be used as a proxy for the dipolar potential. We conclude by studying the gas-liquid phase transition, finding that the phase transition disappears beyond a threshold degree of chaining.

12:39PM T26.00008 A new lattice Monte-Carlo simulation for the dielectric inhomogeneity of ion-containing liquids, XIAOZHENG DUAN, ISSEI NAKAMURA, State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences — We develop a novel lattice Monte-Carlo method to capture the effects of the reorientation of solvent dipoles under external electrostatic fields. Our simulation accounts for the effects of saturated dipoles near ions on the angstrom scale and hence spatial variations in the dielectric function. We will discuss the substantial disparity in the dielectric functions between like and unlike charges. Importantly, a contacting cation-anion pair cannot be literally taken as “charge-neutral species” in terms of the solvation energy. On the other hand, even when the two charges are separated by 1 nm, a significant correlation in the dielectric function may arise. Our simulation also provides the dependence of the bulk dielectric value on the ionic strength, which is consistent with experimental data.

12:51PM T26.00009 Energy levels of a particle confined in an ellipsoidal potential well, ROMAN KEZERASHVILII, New York City College of Technology, CUNY, USA, TAMAZ KERESELIDZE, TAMAR TCHELIDZE, Tbilisi State University, Georgia — The Schrodinger equation is solved for a particle confined within the ellipsoidal potential well using the perturbation theory and the Hamiltonian diagonalization method. The explicit expressions are obtained for the energy levels that are size and shape dependent and appropriate wave functions. The calculated energy levels are in a good qualitative and quantitative agreement with the result obtained by numerical solution of the Schrodinger equation. It is revealed that for the lowest states of a given symmetry the region of validity of the perturbation approximation is much larger than it follows from the usual condition of applicability of the perturbation theory. The optical properties of nanoparticles of a prolate and oblate ellipsoidal shape are discussed.

1:03PM T26.00010 Potential and kinetic energetic analysis of phonon modes in varied molecular solids, BRENT KRACZEK, US Army Research Laboratory — We calculate partitioned kinetic and potential energies of the phonon modes in molecular solids to illuminate the dynamical behavior of the constituent molecules. This enables analysis of the relationship between the characteristics of sets of phonon modes, molecular structure and chemical reactivity by partitioning the kinetic energy into the translational, rotational and vibrational motions of groups of atoms (including molecules), and the potential energy into the energy contained within interatomic interactions[1]. We consider three solids of differing size and rigidity: naphthalene (C₁₀H₈), nitromethane (CH₃NO₂) and α-HMX (C₇H₆N₃O₉). Naphthalene and nitromethane mostly act in the semi-rigid manner often expected in molecular solids. HMX exhibits behavior that is significantly less-rigid. While there are definite correlations between the kinetic and potential energetic analyses, there are also differences, particularly in the excitation of chemical bonds by low-frequency lattice modes. This suggests that in many cases computational and experimental methods depend on atomic displacements may not identify phonon modes active in chemical reactivity. 1. Kraczek, Chung, J. Chem. Phys. 138:074505 (2013).
1:15PM T26.00011 Switching mechanisms and role of entropy in chemically controlled hydrazone-based switches. RENE DERIAN, IVAN STICH, Inst. of Physics, Slovak Academy of Sciences — Chemically controlled synthetic rotary switches are important as they resemble rotary motors found in nature. In order to elucidate the recent experiments [1], using hybrid QM/MM methods we have studied chemically controlled hydrazone-based switches in a strongly polar solvent. The experiments indicate a controlled E→Z+H switching by addition of acid and thermal backward isomerization. We have studied the Z→E switching mechanisms and the role of entropy. We find use of explicit MM solvent crucial for understanding the huge dipole moments (>10D) in the Z conformation and significantly smaller (∼5D) in the E conformation and at the transition state, pointing toward very different ordering in those states. Furthermore, the internal and free energy surfaces from thermodynamic integration are qualitatively very different with the free energy surface exhibiting much smaller energy differences between E and Z. In addition, the solvent causes a pronounced shift (∼30°) in the position of the Z states from internal and free energies. Both finding highlight the role of the entropy in the switching process and help a quantitative understanding of the switching in the solvent.


1:27PM T26.00012 Determination of the Torsional Potential Energy Surfaces of the Ortho-, Meta- and Para-Isomers of Dinitrobenzene. PAUL SMITH, MARIO BORUNDA, Oklahoma State Univ — The three unique isomers of dinitrobenzene, the ortho-, meta-, and para-isomers, have widely varying steric hindrances and bond hybridizations. The steric effects and the hybridized bonds cause the molecular energy to be dependent on the rotation of the nitro groups. We have calculated the torsional potential energy surfaces of each of the three dinitrobenzene isomers using density functional theory, obtaining a 33x33 plot of the energy of each molecule as a function of the torsional angles of the C-N bonds. The accuracy of the method used is determined by comparison with previous theoretical and experimental results. The potential energy surfaces provide valuable insight into the mechanics of conjugated molecules, and the method we present can be extended even to proteins, which have very complicated conformations and many conjugated bonds. This method makes the determination of the lowest energy conformations of complex molecules far more computationally accessible.

1:39PM T26.00013 Density Functional Plus Dynamical Mean Field Study of Spin Crossover Molecule. JIA CHEN, Departemtn of Applied Physics and Applied Math, Columbia University, ANDREW MILLIS, Departmentn of Physics, Columbia University, CHRIS MARIANETTI, Departmentn of Applied Physics and Applied Math, Columbia University — We report a density functional plus dynamical mean field study of spin crossover molecule Fe(phen)2(NCS)2. The temperature dependent magnetic susceptibility, Fe-d spectral and total energy were calculated and compared with experimental magnetization, metal L-edge x-ray adsorption spectroscopy. The importance of dynamic effect on energetics is demonstrated by comparison with density functional plus U method, and the role of full charge self-consistency is identified. Moreover, the local spin density plus U (LSDA+U) method with exchange interaction explicitly included is shown to dramatically overemphasize magnetic interaction.

2:03PM T26.00015 Machine learning of single molecule free energy surfaces and the impact of chemistry and environment upon structure and dynamics. RACHAEL MANSBACH, ANDREW FERGUSON, Univ of Illinois - Urbana — The conformational states explored by proteins and polymers can be controlled by environmental conditions (e.g., temperature, pressure, solvent) or molecular chemistry (e.g., chain length, side chains). It is of fundamental interest to quantify the impact upon molecular structure and function, and a prerequisite to the rational engineering of proteins and polymers with desired properties. Using the diffusion map nonlinear manifold learning algorithm, we have developed an approach to: (i) extract from molecular simulations the single molecule free energy surface governing the microscopic molecular behavior, (ii) quantify changes in its topography as a function of environmental conditions and molecular chemistry, and (iii) relate these perturbations to changes in molecular structure and dynamics. In a first application to an n-icosane chain, we have quantified the thermally accessible chain configurations as a function of temperature and solvent conditions. In a second application to a family of polyglutamate-derivative decameric homopeptides, we quantify the stability of the helical state relative to the random coil as a function of side chain length and expose the molecular mechanism underpinning side chain-mediated helix stability.

Thursday, March 5, 2015 11:15AM - 2:15PM
Session T27 DCP: Focus Session: Solvation of Ions and Electrons III 204B - Etienne Garand, University of Wisconsin, Madison

11:15AM T27.00001 Solvation and Organization of Ions at the Air-Water Interface. HEATHER ALLEN, Ohio State University — The air-water interface has been the focus of research in the Allen Lab at Ohio State for more than a decade. We utilize nonlinear and linear optical spectroscopic methods to understand the local intermolecular interactions and organization of water itself with various solutes and monolayers. Motivated by atmospheric aerosol chemistry of marine and urban regions, and biophysical applications related to lung lining and biomembranes, monovalent and divalent cations and anions continue to be investigated by our group using conventional and heterodyne-detection vibrational sum frequency generation (VSFG) spectroscopy. Interest is in the surface propensity and availability for reaction at water surfaces. Ion valency, polarizability, size, shape, and identity of the counterion are critical factors in considering ion organization and subsequent changes in interfacial electric field at the air-water interface. The hydrating water molecules play a key role in the interfacial organization of other species in the solution, and is studied directly as it reveals the details of ion interfacial distributions. Phospholipids and fatty acids are also investigated using both VSFG and Brewster angle microscopy (BAM). Head group differences, especially with regard to hydrogen bonding capability and extent, are discerning factors for surface organization and shape distinction at the water surface.

In collaboration with Wei Hua and Dominique Verreault, Ohio State University.
11:51 AM T27.00002 Sensitivity of ultrafast vibrational dynamics of interfacial water to cations at silica/water interfaces, SHALAKA DEWAN, AASHISH TULADHAR, ERIC BORGUET, Temple Univ — Interfacial water structure is a key player in the chemistry of environmentally relevant processes, e.g., the dissolution of mineral surfaces. Since the properties of water are dominated by its hydrogen-bonding network, understanding the local changes in this structure at the mineral/water interface is important. Vibrational sum-frequency generation (vSFG) spectroscopy is a tool that can probe the hydrogen bonding environment at buried interfaces. Time-resolved vSFG of the OH stretch is further sensitive to the changes in hydrogen bonding at surfaces. vSFG has demonstrated that interfacial water structure at silica is most sensitive to cations at near water pH 6-8. Further, at this pH, increasing the ionic strength slows the vibrational relaxation of O-H stretch of water from ~200 to ~600 fs. Here, we show that the slowing down of O-H dynamics on addition of cations is more pronounced at pH 6 than at pH 12, even though the surface is negatively charged in both cases. This suggests that, in addition to the ion screening the surface charge, the cations actually change the local H-bonding environment of water differently at distinct bulk pH. Our results shed light on the ongoing debate on the role of ions in altering the structure of water at an interface.

12:03 PM T27.00003 Vibrational Spectroscopy of Hydrated MOH Clusters, BRETT MARSH, JONATHAN VOSS, JIA ZHOU, ETIENNE GARAND, Univ of Wisconsin, Madison — Hydrated metal ions have importance in a number of fields of chemistry including environmental chemistry, biochemical chemistry, and catalysis. Although the aqua complexes of transition metals are well studied there is a dearth of information on hydroxide containing metal clusters which have been implicated in catalytic mechanisms of water oxidation. In this work we use cryogenic ion vibrational spectroscopy (CIVS) to interrogate clusters of the form MOH(H2O)n (M = Fe, Co, Ni, Cu, Zn) in the hydride stretching region (2400-3800 cm⁻¹). Comparison of the spectral data to density functional theory calculations allows for unambiguous assignment of the observed spectral features. The resulting spectra show both a metal dependent and size dependent shift of the hydroxide stretching frequency in all clusters. The spectra also reveal that the first solvation shells of Fe, Co, Cu, and Zn containing clusters are composed of 4 ligands while the first solvation shell in Ni clusters is at least 6 ligands. This is markedly different from previous work on Ni(H2O)6+, Cu(H2O)4+, and Zn(H2O)6+ cluster in which the first solvation shells are 4 ligands, 2 ligands, and 3 ligands respectively. Aspects of hydration in the second solvation shell of these clusters will also be discussed.

12:15 PM T27.00004 Exploring Specific Ion Effects on Ion Hydration at Aqueous Interfaces, PAUL CREMER, Penn State University — We used sum frequency generation vibrational spectroscopy to probe the interactions of ions with self-assembled monolayers and proteins at aqueous interfaces. I will discuss the behavior of cations and anions as they relate to the Hofmeister series, which is a rank ordering of the efficacy of these species to influence the physical behavior of colloidal and interfacial systems in solution. Ion specific effects at these interfaces were found to be determined by several factors. These include the sign and magnitude of the surface potential, ion pairing effects in the double layer, as well as the presence of polar and nonpolar interfacial moieties. At negatively charged, hydrophilic surfaces, we found that Na⁺ adsorption and double layer formation were modulated by the type of the counterion in solution. The same ordering was observed for the anions whether this interface was relatively hydrophilic or hydrophobic. Changing the sign of the charge at the interface also led to a similar Hofmeister ordering. Moreover, at negatively charged hydrophilic surfaces, the smallest and best hydrated cations were mostly favored over more poorly hydrated cations. By contrast, well hydrated cations were expelled from more apolar surfaces.

12:15PM T27.00005 Structural properties of simple aqueous solutions from ab initio simulations, ALEX P. GAIDUK, Institute for Molecular Engineering, University of Chicago, FRANCOIS GYGI, Department of Computer Science, University of California, Davis, GIULIA GALLI, Department of Molecular Engineering, University of Chicago — Although water and salt solutions have been studied for many decades, several aspects of their microscopic and electronic properties remain uncertain. One of the open questions is whether simple ions have long-range effects on the structure of liquid water. We performed extensive first-principles molecular dynamics simulations [1] of solutions of a simple salt (NaCl) and found that what Na⁺ does not significantly change the structure of water beyond the first solvation shell. This has far reaching hydrogen-bond-breaking effect. We present an analysis of the structural modifications in terms of molecular polarizabilities and dipole angular correlations. Our results are in agreement with the traditional classification of Cl⁻ as a structure-breaker, but at variance with several theoretical and experimental studies which did not observe significant modifications of the structure of water outside the first solvation shell of ions [2]. We also present an analysis of the electronic properties of the solutions [3].

1:03PM T27.00006 Ultrafast vibrational spectroscopy (2D-IR) of anions in ionic liquids, SEAN GARRETT-ROE, University of Pittsburgh — Ionic liquids hold promise for applications in energy storage as the electrolyte in electric double-layer capacitors and other devices. Further optimizing device performance through their physical and chemical properties requires an improved understanding of the detailed interactions between cation and anion and how they reorganize in the presence of charge. Here we probe the dynamics of thiocyanate ions in several bulk imidazolium bis(trifluoromethylsulfonyl)amide ionic liquids from femtoseconds to 100 ps using ultrafast vibrational spectroscopy. Two-dimensional infrared (2D-IR) spectroscopy of thiocyanate ions detect both inertial motion (on the hundreds of femtosecond timescales) as well as slower, diffusive motions (on the tens of picosecond timescales). The 2D-IR experiments show that the rate of fluctuation of the electrostatic environment around the thiocyanate is sensitive to hydrogen bonding at the 2-position of the imidazolium ring. The correspondence of time-scales with molecular dynamics simulations suggests that the slowest motions we observe are fluctuations around a local free-energy minimum while the faster timescales correspond to the rearrangement of those local intermolecular arrangements. Our measurements implicate the break-up of local ion cages as the activating event for the onset of translational motions which are responsible for viscosity and conductivity. We additionally test our hypothesis that the SCN anion is sensitive to the local environment by introducing co-solutes - counter-cations such as K⁺ and water. We observe contact-ion pairs, i.e., SCN- anions with a K⁺ counter charge in the first solvation shell through a static component in the frequency correlation function. We observe water-bound SCN- through changes in linewidth, population relaxation rates, and dynamics. The SCN- is an eloquent reporter of local structure and dynamics in these complex fluids.

1:39PM T27.00007 Structural dynamics of solvated OH⁻ and H₃O⁺ in liquid water: an ab initio molecular dynamics study using PBE0 hybrid functional with van der Waals’ interaction, LIXIN ZHENG, XIFAN WU, Temple Univ — The nature of solvation structure of hydroxide (OH⁻) and hydronium (H₃O⁺) solvated in liquid water is of fundamental interest, as it is the prerequisite to understand the autoprotolysis process, which is often a crucial step in chemical and biological activities. It has been revealed that the proton transfer (PT) process, especially in hydroxide case, is of great controversy and complexity compared to traditional textbook description. One major source of inaccuracy originates from the delocalization error and lack of dispersion force in the conventional adopted electron exchange correlation function in GGA functional leading to an over-structured H-bond (HB) structure. Now with state-of-the-art PBE0 hybrid density functional, and the inclusion of long-range van der Waals dispersion force, we are able to perform ab initio molecular dynamics with higher accuracy. Through the analysis of mean square displacement of ion, HB geometrical distribution and lifetime, and the strength change of HB, we are presenting a quantitatively accurate picture of proton transfer structural mechanism.

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Work supported by DOE BES DE-SC0008938. Computer time provided by the Argonne Leadership Computing Facility through the INCITE program.
1:51PM T27.00008 Solvation of a Ruthenium Water Oxidation Catalyst, [Ru(tpy)(bpy)(H₂O)]²⁺. ERIN DUFFY, BRETT MARSH, JONATHAN VOSS, ETIENNE GARAND, University of Wisconsin-Madison — The splitting of H₂O into H₂ and O₂ is an important reaction for alternative energy sources, but it is hindered by the water oxidation step due to its unfavorable thermodynamics. Production of a suitable water oxidation catalyst (WOC) has posed a challenge to researchers for decades, and the reaction mechanism is not well understood. One of the most well-known and extensively studied WOCs is [Ru(tpy)(bpy)(H₂O)]²⁺ (tpy = 2,2'-bipyridine and bpy = 2,2'-bipyridine) and its derivatives. In this talk, infrared spectral data (2400-3800 cm⁻¹) obtained by Cryogenic Ion Vibrational Spectroscopy (CIVS) of [Ru(tpy)(bpy)(H₂O)]²⁺ and its water clusters, [Ru(tpy)(bpy)(H₂O)]²⁺·nH₂O, are presented. In particular, the OH stretches are used as a probe of solvation strength, and trends in their spectral shifts are examined as a function of cluster size. Determination of water binding geometries are facilitated with comparison with density functional theory (DFT) calculations. Additionally, IR and mass spectral data of electrochemically-produced intermediates of the water oxidation cycle are shown, which provide evidence of proton-coupled electron transfer (PCET) events, in agreement with proposed mechanisms.

2:03PM T27.00009 Ion Induced Hydrophilicity at Hexane Vapor Water Interface. SHANSHAN YANG, YUDAN SU, CHUANSHAN TIAN, Fudan University, STATE KEY LABORATORY OF SURFACE PHYSICS, DEPARTMENT OF PHYSICS, FUDAN UNIVERSITY TEAM — How ions occupy themselves at hydrophobic interface plays a key role in physical, chemical, atmospheric, and biological processes. However, hydrophobic molecules often gather together on water surface, thus few experiment taking on the adsorption of hydrophobic molecules on aqueous solutions from vapor phase. In this work, we report unexpected mutually promoted adsorption of hydrophobic molecules and ions through unification of contact angle method and sum frequency vibrational spectroscopy (SFVS). We observe oil tends to spread on solutions with higher pH, implying interaction exists between hydrophobic molecules and ions. SFVS suggests that this phenomenon stems from relatively strong Coulomb interaction between hydrophobic molecule and hydroxide ions, the initial hydroxide ion adsorption free energy is calculated. The surface charge density induced at the interface is plotted to show the variation of surface charge density with both hydroxide ion molar fraction and hexane vapor pressure. In addition, we propose a new perspective on explanation of intensity decay of icelike band at high pH (>10) aqueous solution, hydrophobic interfaces, in which the relative relation between Debye length and coherence length plays an essential role.

Thursday, March 5, 2015 11:15AM - 2:15PM — Session T28 GMAG DMP FIAP: Focus Session: Spin-Hall Effect II

11:15AM T28.00001 Spin Hall Effect in Spin Glass Systems, YASUHIRO NIIMI, Univ of Tokyo-Kashiwanaga — The spin Hall effect (SHE) and its inverse play important roles in spintronics devices as they enable interconversions between charge and spin currents. The conversion efficiency, i.e., the spin Hall angle, strongly depends on detailed material properties, such as the electronic band structure and the nature of impurities. While most of the work has focused on the mechanism of the SHE and the magnitude of the spin Hall angle, there are only a few examples to utilize the SHE such as current generated by the SHE is much more sensitive to magnetization measurements.

11:51AM T28.00002 Scaling of the Anomalous Hall Effect in the Low Conductivity Regime³. FRANCES HELLMAN, UC Berkeley Physics Department, JULIE KAREL², UC Berkeley Materials Science and Engineering Department, CATHERINE BORDEL, SIMCA BOUMA, HYEON-JUN LEE, UC Berkeley Physics Department, MATERIALS SCIENCE DIVISION, LAWRENCE BERKELEY NATIONAL LAB TEAM — Temperature-dependent resistivity, magnetization, magnetoresistance and Hall effect were measured in amorphous and epitaxial Fe₇₀Si₃₀ thin films. The resistivity increases as x is decreased, and changes in the temperature coefficient of resistivity (α) are observed with variation in both structure and composition. All films are ferromagnetic and display an anomalous Hall effect (AHE). AHE of the amorphous films is 10 times larger than crystalline films of the same composition. The epitaxial films display a scaling behavior consistent with the intrinsic AHE mechanism. The AHE in the low conductivity regime (amorphous films) shows a scaling with conductivity similar to that seen in low conductivity GaMnAs films despite much larger disorder and carrier concentration in the amorphous films. Amorphous FeₓSi₁₋ₓ in this range of x however is notably not in the insulating hopping regime but is instead a strongly disordered metal, a regime that lacks theoretical understanding of AHE.

12:03PM T28.00003 Anomalous Hall effect and persistent current due to spin chirality in a diffusive regime. KAZUKI NAKAZAWA, HIROSHI KOHNO, Department of Physics, Nagoya University, CONDENSED-MATTER THEORY TEAM — It is known that a non-coplanar spin configuration having spin chirality gives a Berry phase to electrons through the exchange interaction, leading to anomalous Hall effect (AHE). Tatara and Kawamura showed that AHE can result without the concept of Berry phase by treating the exchange coupling perturbatively in a model with discretely distributed spins [1]. Recently, we reexamined the AHE in the same model by considering vertex corrections due to normal impurities [2]. This amounts to electron’s diffusive motion and spin conservation at the scattering from normal impurities, and leads to the expression of AHE conductivity which satisfies spin conservation. We also investigated a persistent current around the spin chirality as a physical origin of the AHE response, and we found that the “typical” value of the persistent current reproduces the AHE conductivity in the diffusive regime.

12:15PM T28.00004 Planar Hall effect (PHE), anisotropy magnetoresistance (AMR), and anomalous Hall effect (AHE) in perpendicularly magnetized synthetic ferromagnets, SEE-HUN YANG, IBM Almaden Research Center, PRISCILA BARBA, AURELIEN MANCHON, KAUST, STUART PARKIN, IBM Almaden Research Center — Chiral spin torque driven domain wall motion (CIDW/M) faster than 300 m/s along the current direction has been reported in perpendicularly magnetized atomically thin Co/Ni bilayers deposited on Pt underlayers [1], making these materials promising for DW-based memory and logic devices. Moreover, most recently even more efficiently domain motion (~ 750 m/s) has been observed from synthetic antiferromagnetic (SAF) racetracks with almost compensated magnetization [2]. In this talk we will present Hall measurement results from SAF Hall bars that exhibit characteristic planar Hall effect and anomalous Hall effect. We discuss the origin of these behaviors.


12:27PM T28.00005 Phase-Sensitive Detection Of The AC Inverse Spin Hall Effect, MATHIAS WEILER, National Institute of Standards and Technology — Spin pumping [1] is a significant source of damping in ultrathin ferromagnet/normal metal bilayers. In these structures, the magnetization relaxation is enhanced via the diffusion of spin currents across the bilayer interface. The pumped spin currents have both a small dc and dominant ac contributions. The nonlinear dc spin current contribution that arises in ferromagnetic resonance (FMR) has been extensively studied in electrical dc measurements that are enabled by means of the inverse spin Hall effect (ISHE) in the normal metal [2]. The ac charge voltage generated in FMR due to the ac ISHE should be linear in the magnetization precession and thus much larger than the corresponding dc voltage for small precession cone angles [3]. However, any measurement of the ac iSHE voltage needs to take the linear inductive voltages due to Faraday’s law into account, as magnetization dynamics in ferromagnet/normal metal bilayers result in both, inductive and possible ac iSHE voltages. These voltage signals are always superimposed and cannot be separated in a measurement scheme that is only sensitive to the magnitude of the signal [4-7]. Moreover, inductive and ac ISHE voltages are estimated to be of the same order of magnitude for typical nm-thick ferromagnetic layers in contact with Pt and share identical symmetry with respect to magnetization orientation. The only qualitative difference between inductive and ac ISHE voltages is their expected phase difference of π/2. We thus use a phase-sensitive, quantitative technique to separate inductive and ac ISHE signals in a variety of Ni$_81$Fe$_{19}$/normal metal thin film bilayers at room temperature. All samples show the expected behavior in terms of damping and dc iSHE voltages from which we find a dc spin Hall angle Θ$_{SH}$=0.1 for Pt [8]. Our ac iSHE experiments [9] are carried out using Ni$_81$Fe$_{19}$/normal metal bilayers deposited simultaneously with the dc structures. Using Ta, W, Pd, Cu or Nb as the normal metal, we find that the inductive contribution dominates over any ac iSHE signal, in agreement with simple estimates based on the extracted dc spin Hall angles for these materials. However, for Pt, we find a surprisingly large ac iSHE contribution that has a significantly different phase than expected. Similar results are also found in Ni$_81$Fe$_{19}$/Cu/Pt trilayers, excluding the possibility of an interfacial origin of the large ac iSHE signal. Modeling of our experimental results in the context of the ac iSHE requires a complex-valued spin Hall angle Ψ$_{SH}$ of Pt with Θ$_{SH}$≈ 1 and arg (Θ$_{SH}$)≈ 110° in the investigated frequency range of 7 to 20 GHz.


1:03PM T28.00006 Skew-scattering contribution to anomalous and spin Hall effects in dilute ferromagnetic alloys, BERND ZIMMERMANN, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — The spin Hall effect (SHE) possesses great potential for the generation of pure spin currents, but it is difficult to measure directly. The closely related anomalous Hall effect (AHE) is much easier to access in experiment via a finite Hall voltage. Phenomenologically, the only difference between the two effects is the ferromagnetic order needed for the AHE. In this work [1], we investigate the skew-scattering contribution to the AHE in dilute ferromagnetic alloys from first principles. We compare three state-of-the-art methods and analyze chemical trends by considering 3d impurities in bcc-Fe, as well as magnetic 3d impurities in fcc Pd, Pt and Au. We arrive at general rules to obtain a large anomalous Hall angle, which represents an efficiency for the conversion of a longitudinal into a transverse current. Moreover, we reveal a clear correlation between the AHE and SHE in the alloy s which are based on a nonmagnetic host material.


1:15PM T28.00007 Epitaxial IrMn3 on MgO(111) by sputter deposition, ALEJANDRO JARA, IGOR BARSUKOV, YU-JIN CHEN, BRIAN YOUNGBLOOD, Univ of California - Irvine, JOHN READ, PATRICK BRAGANCA, HGST, San Jose CA, USA, ILYA KRIVOROTOV, Univ of California - Irvine — Antiferromagnets are promising systems for spintronic applications due to the absence of stray fields and high spin wave group velocity. Coupling between the charge and spin degrees of freedom in metallic antiferromagnets is a topic of high interest. The chemically ordered compensated antiferromagnet IrMn3 has recently been predicted to show anomalous Hall effect (AHE) arising from its noncollinear spin configuration. The AHE would provide a unique opportunity to probe the order parameter of an antiferromagnet via direct electrical measurements, which should be of tremendous utility for antiferromagnetic spintronics. To quantify and further exploit AHE, IrMn3 must be grown in the L12 phase, which supports ordering of the Mn spins on stacked sheets of Kagome spin lattices. Here we present an experimental study of IrMn3 thin films grown on MgO(111) by sputter deposition. We carry out XRD measurements and identify two quasi-epitaxial phases rotated by 60 deg to each other in the film plane. The IrMn3 is strongly (111)-textured with the (111) axis deviating by less than 2 degrees from the film normal due to oblique deposition of the material. The grain size in our films is determined to be 15 nm, while the dimensionless chemical order parameter of the L12 phase is found to be 0.4.

1:27PM T28.00008 Spin Hall effects in CuAu-I-type metallic antiferromagnets, WEI ZHANG, BENJAMIN JUNGFLEISCH, WANJUN JIANG, JOHN PEARSON, AXEL HOFFMANN, Argonne National Laboratory, FRANK FREimuth, YURIY MOKROUSOV, Forschungszentrum Jülich — We investigated the spin Hall effect of CuAu-I-type metallic antiferromagnets by using spin pumping — inverse spin Hall effect via a coplanar waveguide ferromagnetic resonance broadband technique. By studying the ratio of the two voltage components (anisotropic magnetoresistance and inverse spin Hall effect) with the metal layer thickness, the spin diffusion lengths of the materials are directly extracted, which further allows the determination of the spin Hall angle. We performed such analysis for polycrystalline FeMn, PdMn, IrMn, and PtMn. In particular, PtMn showed large spin Hall effect that is comparable to Pt. First principle calculations of the intrinsic spin Hall effect reproduce these results. We also demonstrate the epitaxial growth of these metallic crystals and its influence to the spin Hall effects due to different crystalline orientation. This work highlights the importance of both spin-orbit coupling and the magnetic ordering to the spin Hall effects of metals. W. Zhang, et al., Phys. Rev. Lett. 113, 196602 (2014)

1This work was supported by the U.S. DOE Office of Science, Materials Sciences and Engineering Division and by DFG.
1:39PM T28.00009 Probing the Inverse Spin Hall Effect and Spin-Orbit Coupling in a Broad Range of Transition Metals by $Y_3Fe_5O_{12}$-Based Spin Pumping. HAILONG WANG, CHUNHUI DU, P. CHRIS HAMMEL, FENGYOU YANG, The Ohio State University — Spin-orbit coupling (SOC) is the underlying mechanism for spin Hall physics and it is generally believed that SOC follows $Z^2$ (atomic number) dependence and becomes significant only in heavy elements. We report FMR spin pumping from 20-nm $Y_3Fe_5O_{12}$ (YIG) films into a series of 3d, 4d, and 5d transition metals. We observe surprising large mV-level inverse spin Hall effect (ISHE) voltages in Pt, Ta, W, and Cr and robust ISHE signals in other metals. Using the ISHE voltages and damping enhancement, we determine the spin Hall angles and interfacial spin mixing conductances for these metals. Both 3d and 5d metals exhibit systematic behavior of the spin Hall angle, which reveals the critical role of $d$-electrons in SOC. Our result enriches the understanding of ISHE and broadens the scope of materials available for exploring the rich phenomena enabled by SOC as well as presenting a guidepost for testing theoretical models of SOC in transition metals.

1:51PM T28.00010 Inverse spin Hall effect in Cr metal. DANRU QU, Johns Hopkins University, SSU-YEN HUANG, National Taiwan University, CHIA-LING CHIEN, Johns Hopkins University — Spin Hall angle, which measures the conversion efficiency between spin current and charge current, is the most important quantity in spin current phenomena. Sizable spin Hall angles have thus far been reported exclusively in non-magnetic materials of heavy elements, such as Pt and Au, and recently in ferromagnetic metals, such as Py. In this work, we use the thermal spin injection method to inject a spin current from ferromagnetic insulator YIG into a 3d metal Cr, which is a well-known antiferromagnet (AF) with spin density ordering. We report the observation of inverse spin Hall effect (ISHE) in Cr with a large spin Hall angle, comparable to that of Ta. Through measurements above and below the Neél temperature of the AF ordering, we show that the origin of the large ISHE in Cr is not due to its spin density wave AF ordering. Moreover, there is no magnetic proximity effect that plagued Pt and Ta. These features show that Cr can be a superior spin current generator/detector in pure spin current phenomena and devices. [1] D. Qu, S. Y. Huang, B. F. Miao, S. X. Huang, and C. L. Chien, Phys. Rev. B 89, 140407(R) (2014). [2] B. F. Miao, S. Y. Huang, D. Qu and C. L. Chien, Phys. Rev. Lett. 111, 066602 (2013)

2:03PM T28.00011 Towards the terahertz frequency measurement of the Inverse Spin Hall Effect. EVAN V. JASPER, M. T. WARREN, T. T. MAI, J. BRANCHAM, H. WANG, J. GALLAGHER, F. YANG, R. VALDÉS AGUILAR, Center for Emergent Materials, Department of Physics. The Ohio State University. Columbus, OH 43210 — The Inverse Spin Hall Effect (ISHE) has become an important tool in the spintronics field as a promising route for generation and detection of spin currents via charge currents. In particular, when the magnetization of a ferromagnet is resonantly excited by a radio-frequency field, angular momentum can be transferred to a non-magnetic metal to produce a pure spin current (spin-pumping), and the ISHE provides a way to measure the generated spin current in the metal and extract essential spin pumping parameters. Very recently, theoretical predictions of spin pumping from an antiferromagnetic (AF) insulator to a normal metal have attracted significant interest. We will report results of experiments where terahertz pulses of electromagnetic radiation resonantly excite the AF resonance on the AF insulator NiO coupled with a thin film of Pt, and attempt to measure the ISHE voltage at terahertz frequencies.

Thursday, March 5, 2015 11:15AM - 2:15PM – Session T29 GMAG: Correlated Electron Magnetism II

11:15AM T29.00001 Onset of ferromagnetism in EuB$_6$. NICHOLAS BUTCH, NIST - Natl Inst of Stds & Tech, I-LIN LIU, XIAOHANG ZHANG, University of Maryland, College Park, KATHRYN KRYCKA, JEFFREY LYNN, DANIEL PARSHALL, WILLIAM RATCLIFF, YANG ZHAO, NIST - Natl Inst of Stds & Tech, PRISCILLA ROSA, ZACHARY FISK, UC Irvine — We assess the magnetic experimental signatures of precursor magnetic polarons and characterize the ferromagnetic ordering transition in EuB$_6$. The results of bulk magnetometry and neutron scattering measurements will be discussed.

11:27AM T29.00002 High-pressure magnetotransport measurements of the semimetallic ferromagnet EuB$_6$. DANIELLE SIMMONS, LIUQI YU, STEPHAN VON MOLNAR, PENG XIONG, Florida State University, JUN ZHU, CONG REN, Institute of Physics, Chinese Academy of Sciences, ZACHARY FISK, University of California, Irvine — Hall effect measurements on EuB$_6$ have revealed manifestations of the microscopic electronic phase separation and resulting percolative phase transition in a macroscopic magnetotransport property of this semimetallic ferromagnet: the Hall resistivity as a function of applied field in the paramagnetic phase exhibits two distinct linear regions with a transition point at a single critical magnetization in a broad temperature range, which was interpreted as the percolation point for the more conducting phase. To further understand this phenomenon, magnetotransport measurements were performed on EuB$_6$ under high pressure. Hydrostatic pressure is known to substantially modify the magnetic state of EuB$_6$. EuB$_6$ single crystals were inserted in a high-pressure cell filled with silicone oil and measurements were taken at different pressures up to 1.8 GPa. Increasing hydrostatic pressure caused a decrease in resistivity and an increase in $T_H$, while the ferromagnetic ordering temperature stayed approximately constant. The Hall resistivity in the paramagnetic phase developed an intermediate region between the two previously observed regions. The transition fields between the low-field and intermediate regions depend linearly on temperature and their intercepts increase with pressure similar to the variation of $T_H$ indicated by the resistivity peak. [1] X. H. Zhang et al, Phys. Rev. Lett. 103, 106602 (2009). [2] J.C. Cooley et al, Phys. Rev. B 56, 14541 (1997).

1:39AM T29.00003 Interplay of many-body and single-particle interactions in iridates and rhodates. YURIY SIZYUK, NATALIA PERKINS, Univ of Minn - Minneapolis, PETER WOLFLE, Institute for Condensed Matter Theory and Institute for Nanotechnology, Karlsruhe Institute of Technology — Motivated by recent experiments exploring the spin-orbit-coupled magnetism in 4d- and 5d-band transition metal oxides, we study magnetic interactions in Ir- and Rh-based compounds. In these systems, the comparable strength of spin-orbit coupling (SOC), crystal field splitting (CF) and Coulomb and Hund’s coupling leads to a rich variety of magnetic exchange interactions, leading to new types of ground states. Using a strong coupling approach, we derive effective low-energy super-exchange Hamiltonians from the multi-orbital Hubbard model by taking full account of the Coulomb and Hund’s interactions in the intermediate states. We find that in the presence of strong SOC and lattice distortions the super-exchange Hamiltonian contains various kinds of magnetic anisotropies. Here we are primarily interested in the magnetic properties of Sr$_2$IrO$_4$ and Sr$_2$Ir$_{1-x}$Rh$_x$O$_4$ compounds. We perform a systematic study of how magnetic interactions in these systems depend on the microscopic parameters and provide a thorough analysis of the resulting magnetic phase diagram. Comparison of our results with experimental data shows good agreement. [1] J.C. Cooley et al, Phys. Rev. B 56, 14541 (1997).
11:51AM T29.00004 Impact of spin-orbit coupling on the magnetism of Sr$_3$MIrO$_6$ (M = Ni, Co) , XUEDONG OU, HUA WU, Fudan University, LABORATORY FOR COMPUTATIONAL PHYSICAL SCIENCES TEAM — Recently, Iridates have recently drawn considerable attention due to their significant spin-orbit coupling (SOC) effect and possibly exotic properties [1]. In this work, we demonstrate, using density functional calculations, that the SOC of Ir$^{4+}$ ions plays an essential role in determining the antiferromagnetism of hexagonal spin-chain materials Sr$_3$MgIrO$_6$ (M=Ni, Co) by tuning the crystal-field level sequence and altering the Ir-M inter-orbital interactions. Owing to the SOC effect, the single t$_{2g}$ hole of the Ir$^{4+}$ ion resides on the e$_g$ upper branch and gives rise to the Ir$^{4+}$-M$^{2+}$ antiferromagnetic coupling. In absence of the SOC, however, the single t$_{2g}$ hole would occupy the crystal-field a$_{1g}$ singlet instead, which would mediate an unreal ferromagnetic exchange This work clarifies the nature and the origin of the intra-chain Ising antiferromagnetism of Sr$_3$MgIrO$_6$ (M = Ni, Co) [2].


12:03PM T29.00005 LDA+DMFT Approach to Magnetocrystalline Anisotropy of Strong Magnets , JIAN-XIN ZHU, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, MARC JANOSCHEK, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, RICHARD ROSENBERG, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA, FILIP RONNING, J.D. THOMPSON, MICHAEL A. TORREZ, ERIC D. BAUER, CRISTIAN D. BATISTA, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — The new challenges posed by the need of finding strong rare-earth-free magnets demand methods that can predict magnetization and magnetocrystalline anisotropy energy (MAE). We argue that correlated electron effects, which are normally underestimated in band structure calculations, play a crucial role in the development of the orbital component of the magnetic moments. Because magnetic anisotropy arises from this orbital component, the ability to include correlation effects has profound consequences on our predictive power of the MAE of strong magnets. Here we show [1] that incorporating the local effects of electronic correlations with dynamical mean-field theory provides reliable estimates of the orbital moment, the mass enhancement and the MAE of YCo$_5$.


12:15PM T29.00006 Quantum Indian Rope Tricks: Fluctuation driven magnetic hard-axis ordering in metallic ferromagnets , FRANK KRUGER, CHRIS PEDDER, ANDREW GREEN, London Centre for Nanotechnology, UCL — We demonstrate that the interplay between soft electronic particle-hole fluctuations and magnetic anisotropies can drive ferromagnetic moments to point along a magnetic hard axis. As a proof of concept, we show this behavior explicitly for a generic two-band model with local Coulomb and Hund’s interactions, and a spin-orbit-induced easy plane anisotropy. The phase diagram is calculated within the fermionic quantum order-by-disorder approach, which is based on a self consistent free-energy expansion around a magnetically ordered state with unspecified orientation. Quantum fluctuations render the transition of the easy-plane ferromagnet first-order below a tricritical point. At even lower temperatures, directionally dependent transverse fluctuations dominate the magnetic anisotropy and the moments flip to lie along the magnetic hard axis. We discuss our findings in the context of recent experiments that show this unusual ordering along the magnetic hard direction.


12:27PM T29.00007 New mechanism of kinetic exchange interaction induced by strong magnetic anisotropy , NAOYA IWAHARA, LIVIU CHIBOTARU, Theory of Nanomaterials Group, Katholieke Universiteit Leuven — It is well known that the kinetic exchange interaction between single-occupied magnetic orbitals (s-s) is always antiferromagnetic, of the order $-t^2/U$, where $t$ is the transfer parameter and $U$ is the electron promotion energy. At the same time the exchange interaction between single- and double-occupied orbitals, s-d, is always ferromagnetic, of the order $t^2U/JU$, where $J$ is the Hund’s rule coupling parameter ($|J/U| \approx 0.1$). Here we show that the exchange interaction between ground doublet states of lanthanide or actinide ions is characterized by equal in magnitude s-s and s-d kinetic exchange interactions, both scaling as $\sim t^2/U$ [1]. Moreover, the s-d kinetic mechanism prevails in many situations, contributing to antiferromagnetic coupling in the case of collinear magnetic ions. In the non-collinear case the s-d kinetic mechanism can cause an overall ferromagnetic exchange interaction of the order of $t^2/U$, already for the angle $\sim \pi/2$ between the main magnetic axes on sites, which appears quite counter-intuitive. This new s-d kinetic mechanism is not operative in the case of exchange interaction between strongly anisotropic magnetic doublets and an isotropic spin.


12:39PM T29.00008 ABSTRACT WITHDRAWN —

12:51PM T29.00009 First-Order Magnetostuctural Phase Transition in AlFe$_2$B$_2$ , BRIAN LEJEUNE, RADHIKA BARUA, Department of Chemical Engineering, Northeastern University, Boston, MA 02115, ENRIC STERN-TAULATS, LLUIS MANOSA, ANTONI PLANES, Departament d’Estructura i Constituents de la Matèria, Facultat de Física, Universitat de Barcelona, 08028 Barcelona, Catalonia, POL LLOVERAS, Departament de Física i Enginyeria Nuclear, ETSEIB, Universitat Politècnica de Catalunya, 08028 Barcelona, Catalonia, L.H. LEWIS, Departament d’Estructura i Constituents de la Matèria, Facultat de Física, Universitat de Barcelona, 08028 Barcelona, Catalonia — Understanding correlations between composition and crystal structure is key to tailoring the response of functional magnetic materials. In particular, the ferromagnetic AlFe$_2$B$_2$ compound with the layered AlMn$_2$B$_2$-type structure is reported to exhibit a magnetic transition of relevance for magnetocaloric cooling, with a reported entropy change $\Delta S \sim 4J/\text{kg} \cdot K$ at an applied magnetic field of 2 T [1].[2] New results derived from magnetic, structural and calorimetric probes confirm a thermodynamically first-order magnetic phase change in AlFe$_2$B$_2$ in the vicinity of the Curie temperature of $\sim 300$ K. The transformation from the ferromagnetic to the paramagnetic state is accompanied by a non-uniform 1% unit cell volume expansion upon heating, signifying that application of magnetic field is anticipated to have a similar effect (stabilizing the ferromagnetic phase) as the application of chemical or hydrostatic pressure. Relevant barocoralic effects are expected in this compound.


[2] 12:03PM T29.00010 Pressure tuning of itinerant magnetism in Mo$_5$Sb$_7$ , YISHU WANG, Univ of Chicago, JINGJUN CHENG, Chinese Academy of Sciences, ALEXANDER PALMER, DANIEL SILEVITCH, THOMAS ROSENBAUM, Univ of Chicago, JIAQIANG YAN, BRIAN SALES, Oak Ridge National Laboratory, YOSHIYA UWATOKO, University of Tokyo, YEJUN FENG, Argonne National Laboratory — Mo$_5$Sb$_7$ is a recently discovered itinerant antiferromagnet with a magnetic phase formed by spin dimerization at 53 K and ambient pressure, followed by a 2.3 K superconducting phase. In concert with the dimer pairing of S=1/2 Mo ions, a contraction of the crystalline lattice breaks the cubic symmetry. Here we use both high pressure x-ray single crystal diffraction and electrical transport techniques to investigate the magnetic behavior and map out the Pe-T phase diagram of Mo$_5$Sb$_7$. Our results demonstrate that the magnetic phase is eventually suppressed by high pressure, where the lattice structure returns to cubic. The disappearance of the antiferromagnetic phase in Mo$_5$Sb$_7$ could influence the evolution of the superconducting state.
Au faster than the superexchange interaction, favoring a spin-spiral state. For realistic values of double exchange. We find that, contrary to earlier reports, the ground state in standard density functional theory is ferromagnetic, induced by a competition between the short-range antiferromagnetic exchange and a long-range interaction induced by the polarization of Au bands, similar to double exchange. We find that, contrary to earlier reports, the ground state in standard density functional theory is ferromagnetic, whereas the other compounds order antiferromagnetically. Preliminary studies on single crystals of SmCuGa indicate that the spiral state is still not clear. The spiral cannot be explained via relativistic effects due to the short pitch of the spiral and the weakness of the spin-orbit interaction in LnCuGa, with the largest being 16% in Ce at only 0.7 GPa but 6% in Dy at 73 GPa, possibly a sign that the magnetic state has become unstable. Recent electrical resistivity measurements on Dy reveal a highly non-monotonic dependence of $T_c$ on pressure. Immediately above $P_{cr}, T_c(P)$ in Dy shows a dramatic increase, extrapolating to values near 400 K at 160 GPa (1.6 Mbar). Interestingly, the pressure dependence of the magnetic spin-disorder resistivity $\rho_{sd}(P)$ tracks that of $T_c(P)$.

2:17PM T29.00013 CF excitations of CeCu$_2$Si$_2$: Revisited employing a single crystal and triple-axis spectrometers, MICHAEL LOEVENHAPPT, Tech Univ Dresden, SERGEY DANILKIN, GUOCHU DENG, ANSTO, KLAUDIA HRADIL, TU Wien, OLIVER STOCKERT, MPI-CPS, ASTRID SCHNEIDEWIND, JCNS-MLZ — CeCu$_2$Si$_2$ is the famous heavy-fermion system showing unconventional superconductivity mediated by low-energy magnetic excitations of the CF ground-state doublet. From the point symmetry of the Ce$^{3+}$ ions in the tetragonal crystal lattice a CF splitting into 3 doublets is expected for the (J=5/2) multiplet. First INS measurements on polycrystalline samples of CeCu$_2$Si$_2$ employing a time-of-flight technique revealed a CF level scheme of 0-12-30 meV but were disputed by more advanced INS data in subsequent years. Finally it was accepted that the CF excitations of CeCu$_2$Si$_2$ consist of only one very broad transition with 30 meV from the ground-state doublet to both of the more or less degenerated excited CF states, the so-called “quasi-quartet.” Employing a large single crystal of CeCu$_2$Si$_2$ and the thermal neutron triple-axis spectrometers PUMA at FRM II and TAIPIAN at OPAL we revisited the CF-transitions to verify or falsify this interpretation. We performed TAS measurements for different crystallographic directions. From our results we infer that the quasi-quartet actually consists of two doublets situated at 30 and 35 meV exhibiting a strong directional dependence of their transition matrix elements to the ground state doublet.

1:51PM T29.00014 Magnetism and magnetic ordering in LnCuGa$_3$ ($\text{Ln} =$ lanthanide), MICHAEL GRAF, RYAN POLISCHUK, MARKIAN BOJKO, STEPHEN TRUDEAU, ELENI HUGHES, REBECCA DALLY, Boston College, UDUMULA SUBBARAO, SEBASTIAN PETER, Jawaharlal Nehru Centre for Advanced Scientific Research — We report structural characterization and magnetization and transport measurements on LnCuGa$_3$ ($\text{Ln} =$ La, Ce, Pr, Nd, Sm, Eu, and Gd) intermetallics. Magnetization in fixed field was measured for high quality polycrystalline samples at temperatures between 1.8 and 300 K, along with the isothermal variation of magnetization with field, while the temperature dependent resistivity was measured down to $T = 0.3$ K. All members of this family, except for the PrCuGa$_3$ and non-magnetic LaCuGa$_3$ compounds, exhibit magnetic ordering above 1.8 K at temperatures ranging from 2 K (CeCuGa$_3$) to 75 K (EuCuGa$_3$). The Eu and Sm based compounds exhibit multiple magnetic transitions. SmCuGa$_3$ appears to be ferromagnetic, whereas the other compounds order antiferromagnetically. Preliminary studies on single crystals of SmCuGa$_3$ indicate that the ordered moments lie parallel to the $c$-axis in the low temperature magnetically ordered phase of this tetragonal system.

1:39PM T29.00011 Possible Correlation-Enhanced Magnetic Ordering at Anomalously High Temperatures in Dy under Extreme Compression, JINHYUK LIM, Washington University in St. Louis, GILBERTO FABBRIX, Argonne National Lab/Washington University in St. Louis, DANIEL HASKEL, Argonne National Lab, JAMES SCHILLING, Washington University in St. Louis — Most lanthanides order magnetically at temperatures $T_c$, well below ambient, the highest being 292 K for Gd. The highly localized magnetic state of the heavy lanthanoids should become unstable at sufficiently high pressure, leading to a competition between the RKKY interaction and Kondo physics. Most lanthanoids undergo a volume collapse at a critical pressure $P_{cr}$, the largest being 16% in Ce at only 0.7 GPa but 6% in Dy at 73 GPa, possibly a sign that the magnetic state has become unstable. Recent electrical resistivity measurements on Dy reveal a highly non-monotonic dependence of $T_c$ on pressure. Immediately above $P_{cr}, T_c(P)$ in Dy shows a dramatic increase, extrapolating to values near 400 K at 160 GPa (1.6 Mbar). Interestingly, the pressure dependence of the magnetic spin-disorder resistivity $\rho_{sd}(P)$ tracks that of $T_c(P)$. The results of parallel experiments on Gd and further heavy lanthanoids will also be presented.

2:03PM T29.00015 Magnetic spiral induced by strong correlations in MnAu$_3$, JAMES GLASBRENNER, NRC/NRL, KONRAD BUSSMANN, IGOR MAZIN, NRL — The compound MnAu$_3$ is one of the oldest known spin-spiral materials, yet the nature of the spiral state is still not clear. The spiral cannot be explained via relativistic effects due to the short pitch of the spiral and the weakness of the spin-orbit interaction in Mn, and another common mechanism, nesting, is ruled out as direct calculations show no features at the relevant wave vector. We propose that the spiral state is induced by a competition between the short-range antiferromagnetic exchange and a long-range interaction induced by the polarization of Au bands, similar to double exchange. We find that, contrary to earlier reports, the ground state in standard density functional theory is ferromagnetic, i.e., the latter interaction dominates. However, an accounting for Coulomb correlations via a Hubbard $U$ suppresses the Schrieffer-Wolff type $s-d$ magnetic interaction between Mn and Au faster than the superexchange interaction, favoring a spin-spiral state. For realistic values of $U$ the resulting spiral wave vector is in close agreement with experiment.

Thursday, March 5, 2015 11:15AM - 2:15PM — Session T30:GMAG DMP: Focus Session: Exchange Spring Magnets and Multilayers
11:15AM T30.00001 Depth dependent magnetization profiles of hybrid exchange springs , R. KNUT, Uppsala University - Sweden, T-N. ANH NGUYEN, S. CHUNG, Q. TUAN LE, S.M. MOHSEN, Royal Institute of Technology - Sweden, V. FALLAH, Amirkabir University of Technology - Iran, S. PERDEKOV, Lund University - Sweden, O. KARIS, Uppsala University - Sweden, R.K. DUMAS, University of Gothenburg - Sweden, C.W. MILLER, Rochester Institute of Technology - USA, J. AKERMAN, Royal Institute of Technology - Sweden — We report on the magnetization depth profile of a hybrid exchange spring system in which a Co/Pd multilayer with perpendicular anisotropy is coupled to a CoFeB thin film with in-plane anisotropy. Such materials allow for additional control of the magnetization dynamics in magnetic nanostructures, and suggest the possibility of improved spin transfer torque-MRAM switching behavior and thermal stability. The competition between these two orthogonal anisotropies promotes a strong depth dependence of the magnetization orientation. The angle of the magnetization vector is sensitive both to the strength of the individual anisotropies and to the local exchange constant, and is thus tunable by changing the thickness of the CoFeB layer and by substituting Ni for Pd in one layer of the Co/Pd stack. The resulting magnetic depth profiles are directly probed by element-specific x-ray magnetic circular dichroism of the Fe and Ni layers located at different average depths. The experimental results are corroborated by micromagnetic simulations.

11:27AM T30.00002 Quadratic magneto-optical Kerr effect and chirality of magnetization reversal in Py/SmFe/Py exchange spring magnet thin films , JIYEONG GU, HANNING YUAN, California State University, Long Beach — Magnetic switching behavior of the exchange spring magnet, Py(Permalloy)/SmFe/Py thin films, was investigated by magneto-optical Kerr effect (MOKE). Exchange spring magnet shows a unique magnetic hysteresis loop due to the non-collinear magnetization developed by magnetic coupling of the soft and hard magnetic layers. Py/SmFe/Py thin films were deposited on silicon substrate by DC magnetron sputtering. Experimental Kerr rotation measurement showed asymmetric hysteresis loops as a result of superimposed quadratic MOKE (QMOKE) contribution to linear MOKE (LMOKE). Overall MOKE signal was separated into LMOKE and QMOKE signals using loop symmetrization and antisymmetrization operation. The longitudinal ($M_z$) and transverse ($M_T$) magnetization components with respect to the plane of light incidence were extracted and QMOKE signal was simulated from the two mixed terms, $M_z$ and $M_T$. QMOKE signal not only showed the nature of magnetization reversal in exchange spring magnet system from the information of $M_T$ at switching field but also determined the direction of magnetization rotation from the positions of the peaks. Our work demonstrated that the chirality of magnetization reversal can be determined from analysis of QMOKE signal.

11:39AM T30.00003 Nanoscale Engineering Toward Bulk Exchange-Spring Permanent Magnetic Fe/MnAl Nanocomposites , LUK G. MARSHALL, IAN J. MCDONALD, LAURA H. LEWIS, Department of Chemical Engineering, Northeastern University, Boston, MA 02115, USA — The ability to amplify the performance of exchange-spring nanocomposites through correlation and tailoring of chemical order, microstructural scale and magnetic response is necessary for the development of novel high-performance permanent magnets. To this end, rapid solidification of near-equiatomic MnAl for incorporation into the model exchange-spring Fe/MnAl system has produced alloys containing 20-30% ferromagnetic Fe/MnAl with the high-temperature parent hexagonal $\alpha$-MnAl phase composing the balance. While typically formed by briefly annealing the quenched $\alpha$-phase, this work has confirmed direct attainment of nanoscale $\tau$-MnAl via cryogenic milling. Magnetic and structural data indicate a significantly decreased chemical order accompanied by increased lattice strain with increased milling time. Control of the chemical order and nanostructure of near-equiatomic MnAl will favor metastable configurations to foster robust exchange coupling between $\tau$-MnAl and $\alpha$-Fe to create high performance magnetic nanocomposites.

1This work is supported by the U.S. Office of Naval Research and the U.S. Army Research Office.

11:51AM T30.00004 Micromagnetic Modeling of Reversal Nucleation in Core/Shell Exchange-Spring Structures , J.S. JIANG, SAM BADER, Argonne National Laboratory — Nanocomposite exchange-spring permanent magnet materials promise superior performance and are a potential solution to the supply criticality of rare earth elements [1]. The nucleation of magnetization reversal in cylindrical and spherical soft core/hard shell exchange-spring structures has been investigated by solving the linearized Brown’s equation perturbatively, and has been verified with numerical simulations [2]. Accounting for the magnetostatic self-interaction field leads to a modification to the proposed quasi-coherent “bulging” mode of nucleation for small core sizes. The modified curling mode, where the magnetization configuration is vortex-like and flux-closed, becomes favored at large core sizes. The mode crossover occurs at a core diameter of approximately twice the exchange length for the cylindrical geometry. Since flux-closure allows magnetic elements to be densely packed without affecting the nucleation field, a potential direction for improving permanent magnet materials is to induce the modified curling mode by creating a soft-cylinder-in-hard-matrix exchange-spring microstructure.

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

12:03PM T30.00005 Fabrication and Characterization of MnBi/Co and MnBi/FeCo Nanocomposite Bulk Magnets , NARAYAN POUYDAL, KINJAL GANDHA, WEI WANG, XIAOTONG LIU, ZHAOGUO QIU, KEVIN ELKINS, JING LIU, Department of Physics, the University of Texas at Arlington, Texas 76019, USA; JUN CUI, Energy and Environment Directorate, Pacific Northwest National Laboratory, Richland, Washington 99352, USA, DEPARTMENT OF PHYSICS, THE UNIVERSITY OF TEXAS AT ARLINGTON, TEXAS 76019, USA TEAM, ENERGY AND ENVIRONMENT DIRECTORATE, PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WASHINGTON USA COLLABORATION — We report the fabrication of MnBi/Co and MnBi/FeCo nanocomposite bulk magnets by consolidating the hard and the soft phase powder particles under a magnetic field followed by subsequent sintering process. The anisotropic micro and submicron hard magnetic MnBi particles were first prepared by low energy cryo ball milling at liquid nitrogen temperature. MnBi/Co and MnBi/FeCo nanocomposite powders were then prepared by using different fraction of chemically synthesized Co nanowires and FeCo nanoparticles as the soft magnetic phase. The saturation magnetization ($M_s$) of the composite magnets increases with addition of the soft phase while the coercivity first increases and then decreases. The MnBi/Co and MnBi/FeCo nanocomposite bulk magnets have reached an enhanced magnetization value ($M_s = 78$ and 80.6 emu/g) with 30 wt. % of Co nanowires and FeCo nanoparticles, respectively compared to the single phase MnBi bulk magnet ($M_s = 52$ emu/g).

12:15PM T30.00006 ABSTRACT WITHDRAWN —
12:27PM T30.00007 Direct measurement of interlayer interaction in Permalloy/Gd nanodots\(^1\). PAVEL LAPA, Argonne National Laboratory, Texas A&M University, JUNJIA DING, VALENTINE NOVOSAD, AXEL HOFFMANN, Argonne National Laboratory — Antiferromagnetic interaction at the interfaces of ferromagnetic transition metals (TM) and Gd is well known phenomenon. However, quantitative description of this interaction still lack understanding. The main reason is that most experimental data were obtained by inspecting the hysteresis loops of TM/Gd multilayers. First, in plane domain structures of TM and Gd films complicates the description of the magnetization reversal process. Second, experimentally measured parameters are averaged over the domains obfuscating the microscopical picture. We make an effort to overcome these limitations by studying the magnetization reversal process of Permalloy/Gd nanodots. The dots were prepared by combination of optical lithography and magnetron sputtering. Experimentally it is observed that in these dots the antiferromagnetic interlayer interaction tunes magnetic vortex nucleation/annihilation fields. Rise of Gd magnetization at low temperature provides unusual temperature behavior of hysteresis loop. Micromagnetic models in which interlayer interaction energy acts as a fitting parameter is applied to simulate experimental hysteresis curves. The effect of nonmagnetic spacer between Permalloy and Gd is also considered and will be presented.

\(^1\)Supported by the Department of Energy Office of Science, Materials Science and Engineering Division.

12:39PM T30.00008 Detection of Magneto-Crystalline Anisotropy in YIG Films Formed by Aerosol Deposition. SCOOTER JOHNSON, E.R. GLASER, KONRAD BUSSMANN, FREDERICK RACHFORD, FRITZ KUB, CHARLES EDDY, JR., Naval Research Lab — We have employed aerosol deposition (AD) to form dense polycrystalline films of yttrium iron garnet (YIG) at room temperature in thicknesses of 0.3–11 \(\mu\)m onto \(\alpha\)-plane sapphire substrates. AD is a room-temperature process that accelerates a precursor of dry sub-micron-sized crystallites to impact and form a thick dense nano-crystalline film that is well-bonded to the substrate. We present results of ferromagnetic resonance (FMR) taken on the as-deposited films. In addition to the main resonance at 2815 G (in-plane) and 4650 G (out-of-plane) we find a distinct resonance mode \(H'_r\), that depends on film thickness. It appears in the 0.3-\(\mu\)m-thick film, becomes most intense in the 1-\(\mu\)m-thick film, and saturates for thicker films. \(H'_r\) moves with field orientation in the applied field from 4085 G (in-plane) to 3010 G (out-of-plane). FMR performed by rotating the applied field in the film plane shows that \(H'_r\) exhibits an anisotropy that reflects the crystallographic orientation of the substrate. These results suggest that during the early stages of growth a magneto-crystalline anisotropy is created in the interface region of the film that may be oriented to the crystallographic axis of the sapphire possibly caused by local heating that may facilitate recrystallization.

12:51PM T30.00009 The magnetism of TiN. BARBARA JONES, IBM Almaden Res Ctr, CHIUNG-YUAN LIN, SZU-WEN YANG, National Chiao Tung University, Taiwan, PUSHPA RAGHANI, Boise State University, SHRUBA GANGOPADHYYA, University of California Davis — Titanium Nitride is a well-known technological material, used typically in thin 3 micron coatings, in which form it is an extremely hard ceramic. It is the most common PVD coating used today. It shows no evidence of magnetism. We have studied isolated atoms of Ti on a Cu/N/Cu surface, layers of TiN on a Cu surface, and isolated monolayers of TiN, using first-principles density functional theory (DFT). In all of these geometries, TiN is magnetic, its interactions mainly governed by superexchange, resulting in striped magnetic structures. The question of how this dramatic magnetism disappears as more layers are added and TiN approaches bulk is one we have studied using DFT. We discuss the process by which the magnetism of TiN makes the transition between nanoscale and bulk.

1:03PM T30.00010 Role of Cu in exchange bias in FeMn revealed with neutron scattering\(^1\). IGOR V. ROSCHIN, PAVEL N. LAPA, Texas A&M Univ., ARTUR GLAVIC, HAILE AMBAYE, VALERIA LAUTER, Oak Ridge National Lab., SUNGYUN PARK, Pusan National U., TATIANA EGGERS, U. South Florida, CASEY W. MILLER, U. South Florida, Rochester Inst. of Technology — We observed an unusual behavior: a non-magnetic material, copper, modifies magnetic properties of antiferromagnetic FeMn in close proximity. Copper is responsible for the “intrinsic” exchange bias (EB) observed in a multilayered system without a distinct, separate ferromagnetic (FM) layer: Ta(5 nm)/\(\text{FeMn}(5-45\text{ nm})/\text{Cu}(5 \text{ nm})\)/\(\text{Ta}(5 \text{ nm})\) [1]. This EB occurs between pinned and unpinned uncompensated magnetization (UM) in the FeMn layers. The analysis of the remanent magnetization (\(M_r\)) shows that the unpinned (ferromagnet-like) UM is distributed individually throughout FeMn [1]. Since the magnitude of the EB loop shift (\(H_\theta\)) scales with the inverse thickness of the FeMn layer, this EB is clearly an interfacial phenomena. This behavior is similar to that described by Malozemoff’s model for the bilayer (antiferromagnet-ferromagnet) EB systems [2]. Thus, the pinned UM should be located near the FeMn interface. Results of polarized neutron reflectometry experiment show the explanation of how the Cu in the unusual magnetism in these FeMn/Cu multilayers will be presented.

\(^1\)Supported by Texas A&M Univ., US DOE BES (ORNL SNS), NRF Korea - 2011-0031933 (PNU), NSF-CAREER (USF, RIT).

1:15PM T30.00011 Multilayers of Co and Pt: the ultrathin limit. MICHALIS CHARILAOU, ETH Zurich, CATHERINE BORDEL, UC Berkeley, PIERRE-EMMANUEL BERCHE, Université de Rouen, BRIAN MARANVILLE, NIST, FRANCES HELLMAN, UC Berkeley — Magnetic properties of ultrathin (Co/Pt) multilayers, with overall composition 1Co:3Pt, has been investigated in to provide deeper understanding of magnetism in the ultrathin limit and to better understand the alloy. A comparison between a sub-monolayer multilayer and an fcc CoPt\(_2\) alloy film with perpendicular magnetic anisotropy (PMA) attributed to growth-induced Co clustering reveals significant differences in magnetization, despite the presence of thin Co platelets in both cases. Two regimes of the ferromagnetic phase transition, Brillouin and non-Brillouin-like, are seen in the experimental \(M(T)\) data and have been reproduced in Monte Carlo simulations, associated with different distributions of Co-Co nearest neighbors. Both the average number of Co-Co pairs and the width of the distribution are higher for the alloy than the sub-monolayer, leading to surprisingly higher Curie temperature and a nearly linear temperature-dependence of the magnetization of the alloy film, in contrast to the Brillouin-like behavior of the multilayer.

1:27PM T30.00012 Direct surface charging and alkali-metal doping for tuning the interlayer exchange coupling and magnetic anisotropy. TAMENE DASA, VALERI STEPANYUK, Max Planck Institute of Microstructure Physics — Manipulation of surface or interface charges allows one to control the magnetic orders in nanostructures. In this contribution we show two main surface charge alteration techniques for tuning the interlayer exchange coupling and magnetic anisotropy of ferromagnetic layers interspaced with non-magnetic ones. Our ab-initio study reveals that a modest amount of extra charge could switch the mutual alignment of the magnetic layers from anti-ferromagnetic to ferromagnetic or vice versa, taking Fe/NxCu(Pt)/Fe trilayer as model system. We also propose adsorption of alkali metals as a natural way of surface charging mechanism. Clear evidence is found that the interlayer magnetic order can be tuned only by adsorbing alkali metals on the magnetic layer. A combined effect of non-magnetic overlayers and interlayer magnetic order leads to a high perpendicular magnetic anisotropy in FePt thin films. These findings suggest that the interplay of interlayer magnetic coupling with magnetic anisotropy could play a crucial role for magnetic hardening and controlling the spin states.

1:39PM T30.00013 Antiferromagnetic interaction at the interfaces of ferromagnetic transition metals (TM) and Gd is well known phenomenon. However, quantitative description of this interaction still lack understanding. The main reason is that most experimental data were obtained by inspecting the hysteresis loops of TM/Gd multilayers. First, in plane domain structures of TM and Gd films complicates the description of the magnetization reversal process. Second, experimentally measured parameters are averaged over the domains obfuscating the microscopical picture. We make an effort to overcome these limitations by studying the magnetization reversal process of Permalloy/Gd nanodots. The dots were prepared by combination of optical lithography and magnetron sputtering. Experimentally it is observed that in these dots the antiferromagnetic interlayer interaction tunes magnetic vortex nucleation/annihilation fields. Rise of Gd magnetization at low temperature provides unusual temperature behavior of hysteresis loop. Micromagnetic models in which interlayer interaction energy acts as a fitting parameter is applied to simulate experimental hysteresis curves. The effect of nonmagnetic spacer between Permalloy and Gd is also considered and will be presented.
1:39PM T30.00013 Maximization of surface-enhanced transversal magneto-optic Kerr effect in Au/Co/Au thin films¹, EDGAR PATIÑO, CESAR HERREÑO, Universidad de los Andes — In order to maximize the transversal magneto optic Kerr effect (T-MOKE) of a Au/Co/Au structure we propose a method to obtain the optimum thickness values. A criteria based on preserving good plasmonic properties has been included as part of this method. Using the theoretical prediction we grew Au/Co/Au trilayers and perform optical and MO characterization using the Kretschmann configuration. The results admit very easy interpretation in terms of the interaction between the magneto-optical and plasmonic proper-ties dictating the optimal thicknesses of the structure. Moreover we have grown and characterized the optimized structure finding good agreement with theory reaching, for a 532 nm green laser, a maximal surface magneto-optic (MO) signal enhancement of close to nine folds with respect to the signal without plasmonic excitation.

¹This work was supported by “Programa Nacional de Ciencias Básicas” COLCIENCIAS (No. 120452128168), Vicerrectoría de Investigaciones of Universidad de los Andes (Bogotá, Colombia).

1:51PM T30.00014 Investigation of Boundary Magnetization and Exchange Bias of B-doped Chromia, MICHAEL STREET, WILL ECHTENKAMP, CHRISTIAN BINEK, University of Nebraska-Lincoln — This work is devoted to utilize the magnetoelectric material Cr2O3 (chromia) for spintronics. We exploit the electric switchable boundary magnetization (BM) of chromia to manipulate an adjacent exchange-coupled ferromagnetic material. Using a ferromagnetic Co/Pd multilayer deposited on chromia, reversible, room-temperature isothermal switching of the exchange bias (EB) field has been achieved by reversing the electric field in the presence of a constant magnetic field. To use voltage-controlled BM in chromia as a key component in a spintronic device, the Néel temperature must be increased above the bulk value of TN = 307 K. First principle calculations show that boron doping of chromia can increase TN by roughly 10% per 1% O site substitution by B. We have grown B-doped chromia samples in a gaseous decaborane background atmosphere. We diagram structural and magnetic characterizations of pure and B-doped chromia. SQUID measurements of the BM of B-doped chromia samples indicate an enhancement of TN from the bulk value. This finding has been corroborated by spin dependent inverse photoemission spectroscopy [Ref]. Further, we investigate EB systems using a Co/Pd multilayer deposited on B-doped chromia for independent proof of TN increase in the experimental context most relevant for voltage-controlled spintronics. [Ref] M. Street, et al., Appl. Phys. Lett. 104, 222402 (2014). This work was supported in part by C-SPIN, a center of STARnet, a SRC program, sponsored by MARCO and DARPA.

2:03PM T30.00015 Theoretical analysis of magnetic structures in the fcc-Fe/Cu(001) system¹, YASUTOMI TATETSU, The University of Tokyo, SHINJI TSUNEYUKI, The University of Tokyo, Institute for Solid State Physics, YOSHIHIRO GOHDA, The University of Tokyo, Tokyo Institute of Technology — Magnetic thin films have been studied due to its peculiar magnetic behaviors compared to their bulk systems. Fe/Cu magnetic thin films have been studied for the past decades, because of their uncertain magnetic structures. As is well known, the ground state of Fe has the bcc structure, but the fcc-Fe, which is stable above 1184 K, can epitaxially grow on a Cu(001) substrate even below room temperature, since the lattice parameters of Cu (3.62Å) and fcc Fe (3.58Å) are quite close to each other. Many kinds of studies for the systems have been reported, but its ground state is controversial. We applied first-principles calculations to the fcc-Fe/Cu(001) system using a computational code OpenMX for understanding of its electronic and magnetic structures. Our structural model is a slab model consisting of seven Cu layers and several Fe layers capped by a 10-Å vacuum layer. According to our collinear-spin calculations, an antiferromagnetic structure is stable in the 4 to 7-ML systems and a ferromagnetic coupling at the top of its electronic and magnetic structures. Our structural model is a slab model consisting of seven Cu layers and several Fe layers capped by a 10-Å vacuum layer. According to our collinear-spin calculations, an antiferromagnetic structure is stable in the 4 to 7-ML systems and a ferromagnetic coupling at the top of its electronic and magnetic structures.

¹This work was supported by the Elements Strategy Initiative Center for Magnetic Materials under the outsourcing project of MEXT and was done by using K computer.

Thursday, March 5, 2015 11:15AM - 2:15PM – Session T31 GMAG DMP: Focus Session: Ruthenates and Other Oxides

207A - Dennis Meier, ETH Zuerich

11:15AM T31.00001 Field-induced antiferromagnetic order in Sr3Ru2O7 - CHRISTOPHER LESTER, STEPHEN HAYDEN, University of Bristol, UK, SILVIA RAMOS, University of Kent, UK, ROBIN PERRY, UCL, UK, THOMAS CROFT, University of Bristol, UK, ROBERT BEWLEY, TATIANA GUIDI, PASCAL MANUEL, DMITRY KHALYAVIN, ISIS Neutron Source, UK — Many novel electronic ground states form in close proximity to quantum critical points, that is, the point where a continuous phase transition occurs at zero temperature. By suppressing the metamagnetic transition in Sr3Ru2O7 to low temperatures via the application of a magnetic field, the system is driven into a ‘nematic’ phase. This phase occurs at temperatures below approximately 1 K and at fields μ0Hc2 ≈ 8 T. The phase is often described as nematic since transport properties display pronounced anisotropic tendencies which are not present in the underlying crystal lattice. Using elastic neutron scattering we have found evidence for two adjacent magnetically ordered phases near μ0Hc1 in this material. The period of the order in both phases is incommensurate with the underlying lattice and most likely determined by the electronic band structure. The presence of static antiferromagnetic order provides a very natural explanation for the anisotropic transport properties that have been observed in this system. Our observation of field-induced antiferromagnetic order in a clean metal provides valuable insights into the physics of novel phase formation near quantum critical points.

11:27AM T31.00002 Possible spin-momentum locking and band-dependent coherence in Sr3Ru2O7 revealed by angle-dependent magneto thermolectric measurements, CHENYI SHEN, HUI XING, Department of Physics, Zhejiang University, XINXIN CAI, Department of Physics and Materials Research Institute, Pennsylvania State University, DAVID FOBES, Department of Physics, Tulane University, MINGLIANG TIAN, High Magnetic Field Laboratory, Chinese Academy of Science, ZHIQIANG MAO, Department of Physics, Tulane University, ZHUAN XU, Department of Physics, Zhejiang University, YING LIU, Department of Physics and Materials Research Institute, Pennsylvania State University — The bilayer member of the Roddedson-Popper(R-P) series, Sr3Ru2O7, with its complex phenomena such as a magnetic field orientation dependent metamagnetic transition and the possible existence of a nematic phase, has attracted much attention. Both INS and NMR studies suggested that the metamagnetic transition is band dependent and some bands of Sr3Ru2O7 are heavily renormalized according to the ARPES experiment. However, the underlying electronic and magnetic properties of these bands are yet to be clarified. We explored band dependent electronic and magnetic properties in Sr3Ru2O7 by using angle-dependent magnetoresistance and magneto thermolectric measurements on crystals cut along two specific crystalline directions and a magnetic field rotating in the ab plane. We found evidence supporting the presence of spin-momentum locking and the emergence of a coherent state with unconventional magnetism phase formed in a two-dimensional band in Sr3Ru2O7.
11:39AM T31.00003 Soft magnetic excitations and quantum critically in Sr$_3$Ru$_2$O$_7$ . STEPHEN HAYDEN, C. LESTER, University of Bristol, R. RAMOS, University of Kent, R. PERRY, University College London, T. CROFT, University of Bristol, R. BEWLEY, T. GUIDI, Rutherford Appleton Laboratory, E. FORGAN, University of Birmingham — The application of a magnetic field of approximately $B_H = 8$ T induces quantum critical behavior in Sr$_3$Ru$_2$O$_7$. Near $B_c$, the resistivity shows an anomalous power law temperature dependence and the linear specific heat becomes large. In addition, new ordered phases with strong nematic tendencies appear below 1 K near $B_c$. These phases have recently been identified as spin density wave order. Here we report an inelastic neutron scattering study of the low-energy magnetic excitations. We find a dramatic field-induced softening of the collective magnetic excitations in the region surrounding $B_c$. This suggests that the quantum critically observed in Sr$_3$Ru$_2$O$_7$ is magnetic in origin. The presence of additional magnetic excitations can also explain the increase in entropy and specific heat present near $B_c$.

11:51AM T31.00004 Double metamagnetic transition in Sr$_3$Ru$_2$O$_{10}$ investigated by low temperature magnetization measurements1 . DAGMAR FRANZISKA WEICKERT, LEONARDO CIVALE, MARCELO JAIME, BORIS MAIOROV, ROMAN MOVSHOVICH, Los Alamos National Laboratory, R. FITTIPALDI, V. GRANATA, A. VECCHIONE, University of Salerno, Via Giovanni Paolo II, I-84084 Fisciano, Italy, TENG TAN, Temple University, Philadelphia, Pennsylvania 19122, USA, MYRON SALAMON, University of Texas at Dallas, Richardson, TX 75080, Dallas, USA — We report a study of the magnetization of the n = 3 member of the Sr$_{n+1}$Ru$_2$O$_{3n+1}$ Ruddlesden-Popper series down to 1 K temperatures. Sr$_3$Ru$_2$O$_{10}$ exhibits ferromagnetism below 105 K with magnetic moments aligned along the crystallographic c-direction in the tetragonal crystal structure. Metamagnetism is observed at about 2 T below 50 K when a magnetic field is applied in the ab-plane. A recent study on high quality samples revealed that the magnetization has a substructure [1]. We extend the studies to very low temperatures and found i) a clear double peak in δM/dH, ii) that the metamagnetism is accompanied by a reduction of the magnetic moment and iii) no further splitting of the metamagnetic anomalies to the lowest temperatures of 0.46 K. Furthermore, the measurements indicate a shift of both metamagnetic signatures to higher fields by rotating from $H//ab$ to $H//c$. We will discuss the phase diagram and possible ordered states.


1Research at LANL (magnetometry and data analysis) was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.

12:03PM T31.00005 Optical Response of Sr$_2$RuO$_4$ Reveals Universal Fermi-liquid Scaling and Quasiparticles Beyond Landau Theory1 . DAMIEN STRICKER, University of Geneva, JERNEJ MRAVLJE, Ecole Polytechnique CNRS, CHRISTOPHE BERTHOD, University of Geneva, ROSALBA FITTIPALDI, ANTONIO VecCHIONE, Università di Salerno, ANTOINE GEORGES, Ecole Polytechnique CNRS, DIRK VAN DER MAREL, University de Geneva — We report optical measurements demonstrating that the low-energy relaxation rate $1/\tau$ of the conduction electrons in Sr$_2$RuO$_4$ obeys scaling relations for its frequency ($\omega$) and temperature (T) dependence in accordance with Fermi-liquid theory. In the thermal relaxation regime, $1/\tau \propto (h\omega^2 + p(T^2))^{2}$ with $p = 2$, and $\omega/T$ scaling applies. Many-body electronic structure calculations using dynamical mean-field theory confirm the low-energy Fermi-liquid scaling, and provide quantitative understanding of the deviations from Fermi-liquid behavior at higher energy and temperature. In this regime, evidence for electron-like “resilient” quasiparticle excitations with a scattering rate deviating from Landau’s theory. In the thermal relaxation regime, $1/\tau \propto (h\omega^2 + p(T^2))^{2}$ with $p = 2$, and $\omega/T$ scaling applies. Many-body electronic structure calculations using dynamical mean-field theory confirm the low-energy Fermi-liquid scaling, and provide quantitative understanding of the deviations from Fermi-liquid behavior at higher energy and temperature. In this regime, evidence for electron-like “resilient” quasiparticle excitations with a scattering rate deviating from Landau’s theory.


12:15PM T31.00006 Commensurate-incommensurate magnetic phase transition in the Fedoped ruthenate bilayer Ca$_3$Ru$_2$O$_7$ . XIANGLIN KE, M. ZHU, Michigan State University, W. TIAN, T. HONG, Oak Ridge National Laboratory, J. PENG, Z.Q. MAO, Tulane University — Neutron diffraction studies have revealed an uncommon commensurate-incommensurate magnetic phase transition with decreasing temperature in the (~ 5%) Fe-doped bilayer ruthenate Ca$_3$(Ru,Fe)$_2$O$_7$. An incommensurate phase formed of a cycloidal spiral spin structure coexists with a commensurate one below the phase transition at 42 K and persists down to the lowest temperature, accompanied by higher-order magnetic satellite peaks which indicate the formation of a magnetic soliton lattice. We ascribe these findings to the competing magnetic interactions in Ca$_3$Ru$_2$O$_7$. This study demonstrates an effective approach to tune novel magnetic and electronic properties of this complex system via 3d magnetic transition-metal substitution.


12:27PM T31.00007 ARPES and spin ARPES measurements of nonmagnetic centrosymmetric crystal LaBiO$_2$. JUSTIN VAUGH, XIAOQING ZOU, HAOXING LI, THOMAS NUMMY, STEPHEN PARHAM, QIHANG LIU, XIUWEN ZHANG, Univ of Colorado - Boulder, JASMINKA ZURIC, University of Kentucky, XIANGDE ZHU, Chinese Academy of Sciences, GANG CAO, University of Kentucky, ALEX ZUNGER, DANIEL DESSAU, Univ of Colorado - Boulder — Spin polarized bands are traditionally expected to exist only under global bulk symmetry breaking. LaBiO$_2$ has a centrosymmetric structure thus expected to have no spin polarization. However, it is predicted to have local inversion-asymmetric structure, leading to spin polarization localized on the individual Bi$_2$O$_2$ sublayers. This spin polarization theoretically presents itself in energetically doubly degenerate bands that are spatially separated on different Bi$_2$O$_2$ layers. We measured ARPES and spin ARPES on the inversion-symmetric bulk crystal LaBiO$_2$ in search of such a hidden spin polarization. Our measurements show band structure to have qualitative agreement with DFT calculations. We additionally observe spin polarization in the valence band and will discuss its spin orientation in this talk. This work is supported by NSF DMREF project 1334170.

12:39PM T31.00008 Anisotropic Magnetocaloric Effect in Single Crystalline CoSb$_2$O$_6$. AARON B. CHRISTIAN, JOHN J. NEUMEIER, Montana State Univ., YI-KUO YU, National Center for Biotechnology Information — The quasi one-dimensional spin chains of CoSb$_2$O$_6$ are oriented along [110] at $z = 0$ and [100] at $z = 1/2$. Application of magnetic field $H$ parallel to [110] is therefore parallel to one set of chains and perpendicular to the other. $H > 2$ tesla, applied parallel to [110], lowers the Néel temperature ($T_N = 13.4$ K) for one set of chains, leaving the other set unaffected. This gives rise to two peaks in the heat capacity $C_p$, which are separated by 3.8 K when $H = 8$ tesla. Integrating $C_p(T,H)/T$ with respect to temperature yields a change in entropy $\Delta S_T$, from which the change in magnetic entropy $\Delta S_M$, determined. Near 12 K we find that $\Delta S_M$(8 T) = 2.97 J/kg K for measurements with $H // 110$ or $100$ and $\Delta S_M$(8 T) = 0.44 J/kg K for $H // [001]$. This anisotropy implies that rotation of the sample in constant magnetic field could induce a change in sample temperature.

1Supported by NSF Grant DMR-0907036.
12:15PM T31.00009 Hall effect of triplons in a dimerized quantum magnet. JUDIT ROMHANYI, Max Planck Institute for Solid State Research, Stuttgart, Germany, KARŁO PENC, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, RAMACHANDRAN GANESH, The Institute of Mathematical Sciences, Chennai, India — SrCu$_2$(BO$_3$)$_2$ is the archetypal quantum magnet with a gapped dimer-singlet ground state and triplon excitations. It serves as a realisation of the Shastry Sutherland model, up to small anisotropies arising from Dzyaloshinskii-Moriya (DM) interactions. We demonstrate that the DM couplings give rise to topological character in the triplon band structure. The triplons form a new kind of a Dirac cone with three bands touching at a single point, a spin-1 generalization of graphene. An applied magnetic field opens band gaps and as a result topological bands with Chern numbers $\pm 2$ develop. Thus SrCu$_2$(BO$_3$)$_2$ is a magnetic analogue of the integer quantum Hall effect and supports topologically protected edge modes. At a critical value of the magnetic field set by the strength of DM interactions, the three triplon bands touch again in a spin-1 Dirac cone, and lose their topological character. We predict thermal Hall signature in the topological regime.

1:03PM T31.00010 Spin induced ferroelectric-like structural transition in a metal. YANFENG GUO, Department of Physics, University of Oxford, HAI FENG, National Institute for Materials Science, PRINCEP ANDREW, Department of Physics, University of Oxford, PASCAL MANUEL, ISIS Facility, Rutherford Appleton Laboratory, KAZUNARI YAMAURA, National Institute for Materials Science, BOOTHROYD ANDREW, Department of Physics, University of Oxford — LiOsO$_3$ represents a previously only known example of “ferroelectric metal,” a concept presented by Anderson and Blount in 1965, with the properties being promoted by electron lattice coupling involving Li$^+$ ions displacement in the crystal structure [Y. Shi et al., Nat. Mater. 12, 1024(2013)]. We report that in Pb$_2$CoO$_4$, a new ordered double-perovskite with a centrosymmetric monoclinic space group of $P2_1/n$, a ferroelectric-like structural transition occurs at $\sim$ 38 K in the metallic state, i.e. a continuous second order transition to a noncentrosymmetric structure (space group: P1) associated by appearance of a nominal unique polar axis along the c-axis. The phase transition is coincident with a magnetic transition at the same temperature which corresponds to a long-range antiferromagnetic order. The magnetic structure analysis and theoretical calculations prove that the antiferromagnetic ordering is the driven force for the structural transition in Pb$_2$CoO$_4$ and it ordering involving a magnetic ordering.

1:15PM T31.00011 Anisotropic Magnetocaloric Effect in Single Crystalline NiTa$_2$O$_6$. AARON T. SCHYE, SUELI H. MASUNAGA, AARON B. CHRISTIAN, JOHN J. NEUMEIER, Montana State University, YI-KUO YU, National Center for Biotechnology Information — Magnetic susceptibility and heat capacity measurements were made on the low-dimensional antiferromagnet NiTa$_2$O$_6$. The antiferromagnetic structure most consistent with our measurements is the two sub-lattice model proposed by Law et al.[2] in which magnetic moments in the $z = 0$ plane are aligned parallel to [110] and those in the $z = 1/2$ plane are aligned parallel to [10]. Applying a magnetic field along [110] causes the peak in the heat capacity to split into two with one remaining at $T_N$ and the other shifting to lower temperatures as the field is increased with a maximum $\Delta T \sim 3$ K at 8 T. This splitting indicates that each sub-lattice orders at different Néel temperatures. Calculation of the magnetic entropy change associated with an increase in magnetic field($\Delta S_m(T, \Delta H)$) reveals $\Delta S_m(T, \Delta H) \sim 0.7$ J/kg K for $H \parallel$ [110] and $\Delta S_m(T, \Delta H) \sim 0$ J/kg K for $H \parallel$ [001] if $\Delta H = 8$ T. This anisotropy in the magnetocaloric effect suggests that rotating the sample in constant magnetic field will result in a change in sample temperature.

3Supported by NSF Grant DMR-0907036

1:27PM T31.00012 Transport properties of novel molybdenum bronze oxide materials. JOSEPH HAGMANN, SON LE, National Institute of Standards and Technology, LYNN SCHNEEMEYER, PATTI OLSEN, Montclair State University, THEO SIEGRIST, Florida State University, CURT RICHTER, DAVID SEILER, National Institute of Standards and Technology — Reduced ternary molybdenum oxides, or bronzes, offer an attractive materials platform to study a wide variety of remarkable physical phenomena, including charge density waves [1] and superconductivity [2], in a system with highly varied structural chemistry. Interesting electronic behaviors in these materials arise from the strong hybridization of the 4d states of high-valent Mo with O p orbitals (conditions amenable to itinerancy) and reduced dimensionality arising from ordered O vacancies. This study aims to demonstrate the transport phenomena in a series of novel molybdenum bronze materials, including the new electrochemically-grown molybdenum bronzes, K3LiMo15O47, and the rare earth molybdenum bronze, HoMo16O44, and relate these behaviors to their experimentally-characterized structures. Dependence of the transport behavior on numerous experimental parameters, including temperature, magnetic field and drive current, and gate voltage, is presented to fully reveal charge carrier transport in these materials.


1:39PM T31.00013 Properties of the low dimensional Sr$_2$Cu(W$_{1-x}$Mo$_x$)$_6$O$_{17}$ spin system. OMAR CHMAISSEM, Northern Illinois University, DeKalb IL and Argonne National Laboratory, Argonne IL, MAXIM AVDEEV, SERGEY DANILKIN, Australian Nuclear Science and Technology Organisation, Bragg Institute, Austria, SAMI VASALA, HISAO YAMAUCHI, MAARTEN GARPNEN, Department of Chemistry, Aalto University, Finland — Low-dimensional spin systems have gained much attention in solid state physics. Such systems could have a ground state with no long-range magnetic order and an energy gap in the spin excitation spectrum, offering the possibility of a quantum spin-liquid phase. Quantum fluctuations causing the spin-liquid state are particularly strong in systems with reduced dimensionality and a low spin value, and magnetic frustration can further enhance the fluctuations. Among various low-dimensional spin systems, the S = 1/2 Heisenberg frustrated square lattice model is especially interesting due to its relevance to high-T$_C$ superconducting cuprates, whose undoped parent materials are S = 1/2 square-lattice antiferromagnets. Sr$_2$CuWO$_6$ and Sr$_2$CuMoO$_6$ have been found to be quasi-two-dimensional S = 1/2 magnetic systems with a square lattice of Cu-ions. These compounds show low-dimensional magnetic properties, with no clear indication of long-range order in magnetic susceptibility. I will discuss the materials properties and the observation of long range magnetism by neutron diffraction and other techniques.

1:51PM T31.00014 NMR studies of the internal electric field in a single crystal of the quasi-one-dimensional conductor Li$_{0.8}$Mn$_{0.2}$O$_2$. GUOQING WU, Yangzhou University, BING WU, Fayetteville State University — The quasi-one-dimensional (Q1D) conductor Li$_{0.8}$Mn$_{0.2}$O$_2$ is of considerable interest because it has a highly conducting phase with properties likely associated with a Luttinger liquid, a poorly understood “metal-insulator” crossover at temperature $T_{MI} = 24$ K, and a 3D superconducting phase that may involve triplet Cooper pairs at $T_c = 2.2$ K, while the mechanism for many of its properties has been a long mystery and it presents tremendous experimental challenges. We report the $^7$Li-NMR measurements of the internal electric field with an externally applied magnetic field $B_0 = 9 - 12$ T, and we also show our theoretically calculated result of the electric field based on the structure of the crystal lattice. We find that the $^7$Li-NMR frequency ($\nu_{Q}$) has a value of $\sim$ 45 kHz and the electric field gradient (EFG) at the Li site due to the charges of the surrounding Mo conduction electrons has an axial symmetry with the principle axis ($p_z$) to be along the lattice a-axis. There is no temperature or field dependence for the value of $\nu_{Q}$ or EFG, indicating that the “metal-insulator” crossover has a magnetic origin, rather than the charge density wave (CDW) as one of the possible mechanisms previously thought in literature.
2:03PM T31.00015 ARPES and NMTO of Li$_{0.5}$Mo$_{0.5}$O$_2$: Implications for Unusually Robust Quasi-One Dimensional Behavior$^1$, J.W. ALLEN, U. Michigan, L.M. DUDY, Uni Wuerzburg. J.D. DENLINGER, Lawrence Berkeley Nat’l Lab. J. HE, Clemens U., M. GREENBLATT, Rutgers U., M.W. HAVENKORT, MPI Chem. Phys. Dresden, O.K. ANDERSEN, Y. NOHARA, MPI Stuttgart — Li$_{0.5}$Mo$_{0.5}$O$_2$: displays theoretically interesting $^1$ metallic quasi-one dimensional (1D) behavior that is unusually robust $^2$ against 3D crossover before superconductivity at $\approx 1.9$K, and has large anomalous Luttinger liquid density-of-states exponent $\alpha \approx 0.6$. We present very high resolution, low temperature ($T \approx 6$K-26K) angle resolved photoemission spectroscopy (ARPES) data analyzed with non-linear muffin tin orbital (NOMTO) Wannier function band theory. We confirm a previous conclusion $^3$ that the LDA agrees unusually well with ARPES, implying small Hubbard U, and find in ARPES the dispersion and Fermi surface warping and splitting expected for predicted small but long range inter-chain hoppings ($t_c \approx 10$-15 meV). These various findings imply the likely importance of long range Coulomb interactions for the large $\alpha$ value $^4$ and reaffirm the great puzzle $^2$ of quasi-1D behavior well below the 3D crossover $T$ implied by $t_c$.

$^1$Supported by the US DOE, BES, Materials Science and Engineering Division.

12:03PM T32.00003 Photoinduced phase transitions in vanadium dioxide revealed by ultrafast electron diffraction and mid-infrared spectroscopy$^1$. KUNAL TIWARI, VANCE MORRISON, ROBERT CHATELAIN, McGill University Department of Physics, ALI HENDAOUI, Institut National de la Recherche Scientifique, ANDREW BRUHACS, McGill University Department of Chemistry, MOHAMED CHAKER, Institut National de la Recherche Scientifique, BRADLEY SIWICK, McGill University Departments of Physics and Chemistry — The complex interplay between strong electron-electron correlations and structural distortions is thought to determine the electronic properties of many oxides, but the respective role of these two contributions is often difficult to determine. We report combined radio-frequency compressed ultrafast electron diffraction (RF-UED) and infrared transmissivity experiments in which we directly monitor and separate the lattice and charge density reorganizations associated with the optically induced semiconductor-to-metal phase transition in vanadium dioxide. These studies have uncovered a previously unreported photoinduced transition to a metastable phase retaining the periodic lattice distortion characteristic of the insulating phase, but differing by a reorganization of charge density along the vanadium dimer chains and a transition to metal-like mid IR optical properties. These results demonstrate that UED is able to follow details of both lattice and electronic structural dynamics on the ultrafast timescale.

$^1$Supported by Natural Sciences and Engineering Research Council of Canada, the Canada Foundation for Innovation, the Canada Research Chairs program, NSERC PGS-D and CGS-D fellowships, and Fonds de Recherche du QuébecNature et Technologies.
12:15PM T32.00004 Elucidating the Band Gap of Niobium Dioxide . ANDREW O'HARA, The University of Texas at Austin, DEREK VIGIL-FOWERLER, STEVEN G. LOUIE, University of California - Berkeley and Lawrence Berkeley National Lab, ALEXANDER A. DEMKOV, The University of Texas at Austin — Like VO$_2$, niobium dioxide (NbO$_2$) belongs to the family of transition metal oxides with a temperature-driven metal-to-insulator transition. However, NbO$_2$ has received considerably less attention, and several open questions about the material remain. One such question, of both practical and fundamental importance, is the nature and size of the band gap in the low-temperature, distorted rutile phase with a range reported for the gap of $1$–$1.5$ eV. In this talk, we investigate the band structure utilizing several electronic correlations to extract the electronic energy bands with the standard local density approximation (LDA). LDA+U, hybrid functional, and the GW approximation, to better understand the physics of the band gap in NbO$_2$. Comparisons of the calculations are made to recent experimental work on NbO$_2$ utilizing photoemission spectroscopy and ellipsometry. This work is supported by DOE under the SciDAC program, the NSF, and SRC.

12:27PM T32.00005 Orbital and magnetic states in BaV$_{11}$O$_{15}$ . SACHITH DISSANAYAKE, TIANRAN CHEN, Univ of Virginia, JOOSEOP LEE, MATTHEW STONE, MASAKI MATSUDA, Oak Ridge National Laboratory, TOMOMASA KAZITA, TAKURO KATSUFUJI, Waseda University, SEUNGHUN LEE, Univ of Virginia — BaV$_{11}$O$_{15}$ is a new type of frustrated magnet that exhibits interesting physics due to its charge and orbital ordering which has an average V valance of $2.8^+$. The V ions form a lattice with V “boats,” each of which is made of five V atoms and connected along ab plane. The system undergoes a structural phase transition at $T_s$ = 130 K and shows an antiferromagnetic long range ordering below $T_N$ = 43 K. Although there have been several studies about this complex V spin system, nature of the orbital and magnetic correlations is still unclear. In this talk I will discuss about our elastic and inelastic neutron scattering results obtained from a powder sample and a single crystal of BaV$_{11}$O$_{15}$. We investigated the magnetic ground states of BaV$_{11}$O$_{15}$ by neutron diffraction refinements and observed magnetic excitations below 15 meV were analyzed by performing linear spinwave calculations. Another broad high energy excitation around 33 meV was observed at temperatures below the structural transition $T_s$ = 130 K. Possible orbital and magnetic states for this complex V spin system will be discussed.

12:39PM T32.00006 Pressure-dependent Raman scattering study of CoV$_2$O$_4$ . TAYLOR BYRUM, SAMUEL GLEASON, Univ of Illinois - Urbana, HAIDONG ZHOU, Univ of Tennessee - Knoxville, S. LANCE COOPER, Univ of Illinois - Urbana — The Co$_x$V$_{1-x}$O$_4$ ($A$ = Cd, Mn, Mg, Zn, Co) spinel family provides a fertile ground to explore the crossover between electron localization and itinerancy, which can be tuned with chemical ($A$-site substitution) and/or physical pressure. CoV$_2$O$_4$ resides closest to the predicted itinerant electron limit for the vanadium spinel family. Recent experiments have shown the existence of a critical V-V separation by inducing a metallic transition in CoV$_2$O$_4$ with a pressure of ~6 GPa. While the structure of CoV$_2$O$_4$ has been theoretically suggested to remain cubic through the metallic transition, no structural measurements under pressure have been performed. Raman spectroscopy is well suited to address this issue, as it is sensitive to even subtle structural changes. In this presentation, I present a pressure-dependent Raman scattering study of CoV$_2$O$_4$ to elucidate the role the structure plays in the metallic transition.

1/ Research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Award DE-FG02-07ER46453. T. Byrum was partially supported by the NSF Graduate Research Fellowship Program under Grant Number DGE-1144245.


12:51PM T32.00007 Spin-glass insulating ground state in Y$_2$Os$_3$O$_7$ . ZHIYING ZHAO, Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA, STUART CALDER, Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, MICHAEL MCGUIRE, BRIAN SALES, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, HAIDONG ZHOU, Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA, JIAQIANG YAN, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — 4d/5d transition-metal oxides can display many exotic physical properties due to the interplay between spin-orbit coupling (SOC), Coulomb interaction, crystal field effect, Hund’s coupling, and lattice distortion. The magnetic ground state of systems with $d^4$ electronic configuration is under hot debate since the consensus between experiments and theories has not been achieved. A non-magnetic ground state has been predicted under the $J_{eff}$ scenario in the presence of SOC. However, various ground states are observed in some $d^4$ systems (such as InO$_2$, Os$_2$S, and RuO$_2$). In this talk, I will present our study of Y$_2$Os$_3$O$_7$ with nonmagnetic $Y^{3+}$ at A site which allows us to study the magnetism of Os$^{5+}$ ($d^5$) sublattice. Polycrystalline Y$_2$Os$_3$O$_7$ was synthesized by solid state reaction and was studied by measuring electrical resistivity, magnetic susceptibility, specific heat, and neutron powder diffraction. A spin-glass insulating state is observed in contrast to the long-range magnetic ordered state in Y$_2$Ru$_2$O$_7$.

1:03PM T32.00008 First-principles evidence of Slater-type metal-to-insulator transition in NaOsO$_3$ . BONGJAE KIM, ZEYNEP ERGONENC, CESARE FRANCHINI, Faculty of Physics and Center for Computational Materials Science, University of Vienna — NaOsO$_3$ is thought to be the first example of a three-dimensional Slater insulator where the metal-to-insulator transition (MIT) is driven by the emergence of the (antiferro)magnetism in the system. This picture is fundamentally different from the most widely known Mott-Hubbard (MH) insulators for which the opening of the gap is due to electron correlation. However, there are still experimental evidences for the Slater-type state in NaOsO$_3$ such as the continuous character of the transition and the simultaneous onset of the magnetic and insulating regime at the same temperature ($T_{MIT}=T_N$), both directly and unambiguously indicated by results presented in the theory. Based on ab initio band structure methods, we have studied the origin of the MIT in NaOsO$_3$ and found that the MIT is predominantly driven by magnetic, and only marginally dependent on electronic correlation. A direct comparison between NaOsO$_3$ and other typical MH oxides allows us to analyze and interpret the distinct role of magnetism and the electronic correlation in favoring Slater- or MH-type states. Finally, fingerprints of the Slater behaviour are found in the optical response, that we have computed within a model Bethe-Salpeter scheme.

1:15PM T32.00009 Unconventional electronic state in half-frustrated Ca$_2$Os$_2$O$_7$ . MAREIN RAHN, ROGER JOHNSON, University of Oxford, JAMES VALE, CHRISTIAN DONNERER, University College London, PASCAL MANUEL, DMITRY KHALYAVIN, ISIS Facility, GARETH NISBET, DIAMOND Light Source, DESMOND MCMORROW, University College London, ANDREW BOOTHROYD, University of Oxford — In 5d transition metal oxides ($5d$ TMOS), the combination of strong spin-orbit coupling and electronic correlation can lead to unusual ground states. Orthorhombic calcium osmate is a “half-frustrated” compound with a strange phase transition at $327$ K, enhancing its resistivity by an order of magnitude. We have investigated the concomitant magnetic ordering process by neutron powder diffraction and single crystal resonant x-ray diffraction. Our results reveal a complex reordering process, likely induced by magnetic frustration. Similar coupling of magnetic order and electronic transport has been observed in other families of 5d TMOS. Given the itinerant character of these materials, one cannot explained such behaviour in a Mott-Hubbard scenario. We hope that Ca$_2$Os$_2$O$_7$ will serve as a model system to help understand this peculiar interplay of spin-orbit coupling, correlation and frustration.
1:27PM T32.00010 Magnetic properties of the double perovskite Sr₃FeOsO₉: microscopic insights from ab-initio density-functional theory study. SUDIPTA KANUNGO, BINGHAI YAN, Max Planck Institute for Chemical Physics of Solids, MARTIN JANSEN, Max Plack Institute for Solid State Research, CLAUDIA FELSER, Max Plack Institute for Chemical Physics of Solids — Using density-functional theory calculations, we investigated the electronic and magnetic properties of the ordered 3d-5d double perovskite Sr₃FeOsO₉, which has recently drawn attention for interesting antiferromagnetic (AFM) phase transitions in low temperature observed in experiments. The calculated effective magnetic exchange interactions reveal the importance of long-range super-superexchange interactions in this compound. The competition between the ferromagnetic (FM) Os-O-Fe short-range interaction and AFM Os-O-Fe-O-Os long-range interaction induces strong magnetic frustration along the crystallographic c axis. This strong magnetic frustration is proposed to drive the magnetic phase transition between two AFM phases (AFM1 to AFM2) and related lattice distortion, which were also observed in the experiment. [Ref: Sudipta Kanungo, Binghai Yan, Martin Jansen, and Claudia Felser; Phys. Rev. B 89, 214414 (2014)]

1:39PM T32.00011 Structure and physical properties of R₂Os₂O₇ Pyrochlores ¹ , RYAN RAWL, Univ of Tennessee, Knoxville, STUART CALDER, Oak Ridge National Laboratory, ZHIYING ZHAO, HAIDONG ZHOU, DAVID MANDRUS, JIAQIANG YAN, Univ of Tennessee, Knoxville — The spin-orbit coupling (SOC) in 4d/5d transition metal oxides is enhanced to such a degree, relative to 3d oxides, that it can alter the electronic structure and have a dramatic effect on materials properties. A good example of this is the SOC assisted metal-insulator transition in Sr₂IrO₄, which has been extensively studied in the last few years. In a strong SOC scenario, a nonmagnetic ground state is expected for systems with d⁴ electronic configuration. R₂Os₂O₇ pyrochlores, in which Os⁴⁺ has d⁴ electron count, provides a material playground to study the magnetism of d⁴ and effect of R³⁺-Os⁴⁺ interplay on the ground states. This series has only undergone limited studies, with the only published data investigating the lattice parameters and electrical resistivity at room temperature. In this talk, I will report our study on the magnetic, transport, thermodynamic, and structural properties of R₂Os₂O₇ pyrochlores.

¹Part of the work was supported by the CEM, and NSF MRSEC, under grant DMR-1420451

1:51PM T32.00012 Evolution of symmetry-broken states in the pseudogap regime of cuprates - the atomic structure footprints ¹, EMIL BOZIN, R. Zhong, K.R. Knox, Brookhaven National Laboratory, B.L. Winn, Oak Ridge National Laboratory, G.D. Gu, J.P. Hill, J.M. Tranquada, S.J.L. Billinge, Brookhaven National Laboratory — Revealing the nature of the symmetry broken states in strongly correlated electron systems in general, and in the pseudo-gap (PG) phase of cuprates in particular, is instrumental in understanding the underlying properties. To that effect the knowledge of the local atomic structure may reveal relevant details important for more comprehensive understanding of the character of symmetry broken states in strongly correlated electron systems. Atomic pair distribution function (PDF) is one of the few experimental methods that can speak to this problem. Mounting experimental evidence suggests that the pseudogap phase may represent an electronic state in which the four-fold rotational symmetry of the Cu₂O₂ planes is broken, pointing to stripe or nematic character. Systematic approach has been taken in charting both long and short range structural orders, on an equal footing, across the (x, T) phase diagrams of cuprates. For example, in La₂₋ₓBaₓCuO₄, by combining inelastic neutron scattering and neutron PDF approaches, we find evidence consistent with there being a dynamic symmetry breaking well above the charge ordering temperature and within the pseudogap regime. The response has non-monotonic doping dependence that peaks at 1/8 composition.

¹Work at Brookhaven National Laboratory was supported by US DOE, Office of Science, Office of Basic Energy Sciences (DOE-BES) under contract DE-AC02- 98CH10886.

2:03PM T32.00013 Prediction of novel perovskite-type oxyhydride KTi(O₂H) with two-dimensional electronic states ¹, NOBUYA SATO, SHINJI TSUNEYUKI, Dept. of Phys., The Univ. of Tokyo — Perovskite-type oxides ABO₃ have been widely studied for their dielectricity. The properties of these materials significantly change by substituting A or B cations, while compositions of A and B cations are limited to (A²⁺, B⁴⁺) for charge neutrality. Recently, it has been demonstrated that oxygen anions in BaTiO₃ can be partially substituted with hydride ions (H⁻) suggesting that more varieties of compositions might be realized (e.g., (A¹⁺, B³⁺)) combined with oxygen substitution. In this work, using first-principles calculations, we investigate an unsynthesized model composition with the oxygen substitution, KTi(O₂H). This compound is expected to crystallize into the perovskite-type structure from its tolerance factor. We confirm its stability with the crystal structure optimization. The electronic properties reveal the two-dimensional low-energy electronic states within Ti–O–H planes. For its unconventional composition and the peculiar two-dimensional property, this material may realize novel electronic properties.

¹N. S. was supported by Japan Society for the Promotion of Science through Program for Leading Graduate Schools (MERIT).
11:27AM T33.00002 Conformations of double stranded DNA: the effect of breathing bubbles
AIQUIN HUANG, ANIKET BHATTACHARYA, University of Central Florida — A double stranded DNA (dsDNA) is a natural semi-flexible biopolymer with persistence length \( \approx 50 \) nm, while a single stranded (ss) DNA is very flexible whose persistence length is one order of magnitude smaller (3-5 nm). Depending on the size of a polymer, the sequence and the end groups, the two strands in a dsDNA can locally denature into two single strands and form bubbles along the polymer chain, i.e. dsDNA exists in the form of a combination of double strands and single strands, exhibiting a heterogeneity of bending rigidity. In our study, we adopt a coarse grained model of dsDNA developed by Kim et al. [J. Y. Kim, J. H. Jeon, and W. Sung, J. Chem. Phys. 128, 055101 (2008)] and further improve it by incorporating excluded volume effect and sequence heterogeneity. In this model, a dsDNA is described as two semi-flexible chains paired with each other by hydrogen bonding. The stacking interaction is designed such that the persistence length of the paired chains interpalates 3 nm and 50 nm depending on the fraction of the melted pair base pairs. By performing Langevin dynamics simulation we study the bubble statistics as a function of temperature and sequence and how the bubbles affect local bending rigidity and the chain conformations. We compare our results with those from WLC model.

11:39AM T33.00003 Knots along DNA Confined in Nanochannels
C. BENJAMIN RENNER, MIT, LIANG DAI, SMART, PATRICK DOYLE, MIT — We study the size distribution of spontaneous knots on semiflexible chains confined in square channels using Monte Carlo simulations. The most probable knot size is shown to vary non-monotonically with the channel size. For knotted polymers confined in channels larger than the size of a knot in bulk, our analysis reveals that the metastable knot size in weak confinement is larger than the knot size in absence of confinement because the confinement free energy gained by shrinking the knot is lessened when the chain experiences the confinement of a channel. In the case of strong confinement, the metastable knot size is smaller than the knot size in the absence of confinement because the segments in the core of the knot experience more confinement free energy, and the channels pushes the segments outside of the core of the knot. We demonstrate that a simple theory can capture this non-monotonic behavior and quantitatively explain the metastable knot size as a function of the channel size. These results may have implications for tuning the channel size to either generate or screen knots.

1NSF CBET #1335938 and SMART’s research program in BioSystems and Micromechanics.

11:51AM T33.00004 Protein dynamics from structural ensembles: Diffusive and activated contributions in a linear mode description
JEREMY COPPERMAN, MARINA GUENZA, University of Oregon — We have developed a coarse-grained linear Langevin equation for protein dynamics, which describes proteins as semiflexible objects collapsed into the free energy well representing the folded state of the protein. Fundamental to this approach is the inclusion of internal dissipation, absent in any rigid-body hydrodynamical modeling scheme. The normal mode analytical solution naturally separates into global modes describing the anisotropic tumbling of the object, and internal modes which contain both diffusive and activated glass-like contributions. We show how cooperativity in the dynamical modes is related to the energy barriers to mode diffusion. While molecular dynamics simulations generate the most accurate structural ensembles, we show how sets of NMR conformers can be used to generate the structural ensemble needed as input to the theory, making the approach truly predictive in nature. Results are in good agreement when compared with both nuclear magnetic resonance relaxation, and time correlation functions calculated from molecular dynamic simulations.

1This material is based upon work partially supported by the National Science Foundation under Grant CHE-1362500.

12:03PM T33.00005 Driven Polymer Translocation into a Crosslinked Gel, DAVID SEAN, GARY W. SLATER, University of Ottawa — In a typical polymer translocation setup, a thin membrane is used to separate two chambers and a polyelectrolyte is driven by an electric field to translocate from one side of the membrane to the other via a small nanopore. However, the high translocation rate that results from the forces required to drive this process makes optical and/or electrical analysis of the translocating polymer challenging. Using coarse-grained Langevin Dynamics simulations we investigate how the translocation process can be slowed down by placing a crosslinked gel on the trans-side of the membrane. Since the driving electric field is localized in the neighborhood of the nanopore, electrophoretic migration is only achieved by a “pushing” action from the polymer segment residing in the nanopore. For the case of a flexible polymer we find that the polymer fills the gel pores via multiple “herniation” processes, whereas for a semi-flexible chain in a tight gel there are no hernias and the polymer follows a smooth curvilinear path. Moreover, for the case of a semi-flexible polymer the gel makes the translocation process more uniform by reducing the acceleration at the end of the process.

12:15PM T33.00006 Backfolded Odijk regime for semiflexible polymers confined in nanochannels
ABHIRAM MURALIDHAR, University of Minnesota, DOUGLAS TREE, University of California Santa Barbara, KEVIN DORFMAN, University of Minnesota — The description of properties of DNA confined in a nanochannel with size close to its persistence length represents a major challenge to current theories. Accurate description of DNA in a nanochannel is essential for understanding many applications ranging from DNA translocation to genome mapping technology. We study the effect of channel confinement on DNA conformations using coarse-grained Langevin dynamics. Capturing the electrostatically-driven structural dependence is important for understanding many biological systems. Here, we use single molecule manipulation experiments to collect force-extension behavior on hyaluronic acid (HA), a polysaccharide which is a major component of the extracellular matrix in all vertebrates. By measuring HA elasticity in a variety of salt conditions, we are able to directly assess the contribution of electrostatics to the chain’s self-avoidance and local stiffness. Similar to recent results from a group on single-stranded nucleic acids, our data indicate that HA behaves as a swollen chain of electrostatic blobs, with blob size proportional to the solution Debye length. Our data indicate that the chain structure within the blob is not worm-like, likely due to long-range electrostatic interactions. We discuss potential models of this effect.

12:27PM T33.00007 Electrophoresis of a polyelectrolyte attached to a solid object: A strong influence of the attachment point
MYKKYA V. CHUBYSKYY, GARY W. SLATER, University of Ottawa — In some applications of electrophoresis, a polyelectrolyte (such as the DNA) is attached to an electrically neutral object of an irregular shape (e.g., a globular protein). Because of the hydrodynamic interactions (HI) between the polymer and the object, the amount by which the polymer is slowed down should depend on the shape of the object, especially near the attachment point, and not only on its drag coefficient. To study this effect, we compute the electrophoretic mobility of a short neutral tube closed at one end with a charged polymer attached to the closed end, either inside or outside the tube. Both the polymer and the tube are represented as sets of beads and the HI are pre-averaged. For a short polymer that would occupy only a small part of the tube, the mobility is much lower when the polymer is inside than when it is outside. The mobility ratio depends exponentially on the tube length and exceeds an order of magnitude already when the length of the tube equals its width. As the polymer size is increased and the coil size approaches the tube length, the mobility in the case of inside attachment starts to grow rapidly and then quickly approaches that in the case of outside attachment.

12:39PM T33.00008 Electrostatic effects on hyaluronic acid configuration
JOHN BEREZNEY, OMAR SALEH, University of California, Santa Barbara — In systems of polyelectrolytes, such as solutions of charged biopolymers, the electrostatic repulsion between charged monomers plays a dominant role in determining the molecular conformation. Altering the ionic strength of the solvent thus affects the structure of such a polymer. Capturing this electrostatically-driven structural dependence is important for understanding many biological systems. Here, we use single molecule manipulation experiments to collect force-extension behavior on hyaluronic acid (HA), a polyanion which is a major component of the extracellular matrix in all vertebrates. By measuring HA elasticity in a variety of salt conditions, we are able to directly assess the contribution of electrostatics to the chain’s self-avoidance and local stiffness. Similar to recent results from our group on single-stranded nucleic acids, our data indicate that HA behaves as a swollen chain of electrostatic blobs, with blob size proportional to the solution Debye length. Our data indicate that the chain structure within the blob is not worm-like, likely due to long-range electrostatic interactions. We discuss potential models of this effect.
1:15PM T33.00011 Molecular Dynamics study on the Micellization of Rhamnolipids. ELANGO MUNUSAMY, STEVEN D. SCHWARTZ, Department of Chemistry and Biochemistry, University of Arizona, Tucson, AZ 85721 — Oil spills have become one of the most serious environmental and ecological problems owing to the growth of oil exploitation, production and transportation. Millions of gallons of crude oil are released into the environment each year. Large volumes of surfactants are applied to the ocean as a remediation strategy. Environmental and toxicity issues arise when such a voluminous amounts of chemical surfactants are applied. One prospective solution to this problem is to use greener surfactants that possess excellent biodegradation and toxicity characteristics relative to existing classes of commonly used surfactants. In this context, we are interested in designing and developing greener surfactants that are patterned after naturally occurring glycolipids. In the present work, we concentrate on one of the more commonly studied glycolipid, rhamnolipid (Rha2C10). Despite the available experimental data, the molecular structure, shape and geometry of micelles formed by rhamnolipid is unknown. Molecular Dynamics (MD) simulations were performed to understand the aggregation behavior of rhamnolipids in aqueous solution and at air-water interface. All calculations were performed in NPT ensembles at 300 K using NAMD 2.8, a parallel code designed for high-performance simulation of large biological macromolecules where we use the CHARMM force field. The results obtained from MD simulations on the aggregation of rhamnolipids in water and at air-water interface will be presented.

1:27PM T33.00012 Combining Protein Dynamics and Aggregation Measurements, CURTIS MEUSE, NIST - Natl Inst of Stds & Tech — Infrared spectroscopy has long been used to deduce concentration and structural descriptions of proteins in a variety of static and time resolved experiments. We have developed an infrared order parameter to describe protein conformation variations around the average molecular value. Here we compare our parameter to other techniques including small angle scattering and atomic force microscopy measurements to clarify the characterization of protein structure and aggregation. By combining the information from our suite of methods, we explore the relationship between protein stability, dynamics and aggregation. Our focus is on developing new methods to compare the structure, dynamics and function of nearly identical biopharmaceutical protein ensembles. Examples include lysozyme, albumin cytchrome c and the characterization of amylod beta during aggregation.

1:39PM T33.00013 Wide Field Spectroscopy of Diffusing and Interacting DNA Using Tunable Nanoscale Geometries1, SHANE SCOTT, JASON LEITH, HUGO BRANDAO, SIMON SEHAYEK, ALEXANDER HOFKIRCHNER, JILL LAURIN, DANIEL BERAUD, ALEXANDER VERGE, PAUL WISEMAN, SABRINA LESLIE, McGill University — It remains an outstanding challenge to directly image interacting and diffusing biomolecules under physiological conditions. Many biochemical questions can be posed in the form: Does A interact with B? What are the energetics, kinetics, stoichiometry, and cooperativity of this interaction? To tackle this challenge, we use tunable nanoscale confinement to perform wide-field imaging of interacting DNA molecules in free solution, under an extended range of reagent concentrations and interaction rates. We present the integration of “Convex Lens-induced Confinement (CLIC)” microscopy with image correlation analysis, simultaneously suppressing background fluorescence and extending imaging times. The measured DNA-DNA interactions would be inaccessible to standard techniques but are important for developing a mechanistic understanding of life-preserving processes such as DNA transcription.

1 NSERC

1:51PM T33.00014 Observation of DNA dynamics near silicon nanopores by controlling the ultraviolet light spot, HIROHITO YAMAZAKI, SHINTARO ITO, KEIKO ESASHIKA, TOSHIHARU SAIKI, Keio University — Biopolymer translocation through a nanopore is an attractive phenomenon in the field of biophysics. When the voltage is applied through a nanopore, DNA coils thread into a nanopore by deforming its coil structure and recoil after translocation through a nanopore. Because DNA coil structure is relative with DNA translation, DNA dynamics near a nanopore have a correlation with DNA translocation. To investigate DNA dynamics, we developed the optical nanopore detection system, which has a capability to observe DNA dynamics near nanopore at sub-100-nm and sub-millisecond resolutions. Here, we report our experimental results of DNA dynamics near nanopores by controlling position of light spots. Because silica has high refractive index and extinction coefficient at ultraviolet light, the ultraviolet light creates z- and x-polarized light spot, which locate on nanopores and 50 nm apart from nanopores, respectively. By controlling light polarization, we observed different fluorescence intensity traces between z- and x-polarized light spot. The experimental results showed that fluorescence intensity trance of z-polarized light spot decayed faster than that of x-polarized light spot, which explain DNA dynamics near nanopores change by position from nanopores.

2:03PM T33.00015 Tension-induced binding of semiflexible biopolymers1, PANAYOTIS BENETATOS, Dept. of Physics, Kyungpook National University, Rep. of Korea, ALICE VON DER HEYDT, Inst. for Theoretical Physics, University of Gottingen, Germany, ANNETTE ZIPPELIUS, Inst. for Theoretical Physics at University of Gottingen and Max-Planck Inst. for Dynamics and Self-Organization, Germany — We investigate theoretically the effect of polymer tension on the collective behaviour of reversible cross-links. We use a model of two parallel-aligned, weakly-bending wormlike chains with a regularly spaced sequence of binding sites subjected to a tensile force. Reversible cross-links attach and detach at the binding sites with an affinity controlled by a chemical potential. In a mean-field approach, we calculate the free energy of the system and we show the emergence of a free energy barrier which controls the reversible (un)binding. The tension affects the conformational entropy of the chains which competes with the binding energy of the cross-links. This competition gives rise to a sudden increase in the fraction of bound sites as the polymer tension increases. The force-induced first-order transition in the number of cross-links implies a sudden force-induced stiffening of the effective stretching modulus of the polymers. This mechanism may be relevant to the formation and stress-induced strengthening of stress fibers in the cytoskeleton.

1 We acknowledge support by the Deutsche Forschungsgemeinschaft (DFG) via grant SFB-937/A1.

12:51PM T33.00009 Nuclear Pore Complex Protein Sequences Determine Overall Copolymer Brush Structure and Function?, DAVID ANDO, University of California, Merced, YONGWOOON KIM, KAIST, South Korea, ROYA ZANDI, University of California, Riverside, MICHAEL COLVIN, MICHAEL REXACH, AJAY GOPINATHAN, University of California, Merced — Disordered proteins are an interesting class of unfolded protein biopolymers which are functionally versatile. Their sequences are unconstrained by a structure-sequence relationship, and allow for a wide range of chemical and physical polymer properties. The Nuclear Pore Complex (NPC) contains over one hundred of such proteins (FG nups), which collectively function to regulate the exchange of all materials between the nucleus and cytoplasm. We perform coarse grained simulations of both individual FG nups and grafted rings of nups mimicking the in vivo geometry of the NPC, complemented with polymer brush modeling. Our results indicate that different regions or “blocks” of an individual FG nup can have distinctly different forms of disorder and that this property appears to be a conserved feature across eukarya. Furthermore, this block structure at the individual protein level is critical to the formation of a unique higher-order polymer brush architecture. The interactions between FG nups may be modulated by certain forms of transport factors, our results indicate that transitions between brush morphologies could play an important role in regulating transport across the NPC, suggesting novel forms of gated transport across membrane pores with wide biomimetic applicability.
Thursday, March 5, 2015 11:15AM - 2:03PM –
Session T34 GERA DMP FIAP: Materials for Electrochemical Energy Storage I 210A -

11:15AM T34.00001 Vortex Stabilized Compressed Fusion Grade Plasma1. ADY HERSHCOVITCH, Brookhaven National Laboratory — Inertial confinement fusion schemes comprise of highly compressed dense plasmas. Some involve short pulses of powerful beams (lasers, particles) applied to solid pellets, while others utilize plasma focus to obtain dense pinch plasmas. Although compression factor >1000 has been achieved for starting pressures in the Torr range, the latter is limited by instabilities for initial gas density above 10 Torr. One alternative approach could be shooting electron beams through very dense, atmospheric pressure, vortex stabilized plasma. Large azimuthal magnetic generated by an electron beam can compress and heat the plasma to fusion viable parameters. This configuration is stable against sausage, kink, or beam – plasma instabilities. Based on experimental evidence beam propagation through the plasma is not be an issue. A second possibility is to tangentially squeeze a quasi-neutral plasma focus flow by a surrounding gas vortex. Based on currently available electron beams, the first scheme viability as an electrical power generating reactor does not seem to be promising. But using a plasma cathode electron beam that was developed a while ago, for which DOE has a patent U.S. Patent 4,942,339, could result in net generation of electricity. Calculations will be presented.

3Work supported by Work supported under Contract No. DE-AC02-98CH1-886 with the US Department of Energy.

11:27AM T34.00002 High Thermal Conducting Boron Arsenide: Crystal Growth and Characterization2, BING LV, YUCHENG LAN, TcSUH and Department of Physics, Univ. of Houston, XIQU WANG, TcSUH and Department of Chemistry, Univ. of Houston, QIAN ZHANG, TcSUH and Department of Physics, Univ. of Houston, YONGJIE HU, Dept. of Mechanical Engineering, Massachusetts Institute of Technology, ALLAN J. JACOBSON, TcSUH and Department of Chemistry, Univ. of Houston, DAVID BROIDO, Department of Physics, Boston College, GANG CHEN, Dept. of Mechanical Engineering, Massachusetts Institute of Technology, ZHIFENG REN, CHING-WU CHU1, TcSUH and Department of Physics, Univ. of Houston — Intrigued by recent calculations [Phys. Rev. Lett. 111, 025901(2013)] which predict a remarkably high thermal conductivity of \( \sim 2,000 \text{ Wm}^{-1}\text{K}^{-1} \), comparable to that of diamond, in cubic boron arsenide (BAs) crystals, we have succeeded in synthesizing single crystals of BAs with a zinc blende structure and lattice parameters of \( a = 4.7830(7) \text{ Å} \) characterized by X-ray single crystal diffraction and transmission electron microscopy (TEM). A relatively high thermal conductivity is obtained but still smaller than the predicted value. We attribute the difference of thermal conductivity value to the defect scattering associated with crystal twinning and As vacancies, verified both from experimental evidence and theoretical calculations. The predicted super-thermal-conductivity may be achieved in BAs single crystals with further improvement of crystal growth by removing the defects.

2Lawrence Berkeley National Laboratory, Berkeley California 94720

11:39AM T34.00003 Soft Fusion Energy Path: Isotope Production in Energy Subcritical/Economy Hypercritical D+D Colliding-Beam Mini Fusion Reactor ‘Exyder3’. TIM HESTER, BOGDAN MAGLICH, California Science & Engineering Corporation (CALSEC), CALSEC COLLABORATION — Bethe1 and Sakharov2 argued for soft fusion energy path via isotope production, substantiated by Manheimer3. - Copious T and 1He production4,5 from D(d, p) T and D(d, n) 1He reactions in 725 KeV D+D colliding beams was measured in weak-focusing Self-Collider6,7 radius 0.15 m, in B = 3.12 T, non-linearly stabilized by electron cloud oscillations8 to confinement time = 24 s. Simulations6 predict that by switching to strong focusing9, 10 deuterons 0.75 MeV each, generate 1 1He + IT +1p +1n at total input energy cost 10.72 MeV. Economic value of T and 3He are 65 and 120 MeV/atom, respectively. We obtain economic gain 205MeV/10.72 MeV \( \sim 2,000\% \) i.e. 1He production funds cost of T. If first wall is made of Thorium n’s will breed \( ^{235}U \) releasing 200 MeV/fission, at neutron cost 5.36 MeV versus 160 MeV in beam on target, resulting in no cost 1He production, valued $75K/g. 1. Physics Today, May 1979, p.44; 2. Memoirs, Vintage Books, (1992); 3. Phys. Today, May 2012 p. 12; 4. Phys. Rev. Lett. 54, 796 (1985); 5. Bull. APS, 57, No. 3 (2012); 6. Part. Acc.1, (1970); 7. AНЕУТРОНИЧЕСКАЯ ФИЗИКА NIM A 271 1-167 (1988); 8. Phys. Rev. Lett. 70, 1818 (1993); 9. Part. Acc. 34, 13 (1990).

11:51AM T34.00004 Evidence for Critical Energy for Ion Confinement in Magnetic Fusion Reactors, BOGDAN MAGLICH, TIM HESTER, DAN SCOTT, California Science & Engineering Corporation (CALSEC), CALSEC COLLABORATION — It is shown here that fusion test reactors could not ignite for half-a-century because trials were conducted at thermonuclear ion energies 10-30 KeV, an order of magnitude lower than critical energy [1-2], \( E_c \sim 200 \text{ KeV} \). At subcritical energies, plasma is destroyed by neutralization of ions via lookedover atomic (non-nuclear) charge transfer collisions with giant cross-section, \( 10^9 \text{ barns} \), 100 times greater than that for ionization collisions that counters neutralization. Neutral injection sets limit on ion magnetic confinement time \( <10^{-15} \text{ s vs. } >1 \text{ s} \) required for ignition. In contrast, at energies above \( E_c \), ionization prevails; near \( >1 \text{ MeV} \), stable confinement of 20 s was routinely observed [3] with charged injection. - To render ITER viable, ion energy must be increased to \( >1 \text{ MeV} \); neutral radioactive DT fuel replaced with charged, nonradioactive deuterium, giving rise to compact aneutronic reactor with direct conversion into RF power [4].

1[1] Physics Scripta, 23, 143 (1981);

12:03PM T34.00005 High Performance and Economic Supercapacitors for Energy Storage Based on Carbon Nanomaterials1, VLADIMIR SAMUULOVIĆ, BEHZAD FARSHID, ALEXANDER FRENKEL, Department of Materials Science and Engineering, Sensor CAT, State University of New York at Stony Brook, Stony Brook, NY 11794-2275, USA, SENSOR CAT AT STONY BROOK TEAM — We designed and manufactured very inexpensive prototypes of supercapacitors for energy storage based on carbon nanomaterials comprised of: reduced graphene oxide (RGO) and carbon nanotubes (CNTs) as electrodes filled with polymer gel electrolytes. The electrochemical properties of supercapacitors made using these materials were compared and analyzed. A significant tradeoff between the energy density and the power density was determined; RGO electrodes demonstrated the highest energy density, while composite RGO/CNT electrodes showed the highest power density. The thickness of the RGO electrode was varied to determine its effect on the power density of the supercapacitor and results showed that with decreasing electrode thickness power density would increase. The specific capacitances of over 600 F/g were observed.
12:15PM T34.00006 Nanoporous Hydrogen-Reduced BiVO$_4$: better charge separation with Ni-B, Electrocatalysts for Photoelectrochemical Water Oxidation, JIAYONG GAN, YUEBING ZHENG, Department of Mechanical Engineering, Materials Science and Engineering Program, and Texas Materials Institute, The University of Texas at Austin — Layered Li-excess Li$_2$MnO$_3$ has been of great interest for lithium-ion battery cathodes because of its high theoretical capacity. The compound is also an important component in Li$_2$MnO$_3$:1−x)LiMO$_2$ and other high-capacity cathode materials. It has been reported that Li$_2$MnO$_3$ can be made electrochemically active by acid leaching or charging to high voltages. Several different mechanisms have been proposed to explain its unconventional lithium extraction behavior, including one that involves oxidation at the oxygen site. In this talk, we will present a comprehensive computational approach based on first-principles hybrid density functional defect calculations, and illustrate how it helps uncover the defect physics and chemistry and the intrinsic mechanisms for delithiation and electronic and ionic conduction in layered Li$_2$MnO$_3$. In light of our results, we discuss the relevance of the proposed mechanisms and suggest solutions for improving the electronic conduction and hence the electrochemical performance of Li$_2$MnO$_3$ and related materials.

12:27PM T34.00007 Uncovering the intrinsic delithiation mechanism in Li-excess Li$_2$MnO$_3$ through defect calculations, KHANG HOANG, North Dakota State University — Layered Li-excess Li$_2$MnO$_3$ has been of great interest for lithium-ion battery cathodes because of its high theoretical capacity. The compound is also an important component in Li$_2$MnO$_3$:1−x)LiMO$_2$ and other high-capacity cathode materials. It has been reported that Li$_2$MnO$_3$ can be made electrochemically active by acid leaching or charging to high voltages. Several different mechanisms have been proposed to explain its unconventional lithium extraction behavior, including one that involves oxidation at the oxygen site. In this talk, we will present a comprehensive computational approach based on first-principles hybrid density functional defect calculations, and illustrate how it helps uncover the defect physics and chemistry and the intrinsic mechanisms for delithiation and electronic and ionic conduction in layered Li$_2$MnO$_3$. In light of our results, we discuss the relevance of the proposed mechanisms and suggest solutions for improving the electronic conduction and hence the electrochemical performance of Li$_2$MnO$_3$ and related materials.

12:39PM T34.00008 Bias-dependent local structure of water molecules at an electrochemical interface$^1$, LUANA PEDROZA, ICTP-SAIFR - Brazil, PEDRO BRANDIMARTE, University of Sao Paulo - Brazil, ALEXANDRE R. ROCHA, IFT-UNESP, Brazil, MARIVI FERNANDEZ-SERRA, Stony Brook University — Following the need for new - and renewable - sources of energy worldwide, fuel cells using electrocatalysts can be thought of as a viable option. Understanding the local structure of water molecules at the interfaces of the metallic electrodes is a key problem. Notably the system is under an external potential bias, which makes the task of simulating this setup difficult. A first principle description of all components of the system is the most appropriate methodology in order to advance understanding of electrochemical processes. There, the metal is usually charged. To correctly compute the effect of an external bias potential applied to electrodes, we combine density functional theory (DFT) and non-equilibrium Green's functions methods (NEGF), with and without van der Waals interactions. In this work, we apply this methodology to study the electronic properties and forces of one water molecule and water monolayer at the interface of gold electrodes. We find that the water molecule has a different torque direction depending on the sign of the bias applied. We also show that it changes the position of the most stable structure indicating that the external bias plays an important role in the structural properties of the interface.

$^1$We acknowledge financial support from FAPESP.

12:51PM T34.00009 Effect of Transition Metal Ordering on the Electronic Properties of LiNi$_{1−x}$Co$_x$Mn$_2$O$_4$ Cathode Materials for Li-ion Batteries$^1$, ROBERTO LONGO, FANTAI KONG, SANTOSH KC, University of Texas at Dallas, USA, DONG-HEE YEON, JAEGU YOON, JIN-HWAN PARK, SEOK-KWANG DOO, Samsung Electronics, Republic of Korea, KYEONGJAE CHO, University of Texas at Dallas, USA, MSL TEAM, SAIT TEAM — Current Li-ion batteries use layered oxides as cathode materials, specially LiCoO$_2$ or LiNi$_{1−x}$Co$_x$Mn$_2$O$_4$ (NCM), and graphite as anode. Co alloyed oxides are taken from the high cost and toxicity of cobalt, together with certain instability at high operational temperatures. To overcome these difficulties, the synthesis of novel materials composed of layered oxides with different sets of Transition Metals (TM) has become the most successful way to solve the particular drawbacks of each single-oxide family. Although layered materials can deliver larger capacity than other families of cathode materials, the energy density has yet to be increased in order to match the expectations deposited on the NCM oxides. To acquire a high capacity, they need to be cycled at high operational voltages, resulting in voltage and capacity fading over a large number of cycles. In this work, we examine the phase diagram of the Li-Ni-Co-Mn-O system and the effect of TM ordering on the electronic properties of NCM cathode materials, using density-functional theory. Our findings will provide conceptual guidance in the experimental search for the mechanisms driving the voltage and capacity fading of the NCM family of cathode materials, in an attempt to solve such structural instability problems and, thus, improving the performance of the NCM cathode materials.

$^1$This work was supported by Samsung GRO project.

1:03PM T34.00010 Organic-inorganic hybrid lead iodide perovskite with zero-dipole-moment guanidinium (GA=[C(NH$_3$)$_3$])$^+$ cations: a Density Functional based analysis, GIACOMO GIORGI, Department of Chemical System Engineering, The University of Tokyo, JUN-ICHI FUJISAWA, HIROSHI SEGAWA, Research Center for Advanced Science and Technology, The University of Tokyo, KOICHI YAMASHITA, Department of Chemical System Engineering, The University of Tokyo — BiVO$_4$ photoanode material has attracted broad attention recently as an inexpensive and robust semiconductor for potential application for solar water oxidation. In comparison to pristine BiVO$_4$, the hydrogen-treated BiVO$_4$ (H-BiVO$_4$) show superior photocurrent and electron-hole separation yield of 0.95 at 1.23 V vs. reversible hydrogen electrode (RHE) due to enhanced carrier density and conductivity. Significantly, we adopt a layer of nickel-borate (Ni-B$_4$) complex on the BiVO$_4$ surface as an oxygen evolution catalyst. Modification of H-BiVO$_4$ photoanode with Ni-B$_4$ has yielded a large (∼300 mV) cathodic shift in the onset potential at pH 7. It shows an outstanding performance in the low bias region and the maximum power point for solar water oxidation was achieved at potential as low as 0.75 V vs. RHE with a photocurrent density of 2.25 mA/cm$^2$. We attribute these improved PEC performances to the enhanced charge separation, carrier density and conductivity in these photoanodes.

1:15PM T34.00011 Properties of adsorbed hydrogen films in nanospaces, ELMAR DOHNLKE, ANDREW GILLESPIE, PETER PFEIFER, University of Missouri Columbia — Various high surface area materials were evaluated for their gas storage properties. From supercritical hydrogen isotherms at 77 Kelvin, we estimated the adsorbed film densities, film thicknesses and intrapore gas densities. Intrapore gas density is a measurement of the average hydrogen density within a pore. Furthermore, we investigated the correlation between the isosteric heat of adsorption, surface chemistry, and pore size distribution with an adsorbed film. In most of the samples both saturated film densities and intrapore gas densities exceed the liquid hydrogen density at 1 bar and 20 Kelvin. The saturated film density surpassed it even by 40%. The adsorbed film seems to be independent of the isosteric heat of adsorption or the samples pore size distribution. They behave like a universal constant for all carbon-based surfaces.
1:27PM T34.00012 Pickering Emulsification to Mass Produce Nanoencapsulated Phase-change-material. XUEZHEN WANG, LECHENG ZHANG, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, 77843-3122, USA, S. SAM MANNAN, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, 77843-3122, USA, S. SAM MANNAN, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, 77843-3122, USA, YING CHEN, Soft matter center, Guangdong Province Key Laboratory on Functional Soft Condensed Matter, School of materials and energy, Guangdong University of Tec, ZHENGDONG CHENG, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, 77843-3122, USA. DR. CHENG'S GROUP TEAM — Phase changing materials (PCM) have useful applications in thermal management. However, mass production of micro and nano encapsulated PCM has been a challenge. Here, we present a simple and scalable method via a two-step Pickering emulsification method. We have developed interface active nanoparticles by asymmetric modification of nanoparticles of layered crystal materials. Nanoencapsulated PCM is realized with exfoliated monolayer nanoparticles surfactants using very little energy input for emulsification. Further chemical reactions are performed to convert the emulsions into core-shell structures. The resulted capsules are submicron in size with remarkable uniformity in size distribution. DSC characterization showed that the capssulation efficiency of NEPCM was 58.58% and was thermal stable which was characterized by the DSC data for the sample after 200 thermal cycling.

1:39PM T34.00013 Application of Henry’s Law for Binding Energies of Adsorbed Hydrogen. ANDREW GILLESPIE, ELMAR DOHNIKE, DAVID STALLA, MARK SWEANY, PETER PFEIFFER, University of Missouri — The method of isosteres is the simplest method used to calculate the differential enthalpy of adsorption. However, it is incredibly sensitive to the choice of model and respective fitting parameters. For a set of isotherms measured on a specific sample, most models converge upon a similar value at high coverage, but are inconsistent in the low pressure regime. In this talk, we investigate the application of various models for localized and mobile adsorption at low pressures in order to obtain binding energy of hydrogen to the adsorbent surface. Henry’s Law analysis of the Langmuir Model of adsorption yield binding energies in excellent agreement with those obtained from the Clausius Clapeyron relation.

1Work supported by DOE-EERE, Award No. DE-FG36-08GO18142

11:15AM T36.00001 Chiral and helical superfluid in cold atom system. XIAOHUI LI, TINGPONG CHOY, TAI-KAI NG, The Hong Kong University of Science and Technology — Recently, a chiral spin superfluid has been proposed in weakly interacting boson systems [1]. In this work, we study the properties of bosonic superfluids in a cold atom system with two inequivalent band minima in momentum space related by time reversal symmetry. The system is mapped into an effective spinor-boson model. Without additional symmetries we show that in general there are two possible phases in this model, a ferromagnetic (easy axis) phase and a “x-y” (easy plane) phase. In the presence of nonzero k-space Berry curvature at the two band minima points, we show that the ferromagnetic state is “chiral” and the x-y state is “helical.” The bulk and edge properties of these states are studied where the similarities and differences between the present bosonic superfluids and the corresponding fermionic superconductors are pointed out.


11:27AM T36.00002 Interplay between Kondo screening and local singlets in $SU(N)$-symmetric cold atoms. LEONID ISAEV, ANA MARIA REY, JILA, NIST and Department of Physics, University of Colorado, Boulder, CO, USA — We study collective phenomena in strongly interacting fermionic alkaline-earth atoms (AEAs) loaded in an optical lattice. Owing to the strong decoupling between electronic orbital and nuclear-spin degrees of freedom, AEAs prepared in the two lowest electronic states are predicted to obey an accurate $SU(N > 2I + 1)$ symmetry in their two-body collisions ($I$ is the nuclear spin). The $SU(N)$ symmetric models offer a great opportunity to generate exotic many-body behavior emerging from the increased degeneracy and strict conservation laws. We focus on a parameter regime that realizes an $SU(N > 2)$ (Caoqblin-Schrieffer) generalization of the usual Kondo lattice model, and show that for band fillings above one atom per site, the system exhibits a peculiar interplay between Kondo screening and formation of singlets between localized atoms. In the limit of large Kondo coupling, we derive an effective Hamiltonian and determine its phase diagram. Our results can be tested in experiments with ultracold $^{173}$Yb or $^{87}$Sr atoms and are relevant for the physics of heavy-fermion materials with magnetic frustration.

1Supported by AFOSR, MURI-AFOSR and NSF.

11:39AM T36.00003 Chiral magnetism and spontaneous spin Hall effect of interacting Bose superfluids. XIAOPENG LI, STEFAN NATU, Univ of Maryland-College Park, ARUN PARAMEKANTI, University of Toronto — Recent experiments on ultracold atoms in optical lattices have synthesized a variety of tunable bands with degenerate double-well structures in momentum space. Such degeneracies in the single particle spectrum strongly enhance quantum fluctuations, and may lead to exotic many-body ground states. We consider weakly interacting spinor Bose gases in such bands, and discover a universal quantum “order by disorder” phenomenon which selects a novel chiral spin superfluid with remarkable properties such as spontaneous anomalous spin Hall effect and momentum space antiferromagnetism. For bosons in the excited Dirac band of a hexagonal lattice, such a state supports staggered spin loop currents in real space. We show that Bloch oscillations provide a powerful dynamical route to quantum state preparation of such a chiral spin superfluid. Our predictions can be readily tested in spin resolved time-of-flight experiments.

1QI-NSF-PFC, ARO-Atomtronics-MURI, NSERC of Canada.
11:51AM T36.00004 Engineering Ferromagnetism with Shaken Optical Lattices1, COLIN PARKER.
University of Chicago — Conventional methods of quantum simulation rely on kinetic energy determined by free particle dispersions or simple sinusoidal optical lattices. Solid state systems, by contrast, exhibit a plethora of band structures which differ quantitatively, qualitatively, and even topologically. To what extent does this variety explain the many electronic phenomena observed in these materials? Here we address this question by subjecting an otherwise simple Bose superfluid to a customized band structure engineered by dynamically phase modulating (shaking) an optical lattice. The engineered dispersion contains two minima which we associate with a pseudospin degree of freedom. Surprisingly, in such a system the Bose superfluid exhibits many new behaviors. The pseudospin develops a ferromagnetic order, which can lead to polarization of the entire sample or to sub-division into polarized domains. The excitations of the system also exhibit the roton-maxon structure associated with strong interactions in superfluid helium. I will also discuss recent progress on engineering further exotic behavior.

1Work supported by NSF MRSEC (DMR-0820054), NSF Grant No. PHY-0747907 and ARO-MURI W911NF-14-1-0003

12:27PM T36.00005 Weyl Superfluidity in a Three-dimensional Dipolar Fermi Gas, BO LIU,
Department of Physics and Astronomy, University of Pittsburgh, XIAOPENG LI, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland, LAN YIN, School of Physics, Peking University, W. VINCENT LIU, Department of Physics and Astronomy, University of Pittsburgh & Wilsen Quantum Center, Zhejiang University of Technology — Weyl superconductivity or superfluidity, a fascinating topological state of matter, features novel phenomena such as emergent Weyl fermionic excitations and anomalies. Here we report that an anisotropic Weyl superfluid state can arise as a low temperature stable phase in a 3D dipolar Fermi gas. A crucial ingredient of our model is a direction-dependent two-body effective attraction generated by a rotating external field. Experimental signatures are predicted for cold gases in radio-frequency spectroscopy. The finite temperature phase diagram of this system is studied and the transition temperature of the Weyl superfluidity is found to be within the experimental scope for atomic dipolar Fermi gases. Work supported in part by U.S. ARO, AFOSR, DARPA-OLE-ARO, Charles E. Kaufman Foundation and The Pittsburgh Foundation, JQI-NSF-PFC, ARO-Atomtronics-MURI, and NSF of China.

12:39PM T36.00006 Spin liquid phases of large spin Mott insulating ultracold atoms, TODD C. RUTKOWSKI, Binghamton Univ, MICHAEL J. LAVALER, Binghamton Univ, Cornell Univ — Understanding exotic forms of magnetism, primarily those driven by large spin fluctuations such as the quantum spin liquid state, is a major goal of condensed matter physics. But, the relatively small number of viable candidate materials poses a difficulty. We believe this problem can be solved by Mott insulating ultracold atoms with large spin moments that interact via whole-atom exchange. The large spin fluctuations of this exchange could stabilize exotic physics similar to condensed matter systems, all in an extremely tunable environment. We have approached the problem by performing a mean field theory for spin-f bosons in an optical lattice which is exact in the large-f limit. This setting is similar to that of SU(N) magnetism proposed for alkali-earth atoms but without the SU(N) symmetry. We find that states with long-range order, such as the spin nematic phase of f = 1 Na atom, become highly entangled spin-liquid-like states for f = 3 Cr atoms. This is evidence that the magnetic phase diagram for Mott insulating atoms at larger spins generically contains exotic forms of magnetism.


12:51PM T36.00007 Superfluid-insulator transition in a fermionic optical superlattice, RUBEM MONDAINI, The Pennsylvania State University, PREDRAG NIKLIC, George Mason University, MARCOS RIGOL, The Pennsylvania State University — Despite some of the high-temperature superconductivity properties can be expected in clean and simple cold-atom systems, attempts to simulate the d-wave pairing of cuprates with cold atoms is difficult because the required temperatures are much lower than what is experimentally feasible today. However, the “pseudogap” physics of s-wave pairing is far more accessible. In this paper we consider a simple Mott insulator of tightly bound Cooper pairs as an s-wave analogue of a pseudogap state. The XY transition to a superfluid and the crossover to a band-insulator (conventional unpaired state) in the phase diagram are the phenomena that give this Mott insulator a similar role to the pseudogap of cuprates. We numerically investigate this transition of locally attractive fermions at half-filling and T = 0 in the presence of a checkerboard potential in two dimensions, using quantum Monte Carlo and exact diagonalization. We can identify that it belongs to (2+1)-XY universality class similarly to the superfluid-normal transition in hard-core bosons. Moreover, we show a crossover of charge excitations, in finite systems, from a fermionic to bosonic character when the attraction between the fermions is increased.

1:03PM T36.00008 Spin Liquid Condensate of Spinful Bosons, BIAO LIAN, SHOUCHENG ZHANG, Stanford Univ — We introduce the concept of a bosonic spin liquid condensate (SLC), where spinful bosons in a lattice form a zero-temperature spin disordered charge condensate that preserves the spin rotation symmetry, but breaks the U(1) symmetry due to a spinless order parameter with charge one. It has an energy gap to the spin excitations, and shows many features of SLC. Here we show this SLC shows many behaviors of spin-1/2 fermions. In particular, we analyze the SLC phase diagram in the spin 1/2 case using a mean-field variational wave function method. We show that the SLC shows many new behaviors of spin-1/2 fermions in SLC.

1:15PM T36.00009 Ultracold Molecules in Crystals of Light: A Highly Tunable System for Exploring Novel Materials, Quantum Dynamics, and Quantum Complexity1, LINCOLN CARR, KENJI MAEDA, Colorado Sch of Mines, MICHAEL L. WALL, JILLA, NIST and U. Colorado Boulder — Ultracold molecules trapped in optical lattices present a new regime of physical chemistry and a new state of matter: complex dipolar matter. Such systems open up the prospect of tunable quantum complexity. We present models for the quantum many-body statics and dynamics of present experiments on polar bi-alkali dimer molecules. We are developing Hamiltonians and simulations for upcoming experiments on dimers beyond the alkali metals, including biologically and chemically important naturally occurring free radicals like the hydroxyl free radical (OH), as well as symmetric top polyatomic molecules like methyl fluoride (CHF3). These systems offer surprising opportunities in modeling and design of new materials. For example, symmetric top polyatomics can be used to study quantum molecular magnets and quantum liquid crystals. We use matrix-product-state (MPS) algorithms, supplemented by exact diagonalization, variational, perturbative, and other approaches. MPS algorithms not only produce experimentally measurable quantum phase diagrams but also explore the dynamical interplay between internal and external degrees of freedom inherent in complex dipolar matter. We maintain open source code (openTEBD and openMPS) available freely and used widely.

1 Funded by NSF and AFOSR

1:27PM T36.00010 Spontaneous quantum Hall effect in an atomic spinor Bose-Fermi mixture, ZHI-FANG XU, University of Pittsburgh, XIAOPENG LI, Univ of Maryland-College Park. PETER ZOLLER, University of Innsbruck, W. VINCENT LIU, University of Pittsburgh — We study a mixture of spin-1 bosonic and spin-1/2 fermionic cold atoms, e.g., Rb-87 and Li-6 confined in a triangular optical lattice. With fermions at 3/4 filling, Fermi surface nesting leads to spontaneous formation of various spin textures of bosons in the ground state, such as collinear, coplanar and even non-coplanar spin orders. The phase diagram is mapped out with varying boson tunneling and Bose-Fermi interactions. Most significantly, in one non-coplanar state the mixture is found to exhibit spontaneous quantum Hall effect in fermions and crystalline superfluidity in bosons, both driven by interaction.

[1] C. Senko, P. Richerme, J. Smith, A. Lee, I. Cohen, A. Retzker, and C. Monroe. “Experimental Realization of a Quantum Integer-Spin Chain with Controllable Chain should be experimentally realizable in a recently developed trapped-ion quantum simulator [1]. Our work will enable further study of various topological algorithms, and is also consistent with analytical calculations using renormalization group theory. The topological phase of this long-range interacting spin-1 chain should be experimentally realizable in a recently developed trapped-ion quantum simulator [1]. Our work will enable further study of various topological phases under the presence of long-range interactions.

MAD MAGHREBI, MICHAEL FOSS-FEIG, ALEXEY GORSHKOV, Joint Quantum Institute, NIST/University of Maryland — Topological phases of matter, including symmetry protected topological phases, typically require the underlying many-body system to possess only short-range interactions, such that the notion of locality is well defined. Whether various topological phases can survive in the presence of long-range interactions, however, is largely unknown. Here we show that a paradigmatic example of a symmetry protected topological system, known as the spin-1 Haldane chain, surprisingly remains in its topological phase under arbitrary algebraically-decaying long range interactions. Our conclusion is supported by strong numeric evidence using variational Matrix Product State (vMPS) algorithms, and is also consistent with analytical calculations using renormalization group theory. The topological phase of this long-range interacting spin-1 chain should be experimentally realizable in a recently developed trapped-ion quantum simulator [1]. Our work will enable further study of various topological phases under the presence of long-range interactions.


2:03PM T36.00013 Stoner ferromagnetism in a thermal pseudospin-1/2 Bose gas, JURAJ RADIC, STEFAN NATU, VICTOR GALITSKI, Joint Quantum Institute, NIST/University of Maryland — We compute the finite-temperature phase diagram of a pseudospin-1/2 Bose gas with contact interactions, using two complementary methods: the random phase approximation and self-consistent Hartree-Fock theory. We show that the spin-dependent interactions, which break the (pseudo) spin-rotational symmetry, generally lead to the appearance of a magnetically ordered phase at temperatures above the superfluid transition. In three dimensions, we predict a normal easy-axis/easy-plane ferromagnet for sufficiently strong repulsive/attractive inter-species interactions respectively. The normal easy-axis ferromagnet is the bosonic analog of Stoner ferromagnetism known in electronic systems. For the case of inter-species attraction, we also discuss the possibility of a bosonic analogue of the Cooper paired phase. This state is shown to significantly lose in energy to the transverse ferromagnet in three dimensions, but is more energetically competitive in lower dimensions. Extending our calculations to a spin-orbit-coupled Bose gas with equal Rashba and Dresselhaus-type couplings (as recently realized in experiment), we investigate the possibility of stripe ordering in the normal phase. Within our approximations however, we do not find an instability towards stripe formation.

Thursday, March 5, 2015 11:15AM - 2:15PM — Session T37 GQI: Focus Session: Semiconductor Qubits - Optically Addressed Dots and Impurities II 212A - Danny Kim, HRL Laboratories, LLC

11:15AM T37.00001 All-optical coherent control of energy transfer between a quantum dot and a cavity mode, TAO CAI, RANOJOY BOSE, KAUSHIK CHOUDHURY, Department of Electrical Engineering, University of Maryland, College Park, GLENN SOLOMON, Joint Quantum Institute, University of Maryland, College Park and National Institute of Standards and Technology, Gaithersburg, EDO WAKS, Department of Electrical Engineering, University of Maryland, College Park — Here we demonstrated all-optical coherent control of energy transfer in a quantum dot strongly coupled to a photonic crystal molecule at optical frequency. The photonic crystal molecule comprises two photonic crystal cavities, supporting a pair of strongly coupled normal modes. One of the modes strongly couples with a quantum dot and the other induces a cavity enhanced a.c. Stark shift to rapidly tune the quantum dot resonance on timescales much shorter than the vacuum Rabi period of the strongly coupled dot-cavity system. The quantum dot initially detunes from the cavity mode. By tuning the quantum dot onto resonance with the cavity mode on picosecond timescales, we achieved coherent transfer of energy between a quantum dot and the cavity mode through vacuum Rabi oscillation. We investigated the energy transfer as a function of stark laser power to confirm the coherence of the energy transfer process. We further demonstrated coherent control of light-matter states by implementing a Ramsey-type experiment. These results pave the path for achieving gigahertz controlled generation of quantum states of light and synthesis of photon wavefunctions using integrated semiconductor nano-photonic platform.

11:27AM T37.00002 Control of the cavity reflectivity using a single quantum dot spin, SHUO SUN, HYOCHUL KIM, Univ of Maryland-College Park, GLENN SOLOMON, NIST, EDO WAKS, Univ of Maryland-College Park — The implementation of quantum network and distributive quantum information processing relies on interaction between stationary matter qubits and flying photons. The spin of a single electron or hole confined in a quantum dot is considered as promising matter qubit as it possesses microsecond coherence time and allows picosecond timescale control using optical pulses. The quantum dot spin can also interact with a photon by controlling the optical response of a strongly coupled cavity. Yet all the experimental demonstrations of the cavity spectrum control have used neutral dots. The spin-dependent cavity spectrum for a strongly coupled charged quantum dot and cavity system has not been reported. Here, we report an experimental realization of a spin-photon interface using a strongly coupled quantum dot and cavity system. We show large modulation of the cavity reflection spectrum by manipulating the spin states of the quantum dot. The spin-photon interface is crucial for realizing a quantum logic gate or generating hybrid entanglement between a quantum dot spin and a photon. Our results represent an important step towards semiconductor based quantum logic devices and on-chip quantum networks.
11:39AM T37.0003 Optical Control of Semiconductor Quantum Dot Spin Qubits with Microcavity Exciton-Polaritons , SHRUTI PURI1, PETER L. McMAMON, Ginzton Laboratory, Stanford University, YOSHISUI YAMAMOTO2, Ginzton Laboratory, Stanford University and National Institute of Informatics, Tokyo — The work being presented was carried out at Stanford University. Currently the author is at University of Sherbrooke, Canada

11:51AM T37.0004 Explorations with a new qubit system: Exchange Interactions between Quantum Dot Spin Qubits and Quantum Well Excitons1, PETER McMAMON, Stanford University - Ginzton Lab — In this talk I will present some of our recent work on constructing and optically investigating nanostructures consisting of quantum dots coupled to a nearby quantum well, all embedded in a planar microcavity. The overall goal of this line of work is to develop a platform in which long-range (∼1 micron) two-qubit interactions between quantum dots are possible, following the pioneering proposal of Piermarocchi, Chen, Sham, and Steel (Phys. Rev. Lett. 89 (16) 167402 [2002]). We have succeeded in demonstrating several fundamental aspects of this platform. We have realized a coupled exciton-dot–quantum–well system in a microcavity, and show that quantum dots in this system can be charged (allowing the storage of a spin qubit), and show that both the quantum dots and the quantum well retain favourable optical properties. Most importantly, we have fairly strong evidence suggesting that the operative mechanism of the theoretical proposals, the spin-dependent exchange interaction, is achievable, and an exciton in the quantum well, is observable, and can be engineered to be of the magnitude required for the implementation of universal quantum gate and state manipulation operations. I will discuss these results, and highlight other recent work on site-controlled quantum dots, including with quantum dots in positioned nanowires.

1This work was primarily supported by the JSPS through its FIRST program.

12:27PM T37.0005 Proposed method of optical spin read-out in a quantum dot using the AC Stark effect, EDWARD FLAGG, GARY LANDER, CABOT ZABRISKIE, West Virginia University — We propose a method to read-out the spin-state of a single electron trapped in a quantum dot via a cycling transition induced by the AC Stark effect. Optical spin initialization and manipulation are allowed by a magnetic field in the Voigt configuration, which modifies the polarization selection rules of the transitions. The lack of a cycling transition in the Voigt configuration, however, makes read-out of the spin-state very difficult. We show that cycling transitions can be made possible by a red-detuned, circularly-polarized laser, which modifies the spin eigenstates and polarization selection rules via the AC Stark effect.

12:39PM T37.0006 Ground state initialization in a doubly-charged, vertically-stacked InAs quantum dot molecule1, AARON ROSS, COLIN CHOW, Department of Physics, University of Michigan, LU SHAM, University of California San Diego, ALLAN BRACKER, DANIEL GAMMON, Naval Research Laboratory, DUNCAN STEEL, Department of Physics, University of Michigan — We report on the rapid optical initialization of a subset of the two-electron ground states of a self-assembled, vertically stacked InAs quantum dot molecule, where the states of the electron are approximately localized to separate quantum dots with very little spatial overlap. Four eigenstates, a singlet and three triplets (S, T0, T−1, T−2), arise from the exchange coupling and are identified via bias-dependent photoluminescence measurements. The degeneracy of the triplet states is lifted using an in-plane magnetic field (Voigt geometry). This allows for the determination of the in-plane electron and hole g-factors by differential transmission in the Voigt configuration, however, makes read-out of the spin-state very difficult. We show that optical spin initialization and manipulation can be possible by a red-detuned, circularly-polarized laser, which modifies the spin eigenstates and polarization selection rules via the AC Stark effect.

1This work is supported by NSF, ARO, AFOSR, DARPA, and ONR.

12:51PM T37.0007 Nuclear Spin Locking and Extended Two-Electron Spin Decoherence Time in an InAs Quantum Dot Molecule1, COLIN CHOW, AARON ROSS, DUNCAN STEEL, H. M. Randall Laboratory of Physics, University of Michigan - Ann Arbor, L. J. SHAM, Department of Physics, University of California - San Diego, ALLAN BRACKER, DANIEL GAMMON, Naval Research Laboratory, Washington DC — The spin eigenstates for two electrons confined in a self-assembled InAs quantum dot molecule (QDM) consist of the spin singlet state, S, with J = 0 and the triplet states T−1, T0 and T+1, with J = 1. When a transverse magnetic field (Voigt geometry) is applied, the two-electron system can be initialized to the different states with appropriate laser excitation. Under the excitation of a weak probe laser, non-Lorentzian lineshapes are allowed by a magnetic field in the Voigt configuration, which modifies the polarization selection rules of the transitions. The lack of a cycling transition in the Voigt configuration, however, makes read-out of the spin-state very difficult. We show that cycling transitions can be made possible by a red-detuned, circularly-polarized laser, which modifies the spin eigenstates and polarization selection rules via the AC Stark effect.

1This work is supported by NSF, ARO, AFOSR, DARPA, and ONR.

1:03PM T37.0008 Quantum Dot Molecule Polaritons and a Voltage-Tunable Vacuum Rabi Splitting, PATRICK VORA, George Mason University, ALLAN BRACKER, SAMUEL CARTER, Naval Research Laboratory, MIJIN KIM, Sotera Defense Solutions, Inc., CHUL SOO KIM, SOPHIA ECONOMOU, DANIEL GAMMON, Naval Research Laboratory — InAs quantum dots (QDs) are a popular system for realizing quantum information protocols and studying cavity-QED. An additional class of optical transitions can be accessed by using quantum dot molecules (QDMs); a pair of tunnel-coupled QDs. Recombination can occur within one of the QDs (intradot) or across the tunnel barrier (intertot). Intertot transitions are typically weaker due to reduced wavefunction overlap. Recently, our team embedded a QDM within a GaAs photonic crystal cavity and demonstrated photonic enhancement of a singlet-triplet qubit. Here, we realize a strongly-coupled cavity-QDM system and demonstrate cavity-QED effects inaccessible in single QDs. These include the first observation of molecular polaritons in InAs QDs and a voltage-tunable vacuum Rabi splitting (2γ). The tunable vacuum Rabi splitting can only occur in QDMs and provides an advantage as s is typically fixed post-fabrication. This flexibility could be useful for optical signal processing schemes that exploit the anharmonicity of the Jaynes-Cummings ladder.
1:15PM T37.00009 Screening nuclear field fluctuations to generate highly indistinguishable photons from negatively charged self-assembled InGaAs quantum dots , RALPH MALEIN, TEO SANTANA, JOANNA ZAJAC, Heriot Watt University, PIERRE PETROFF, University of California Santa Barbara, BRIAN GERARDOT, Heriot Watt University — Quantum dots (QDs) can generate highly coherent and indistinguishable single photons. However, a ground-state electron spin interacts with a QD’s nuclear spins to create an effective Overhauser field ($\delta B_n$) of $\sim$30mT. We probe this interaction using resonance fluorescence. We observe the effect of $\delta B_n$ in high resolution (27 MHz) spectroscopy of the elastic and inelastic scattered photons, and characterize the effect of $\delta B_n$ on photon indistinguishability by monitoring the visibility of two-photon interference. With no external magnetic field ($B_z = 0$), $\delta B_n$ effectively splits the ground state, and at low Rabi frequencies we observe two broad ($\Gamma = 200$ MHz) peaks equally spaced by $\sim$100MHz from the central elastic peak. The ratio of elastic to inelastic photons in the spectra gives a dephasing time $T_2 = 0.52T_1 = 400$ps, far from the transform limit. With an external field $B_z > \delta B_n$, we can successfully screen the fluctuating nuclear field. For $B_z = 300$ mT, nearly all photons in the spectrum are elastically scattered and we extract $T_2 = 1.94T_1 = 1512$ps. This transform limited linewidth enables us to demonstrate very high visibility two-photon interference. These results point towards robust generation of indistinguishable photons.

1:27PM T37.00010 Optical Hyperpolarization of Donor Electron Spins in Silicon Using a Widely-Tunable DBR Laser , BRENDON ROSE, Department of Electrical Engineering, Princeton University, GARY WOLFOVICZ, London Centre for Nanotechnology, University College London, ALEXEI TYRYSHKIN, Department of Electrical Engineering, Princeton University, MICHAEL THEWALT, Department of Physics, Simon Fraser University, KOHEI ITOH, School of Fundamental Science and Technology, Keio University, Japan, JOHN MORTON, London Centre for Nanotechnology, University College London, STEPHEN LYON, Department of Electrical Engineering, Princeton University — We report on measurements of isotopically enriched silicon samples (45 ppm Si-29) with very low donor densities (1e12-1e14 cm$^{-3}$). Pushing the donor density limit necessitates optimizing the experimental sensitivity and enhancing spin polarization. Donor spin polarization greater than Boltzmann (hyperpolarization) can be established by optically exciting the no-phonon bound exciton transitions followed by Auger recombination. We established significant donor spin hyperpolarization with a distributed Bragg reflector laser, tunable across all donors including P-31 and Bi-209. For phosphorus doped silicon we observed combined electron-nuclear spin polarizations of 100%-200% depending on donor density. For bismuth donors at a clock transition ($B_z = 80.6$ mT), we observed about 50% spin polarization, and 500% away from the clock transition. This increase in spin polarization allows for single shot measurement of low density samples ($4e12$ P/cm$^3$, and $1e14$ Bi/cm$^3$).

1:39PM T37.00011 Hybrid optical-electrical detection of donor electron spins with bound excitons in silicon , C. C. LO, M. URDAMPILLET, P. ROSS, University College London , M. F. GONZALEZ-ZALBA, Hitachi Cambridge Laboratory, J. MANSIR, University College London, S. A. LYON, Princeton University, M. L. W. THEWALT, Simon Fraser University, J. J. L. MORTON, University College London — Electrical detection of spin resonance is a powerful technique for understanding the dynamics of spins in semiconductors. For electrons bound to shallow donors in silicon, thus far it has been demonstrated by coupling donors to spin readout partners, such as paramagnetic defects or conduction devices, which fundamentally limit the donor coherence times. Here we demonstrate electrical detection of donor bound excitons in a silicon device, and show that the spin-selective bound exciton transition can be exploited for the electrical detection of coherent spin manipulation of isolated donors. We use this method to measure electron spin Rabi oscillations, and we are able to obtain long intrinsic electron spin coherence times, limited only by the donor concentration. Furthermore, we address critical issues for adopting such a hybrid optical-electrical detection scheme for single spin detection in silicon nanodevices, laying the foundations for realizing a versatile readout method for single spin readout with relaxed magnetic field and temperature requirements compared with spin-dependent tunneling. [arXiv:1411.1324]

1:51PM T37.00012 Nearly degenerate light- and heavy-hole trions bound to isoelectronic centers , GABRIEL ETHEIER-MAJCHER, PHILIPPE ST-JEAN, SEBASTIEN FRANCOEUR, Polytechnique Montreal — Many optical quantum control schemes of spin qubits in semiconductors rely on the existence of trion states. In this work, we investigate the fine structure of negative trions bound to isoelectronic centers formed from a pair of nitrogen isovalent impurities in GaAs, which represent interesting candidates for optical quantum information processing. Using optical polarization resolved microluminescence, we find that the fine structure is composed of two unpolarized lines, characteristic of light- and heavy-hole trion states, evolving into two quadruplets under a longitudinal magnetic field. The availability of both light- and heavy-hole states on the same trion could lead to new powerful optical quantum control schemes where both spin initialization and single-shot readout could be conveniently realized.

2:03PM T37.00013 Initialization of a hole spin bound to an isoelectronic center , PHILIPPE ST-JEAN, GABRIEL ETHEIER-MAJCHER, SEBASTIEN FRANCOEUR, Polytechnique Montreal — Hole spins are promising candidates for solid-state qubits because they interact weakly with nuclear spins, leading to long relaxation and coherence times. In this work, we demonstrate the ability to optically initialize a single hole spin bound to an isoelectronic center, which is an atomic defect formed from a small number of isovalent impurities in a semiconductor host. Using time-resolved magneto-photoluminescence of a positive trion bound to a Te dyad in ZnSe, we measured the degree of polarization of the emission under various conditions of excitation and magnetic field. Under non-resonant excitation, the trion emission is partially polarized and becomes completely unpolarized under a longitudinal magnetic field. In contrast, resonant excitation of the heavy-hole valence band of the ZnSe host leads to highly polarized emission, implying that the hole has been initialized in a known spin state.

Thursday, March 5, 2015 11:15AM - 2:15PM — Session T38 GQI: Quantum Characterization and Tomography 212B - Joshua Combes, Perimeter Institute

11:15AM T38.00001 Iterated benchmarking to separate unitary errors from decoherence$^1$, LEV BISHOP, SARAH SHELDON, STEFAN FILIPP, MATTHIAS STEFFEN, JERRY M. CHOW, JAY M. GAMBITTA, IBM TJ Watson Research Center, Yorktown Heights, NY, USA — We describe a scalable experimental protocol for estimating the relative contribution of unitary errors and decoherence to the fidelity of individual quantum gates. As an extension to interleaved randomized benchmarking (Magesan PRL 109, 080505 2012), this protocol consists of interleaving random Clifford gates between $n$-fold repetitions of the gate of interest. The type of error is revealed by the scaling with number of repetitions: linear in the case of errors due to decoherence; quadratic in the case of pure unitary errors. This protocol has recently been implemented experimentally for transmon superconducting qubits and found useful for calibrating microwave pulses as well as identifying new error sources that may be affecting gate fidelity.

$^1$Supported by ARO under contract W911NF-14-1-0124
11:27AM T38.00002 Non-Markovianity in Randomized Benchmarking , HARRISON BALL, ARC Centre for Engineered Quantum Systems, School of Physics, The University of Sydney, NSW 2006 Australia, TOM M. STACE, ARC Centre for Engineered Quantum Systems, University of Queensland, Brisbane 4072, Australia, MICHAEL J. BIERCUK, ARC Centre for Engineered Quantum Systems, School of Physics, The University of Sydney, NSW 2006 Australia — Randomized benchmarking is routinely employed to recover information about the fidelity of a quantum operation by exploiting probabilistic twirling errors over an implementation of the Clifford group. Standard assumptions of Markovianity in the underlying noise environment, however, remain at odds with realistic, correlated noise encountered in real systems. We model single-qubit randomized benchmarking experiments as a sequence of ideal Cliffords operations interleaved with stochastic dephasing errors, implemented as unitary rotations about $\sigma_z$. Successive error rotations map to a sequence of random variables whose correlations introduce non-Markovian effects emulating realistic colored-noise environments. The Markovian limit is recovered by turning off all correlations, reducing each error to an independent Gaussian-distributed random variable. We examine the dependence of the statistical distribution of fidelity outcomes on these noise correlations, deriving analytic expressions for probability density functions and related statistics for relevant fidelity metrics. This enables us to characterize and bear out the distinction between the Markovian and non-Markovian cases, with implications for interpretation and handling of experimental data.

11:39AM T38.00003 Hyperaccuracy and Error Scaling in Gate Set Tomography1, KENNETH RUDINGER, ERIK NIELSEN, JOHN KING GAMBLE, ROBIN BLUME-KOHOUT, Sandia National Laboratories — Standard quantum tomographic procedures are limited in their usefulness by errors in the prior knowledge of the implemented POVMs and prepared states. Gate set tomography (GST) is a tomographic framework introduced to solve this problem of self-referential calibration [arXiv:1310.4492]. GST seeks to simultaneously and self-consistently characterize the set of implemented gates, prepared states, and POVMs. This talk will provide detailed analysis of imperfections in GST-based estimations. From simulations, we establish 1) lower bounds on the experimental resources required to ensure that GST will provide a reliable and useful estimate of the gates, and 2) the scaling of GST’s accuracy with number of samples per experiment, maximum length of experiment, and rate of incoherent error. These results demonstrate that GST can be far more accurate than standard tomography. Lastly we show (from both simulations and experiments) that experiment-by-experiment $\chi^2$ tests are extremely effective at diagnosing inconsistencies in the model caused by non-Markovian noise.

1Sandia National Laboratories is a multi-program lab managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corp., for the U.S. Dept. of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

11:51AM T38.00004 Gate Set Tomography on a trapped ion qubit, ERIK NIELSEN, ROBIN BLUME-KOHOUT, JOHN GAMBLE, KENNETH RUDINGER, JONATHAN MIKRACHI, JOHATHAN STERK, PETER MAUNZ, Sandia National Laboratories — We present enhancements to gate-set tomography (GST), which is a framework in which an entire set of quantum logic gates (including preparation and measurement) can be fully characterized without need for pre-calibrated operations. Our new method, “extended Linear GST” (eLGST) uses fast, reliable analysis of structured long gate sequences to deliver tomographic precision at the Heisenberg limit with GST’s calibration-free framework. We demonstrate this precision on a trapped-ion qubit, and show significant (orders of magnitude) advantage over both standard process tomography and randomized benchmarking. This work was supported by the Laboratory Directed Research and Development (LDRD) program at Sandia National Laboratories. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000.

12:03PM T38.00005 Gate Set Tomography of a 3D Transmon Qubit, YUDAN GUO, Dept. of Physics, Reed College, SERGEY NOVIKOV, Dept. of Physics, University of Maryland-College Park, DANIEL GREENBAUM, ANDREW SKINNER, Altamira Technologies Corporation, B.S. PALMER, Lab. for Physical Sciences — Quantum gate set tomography is a recently developed tool for characterizing quantum gates that does not suffer from the inaccuracies inherent in standard quantum process tomography. We present the results of a gate set tomography (GST) experiment done on a superconducting 3D transmon qubit. $\pi$ and $\pi/2$ rotations over the $x$- and $y$-axes were used as the initial calibrated gates. We performed linear inversion on data from a 4-fiducial experiment to obtain an initial tomographic estimate, which was then used as the starting point for a maximum likelihood procedure. The calibrated gates all achieved fidelity above 98%, which was further verified by randomized benchmarking. The robustness of GST was also examined by introducing errors deliberately. We show that GST with maximum likelihood estimation is able to discern errors due to a mixed initial state, as well as due to a tilted rotation axis in our gate operation.


12:15PM T38.00006 Self-consistent verification of quantum measurements properties1, MARCUS DA SILVA, Raytheon BBN Technologies — Measurements are an important aspect of quantum mechanics, as they represent the controlled extraction of information about quantum systems. Recent approaches for quantum tomography, such as gate-set tomography, have demonstrated that is is possible to recover a self-consistent description of a quantum system (including measurements) without assuming perfect knowledge about any of its components. However, these approaches typically focus on destructive measurements, and the inherent gauge freedom of quantum experiments makes many of the familiar properties quantum measurements (e.g., efficiency and projectiveness) difficult or impossible to verify. Here we describe how the characterization of non-destructive measurements avoids some of these problems, and propose alternate measurement properties that have the advantage of being gauge invariant, so that can be verified through experiments.

1M.S. would like to acknowledge the support of ARO under U. S. Army Research Office contract W911NF-14-C-0048.

12:27PM T38.00007 Precision measurements with a single quantum system, KLAUS MOLMER, ALEXANDER KILERICH, PINJA HAIKKA, Department of Physics and Astronomy, Aarhus University — Continuous probing of a single quantum system provides information about physical parameters that govern its evolution. The stochastic character of the quantum measurement process and the back action on the system accompanying different outcomes makes the extraction of precision information a dynamical process. Quantum trajectory theory of light emitting systems yields an efficient Bayesian estimation, and full photodetection records reveal much more information than integrated signals [1,2]. We present an analysis of the Cramer-Rao bound, quantifying the asymptotic scaling of the estimation error after long time probing of light from a single emitter [2]. The choice of measurement strategy significantly influences the estimation sensitivity of different parameters, but for Markovian decay, a deterministic equation provides the maximally possible estimation sensitivity by any measurement on the system and its emitted radiation [3]. 1. S Gammelmark and K Molmer, Bayesian parameter inference from continuously monitored quantum systems; Phys. Rev. A 87, 032115 (2013). 2. A. H. Kilerich and K. Molmer, Estimation of atomic interaction parameters by photon counting, Phys. Rev. A 89, 052110 (2014). 3. K. Molmer, Hypothesis testing with open quantum systems; arXiv:1408.4568
12:39PM T38.00008 Applying Model Selection to Quantum State Tomography: Choosing Hilbert Space Dimension. TRAVIS SCHOLTEN, University of New Mexico. Sandia National Laboratories — Reconstructing the quantum state of a continuous variable system (e.g., an optical mode) using quantum tomography presents a unique problem: the dimension of its Hilbert space is infinite. Its density matrix has infinitely many parameters, which cannot all be estimated from finite data. Brute force reconstruction (e.g., via the Radon transform or deconvolution) produces undesirable overfitting artifacts. Smoothing is one solution, but lacks a good theoretical justification. I introduce a statistically well-motivated approach based on model selection and log likelihoods. Maximum likelihood estimates in a sequence of D-dimensional subspaces (spanned by the first D Fock states) are ranked by their log likelihood. This ranking allows one to find an estimate whose dimension is smaller while simultaneously providing a good fit to data. I apply this method to heterodyne tomography and demonstrate the method can indeed eliminate overfitting by choosing a good dimension (D) in which to reconstruct optical states. Sandia is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the US Department of Energy’s National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

12:51PM T38.00009 Informationally complete measurements from compressed sensing methodology. AMIR KALEV, University of New Mexico, CARLOS RIOFRIO, Freie Universitat Berlin, ROBERT KOSUT, SC Solutions, IVAN DEUTSCH, University of New Mexico — Compressed sensing (CS) is a technique to faithfully estimate an unknown signal from relatively few data points when the measurement samples satisfy a restricted symmetry property (RIP). Recently this technique has been ported to quantum state tomography with a substantially reduced number of measurement settings. In this work we show that the constraint that a physical density matrix is positive semidefinite provides a rigorous connection between the RIP and the informational completeness (IC) of a POVM used for state tomography. This enables us to construct IC measurements that are robust to noise using tools provided by the CS methodology. The exact recovery no longer hinges on a particular convex optimization program; solving any optimization, constrained on the cone of positive matrices, effectively results in a CS estimation of the state. From a practical point of view, we can therefore employ fast algorithms developed to handle large dimensional matrices for efficient tomography of quantum states of a large dimensional Hilbert space.

1 Supported by the National Science Foundation

1:03PM T38.00010 Quantum Bootstrapping via Compressed Quantum Hamiltonian Learning. NATHAN WIEBE, Microsoft Research, CHRISTOPHER GRANADE, DAVID CORY. Institute for Quantum Computing — Recent work has shown that quantum simulation is a valuable tool for learning empirical models for quantum systems. We build upon these results by showing that a small quantum simulator can be used to characterize and learn control models for larger devices for wide classes of physically realistic Hamiltonians. This leads to a new application for small quantum computers: characterizing and controlling larger quantum computers. Our protocol achieves this by using Bayesian inference in concert with Lieb-Robinson bounds and interactive quantum learning methods to achieve compressed simulations for characterization. Whereas Fisher information analysis shows that current methods which employ short-time evolution are suboptimal, interactive quantum learning allows us to overcome this limitation. We illustrate the efficiency of our bootstrapping protocol by showing numerically that an 8-qubit Ising model simulator can be used to calibrate and control a 50 qubit Ising simulator while using only about 750 kilobits of experimental data.

1:15PM T38.00011 Practical variational tomography for critical 1D systems. JONG YEON LEE, OLIVIER LONDON-CARDINAL, California Institute of Technology — We further investigate a recently introduced efficient quantum state reconstruction procedure targeted to states well-approximated by the multi-scale entanglement renormalization ansatz (MERA). First, we introduce an improved optimization scheme that can be easily generalized for MERA states with larger bond dimension. Second, we provide a detailed analysis of the error propagation and quantify how it affects the distance between the experimental state and the reconstructed state. Third, we explain how to bound this distance using local data, providing an efficient scalable certification method. Fourth, we examine the performance of MERA tomography on the ground states of several 1D critical models.

1:27PM T38.00012 Controlling qubit drift by recycling error correction syndromes. ROBIN BLUME-KOHOUT, Computing Science Research Institute, Sandia National Laboratories — Physical qubits are susceptible to systematic drift, above and beyond the stochastic Markovian noise that motivates quantum error correction. This parameter drift must be compensated — if it is ignored, error rates will rise to intolerable levels — but compensation requires knowing the parameters' current value, which appears to require halting experimental work to recalibrate (e.g. via quantum tomography). Fortunately, this is untrue. I show how to perform on-the-fly recalibration on the physical qubits in an error correcting code, using only information from the error correction syndromes. The algorithm for detecting and compensating drift is very simple — yet, remarkably, when used to compensate Brownian drift in the qubit Hamiltonian, it achieves a stabilized error rate very close to the theoretical lower bound. Against 1/f noise, it is less effective only because 1/f noise is (like white noise) dominated by high-frequency fluctuations that are uncompensatable.

1 Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE

1:39PM T38.00013 Heat bath algorithmic cooling using electron-nuclear spin ensemble in the solid state: characterization of the open quantum system control. KYUNGDEOCK PARK, ROABEDEH DARABAD, GUANRU FENG, STEPHANE LABRUYERE, JONATHAN BAUGH, Institute for Quantum Computing, University of Waterloo, RAYMOND LAFLAMME, Institute for Quantum Computing, University of Waterloo, Perimeter Institute for Theoretical Physics — The ability to perform multiple rounds of Quantum Error Correction (QEC) is an essential task for scalable quantum information processing, but experimental realizations of it are still in their infancy. Key requirements for QEC are high control fidelity and the ability to extract entropy from ancilla qubits. Nuclear Magnetic Resonance (NMR) quantum processors have demonstrated high control fidelity with up to 12 qubits. A remaining challenge is to prepare nearly pure ancilla qubits to enable QEC. Heat Bath Algorithmic Cooling (HBAC) is an efficient tool for extracting entropy from qubits that interact with a heat bath, allowing cooling below the bath temperature. For implementing HBAC with spins, a hyperfine coupled electron-nuclear system in a single crystal is more advantageous than conventional NMR systems since the electron, with higher polarization and faster relaxation, can act as a heat bath. We characterize 3 and 5 qubit spin systems in gamma-irradiated malonic acid and present simulation and experimental results of HBAC to benchmark our quantum control. Two control schemes are compared: electron nuclear double resonance and indirect control of nuclei via the anisotropic hyperfine interaction.
1:51PM T38.00014 Characterization of Qudit Entanglement Through the Visualization of Spin-Coherent-State Wigner Functions, TODD TILMA, Tokyo Institute of Technology, MARK EVERITT, Loughborough University, KAE NEMOTO, National Institute of Informatics, WILLIAM MUNRO, NTT Basic Research Labs — The purpose of our research is to determine whether or not there is a general relationship between the degree of entanglement and the total amount of negativity in the Wigner function of various combinations of finite-dimensional quantum states. Specifically, by using the Stratonovich-Weyl correspondence we can take the density matrix of a known, finite-dimensional quantum state (hereafter known as a “qudit”) and generate its corresponding, finite-dimensional Wigner function. This Wigner function reproduces the qudit density matrix through a known volume integral. By doing the same volume integral, but with the absolute value of the Wigner function as the kernel, we get a measure of the total amount of negativity of the Wigner function instead of reproducing the density matrix. Our question is thus, is this “negative volume” equivalent to the amount of entanglement in the initial qudit state? Our results for general two-qudit states have confirmed a monotonic relationship between concurrence and this negative volume for specific cases. By analyzing the various Wigner functions of three and more qubits, as well as qubit-qudit Wigner functions we hope to build a consensus on whether or not the negativity in the Wigner function is a measure of, or witness to, entanglement.

2:03PM T38.00015 Adaptive characterization of coherent states1, MARKKU P.V. STENBERG, KEVIN PACK, FRANK K. WILHELM, Theoretical Physics, Saarland University, 66123 Saarbrucken, Germany — We present a method for efficient characterization of an optical state. Our algorithm significantly outperforms nonadaptive schemes. While our standard approach works when we are interested in (i) searching a crude estimate, (ii) rapidly improving the accuracy, and (iii) the phase where the improvement of the accuracy slows down due to the quantum nature of the coherent state. Our algorithm significantly outperforms nonadaptive schemes. While our standard approach works when we are interested in the phase of an unknown frequency, our adaptive algorithm uses sequential weak measurements of a Bell state that are implemented with four superconducting qubits. In this second of two talks, we present experimental detail on the measurement of the CHSH correlator and the analysis of error mechanisms.

Thursday, March 5, 2015 11:15AM - 2:15PM — Session T39 GQ1: Focus Session: Quantum Foundations Studies with Superconducting Qubits

11:15AM T39.00001 Continuous measurement of two spatially separated superconducting qubits: quantum trajectories and statistics, NICOLAS ROCH, CNRS and Universite? Grenoble Alpes, Institut N?el, 38042 Grenoble, France — Measurement can be harnessed to probabilistically generate entanglement in the absence of local interactions, for example between spatially separated quantum objects. Continuous weak measurement allows us to observe the dynamics associated with this process. In particular, we perform joint dispersive readout of two superconducting transmon qubits separated by one meter of coaxial cable. We track the evolution of a joint quantum state under the influence of measurement, both as an ensemble and as a set of individual quantum trajectories. Analyzing the statistics of such quantum trajectories can shed new light on the underlying entangling mechanism.

11:51AM T39.00002 Quantum Measurement in Superconducting Circuits, KATER MURCH, Physics Department, Washington University, St. Louis — In recent years, there has been immense progress in the ability to control and measure superconducting circuits. These abilities have enabled several different experiments that address the fundamental physics of quantum measurement, ranging from the observation of non-classical weak values, to the generation of entanglement through measurement and the tracking of individual quantum trajectories. I will review recent progress in the field and discuss how these advances add to the foundations of quantum mechanics.

12:27PM T39.00003 Steady-state entanglement of spatially separated qubits via quantum bath engineering, CAMILLE ARON, Princeton University, MANAS KULKARNI, New York City College of Technology, HAKAN TURECI, Princeton University — We propose a scheme for driving a dimer of spatially separated qubits into a maximally entangled non-equilibrium steady state. A photon-mediated retarded interaction between the qubits is realized by coupling them to two tunnel-coupled leaky cavities where each cavity is driven by a coherent microwave tone. The proposed cooling mechanism relies on striking the right balance between the unitary and driven-dissipative dynamics of the qubit subsystem. We map the dimer to an effective transverse-field XY model coupled to a non-equilibrium bath that can be suitably engineered through the choice of drive frequencies and amplitudes. We show that both singlet and triplet states can be obtained with remarkable fidelities. The proposed protocol can be implemented with a superconducting circuit architecture that was recently experimentally realized and paves the way to achieving large-scale entangled systems that are arbitrarily long lived.

12:39PM T39.00004 Experimental violation of a Bell-Leggett-Garg inequality using weak measurements, Part I: Avoiding loopholes, J. DRESSEL, UC Riverside, T. WHITE, UC Santa Barbara, J. MUTUS, R. BARENDS, Google, Santa Barbara, A. MEGRANT, UC Santa Barbara, E. JEFFREY, D. SANK, Google, Santa Barbara, J. KELLY, B. CAMPBELL, UC Santa Barbara, Y. CHEN, Google, Santa Barbara, Z. CHEN, B. CHIARO, A. DUNSWORTH, I.-C. HOI, C. NEILL, P.J.J. O’MALLEY, UC Santa Barbara, P. ROUSHAN, Google, Santa Barbara, C. QUINTANA, A. VAINSENCHER, J. WENNER, UC Santa Barbara, A. FOWLER, Google, Santa Barbara, A. N. CLELAND, UC Santa Barbara, A. N. KOROTKOV, UC Riverside, A. N. CLELAND, UC Santa Barbara, J. M. MARTINIS, University of California and Google, Santa Barbara — We demonstrate the violation of a hybrid Bell-Leggett-Garg inequality that avoids both the disjoint sampling and fair sampling loopholes that are common to traditional Bell inequalities. Our algorithm uses sequential weak measurements of a Bell state that are implemented with four superconducting Xmon qubits. In this first of two talks, we detail the high-fidelity partial projections that are needed for this violation, which are realized by entangling an ancilla qubit to each data qubit using a controlled-Z two-qubit gate. After calibration of the ancilla readout, these partial projections indirectly measure qubit expectation values with a tunable amount of state disturbance. For sufficiently weak disturbance, the inequality can be violated using all the data collected in a single configuration.

12:51PM T39.00005 Experimental violation of a Bell-Leggett-Garg inequality using weak measurements, Part II: The Violation, T.C. WHITE, UC Santa Barbara, J. MUTUS, Google Santa Barbara, J. DRESSEL, UC, Riverside, J. KELLY, UC Santa Barbara, R. BARENDS, Google, Santa Barbara, A. MEGRANT, UC Santa Barbara, E. JEFFREY, D. SANK, Google, Santa Barbara, B. CAMPBELL, UC Santa Barbara, Y. CHEN, Google, Santa Barbara, Z. CHEN, B. CHIARO, A. DUNSWORTH, UC Santa Barbara, A. FOWLER, Google, Santa Barbara, I.-C. HOI, C. NEILL, P.J.J. O’MALLEY, UC Santa Barbara, P. ROUSHAN, Google, Santa Barbara, C. QUINTANA, A. VAINSENCHER, J. WENNER, UC Santa Barbara, A. N. KOROTKOV, UC Riverside, A. N. CLELAND, UC Santa Barbara, J. M. MARTINIS, University of California and Google, Santa Barbara — We experimentally demonstrate the violation of a hybrid Bell-Leggett-Garg inequality that avoids both the disjoint sampling and fair sampling loopholes that are common to traditional Bell inequalities. Our algorithm uses sequential weak measurements of a Bell state that are implemented with four superconducting Xmon qubits. In this second of two talks, we present experimental detail on the measurement of the CHSH correlator and the analysis of error mechanisms. We find that the dependence of the correlation (i) on the measurement strength shows excellent agreement with theoretical predictions, but the magnitude of the correlator varies greatly with system fidelity. For sufficiently weak and high fidelity measurements, we achieve a violation that is many standard deviations above the classical limit.
In the presence of realistic experimental noise, the cost advantage of unambiguous state discrimination is completely destroyed; however, other cost bound violations are more robust, and thus could be experimentally tested with modern superconducting qubit implementations.

Casimir-Polder-like Effect in a Superconducting Circuit System. PETER GROSKOWSKI, EDUARDO MARTIN-MARTINEZ, CHRIS WILSON, Univ of Waterloo, FRANK WILHELM, Saarland University — Casimir-type forces arise when the ground state energy of a quantum field depends on a classically-treated degree of freedom. The first example of such forces was proposed by Casimir, when he considered the attractive force that arises between two neutral, conducting plates placed in a vacuum. In this talk, we will discuss a variation of the Casimir-Polder effect, the force between an atom and a conducting plate, in a superconducting circuit consisting of a tunable cavity coupled to a qubit. We will describe an analogus "Casimir force" on the cavity's effective boundary condition, outline the consequences of longitudinal versus transverse coupling between the qubit and cavity, and discuss the relevance of the field self-interaction term $\mathcal{A}$. Finally, we will briefly touch on prospects related to measurement.

Vacuum-Induced Berry Phase Measured Via a Phase-Tunable Atom-Field Interaction. S. GASPARINETTI, S. BERGER, A. A. ABDUMALIKOV, M. PECHAL, S. FILIPP, A. WALLRAFF, ETH Zurich — Geometric phases incorporate a fundamental aspect of quantum mechanics. They are at the heart of many quantum phenomena in solid-state physics, from the quantum Hall effect to topologically protected phases, and may provide a resource for quantum computation. We present the first experimental observation of the vacuum-induced Berry phase [1], a geometric effect that arises when the phase of a quantized field mode coupled to an atom is adiabatically steered. Our atom-field system is a transmon embedded in a 3D microwave cavity. A phase-coherent microwave tone induces a tunable interaction between the third level of the transmon and a long-lived mode of the cavity [2]. By adiabatically steering the phase of the interaction, we demonstrate that the qubit accumulates a geometric phase even when the cavity mode is empty. We characterize this effect by varying the effective atom-field detuning as well as the photon number in the cavity mode.

11:27AM T41.00002 Effects of temperature on structure and mechanical properties of alkane-
ethiol coated gold nanoparticle membranes1. K. MICHAEL SALERNO, GARY GREST, Sandia National Laboratories — Single-
nanoparticle-thick membranes have a variety of potential uses due to unique mechanical properties. While these membranes have been studied experimentally and computationally at 300K, the effects of thermal annealing on structure and properties have not been investigated. We present atomistic molecular dynamics simulations that study the effects of temperature on nanoparticle membrane properties. Nanoparticles are made of a gold core coated with organic oligomer ligands. At high grafting density, ligands with CH$_3$ end groups exhibit local crystallinity at 300K while those with COOH end groups orient to form dimers due to electrostatics. Both features influence membrane mechanical properties. As temperature increases ligand crystallinity and COOH affinity are disrupted, and mechanical strength is reduced. Immediately after cooling back to 300K, membranes are weaker and more soluble and ligand interdigitation and COOH affinity are reduced. Over time, interdigitation and end-group interactions rejuvenate and samples that undergo high-temperature annealing have mechanical properties comparable to the original membranes. The structure/property temperature dependence points to ways that membranes could be tailored for temperature-dependent/resistant properties.

1Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s NNSA under contract DE-AC04-94AL85000.

11:39AM T41.00003 Quantitative Analogy Between Polymer Grafted Nanoparticles and
Patchy Particles2, MAKOTO ASAI, Chemical Engineering, Columbia University, ANGELO CACCIUTTO, Chemistry, Columbia University, SANAT KUMAR, Chemical Engineering, Columbia University — We establish a quantitative analogy between polymer grafted nanoparticles (PGNPs) and patchy nanoparticles (NPs). Over much of the experimentally relevant parameter space, we show that PGNPs behave quantitatively like Janus NPs, with the patch size having a universal dependence on the number of grafted chains and the ratio of the size of the NPs to the grafted chain size. The widely observed anisotropic self-assembly of PGNPs into superstructures can thus be understood through simple geometric considerations of single patch model, in the same spirit as the geometry-based surfactant models of Israelachvili

2The authors thank the National Science Foundation for financial support of this work. AC acknowledges financial supported from the National Science Foundation under CAREER Grant No. DMR-0846426.

11:51AM T41.00004 Reversible Thermal-Stiffening in Polymer Nanocomposites. ERKAN SENSES,
PINAR AKCORA, Stevens Institute of Technology — Silica nanoparticles adsorbed with a high glass-transition temperature polymer, PMMA (T$_g$: 130 °C) are shown to uniformly disperse in a low-T$_g$ polymer matrix, PEO (T$_g$: -60 °C). These nanocomposites exhibit an unusual reversible liquid-to-solid transition at temperatures above T$_g$s of both polymers. Mechanical adaptivity of PEO nanocomposites to temperatures underlies the existence of dynamically asymmetric bound layers on particles, and more importantly their impact on mechanical behavior, which sets these materials apart from conventional polymer composites that soften upon heating. Moreover, the growth rate of elastic moduli at temperatures above T$_g$ of PMMA presents an Arrhenius-type relaxation with activation energy well-matching with the α-β merging region of PMMA. These results suggest that the mobility of the surface-bound polymer is essential for reinforcement contrary to commonly accepted glassy-layer hypothesis.

12:03PM T41.00005 SANS Study on the Behaviors of Polymeric Ligands on the Nanoparticle Surfaces, SEYONG KIM, Department of Chemical and Biological Engineering, Korea Univ., SOO-HYUNG CHOI, Department of Chemical Engineering, Hongik Univ., JUNE HUH, JOONA BANG, Department of Chemical and Biological Engineering, Korea Univ. — In this work, we employed small angle neutron scattering (SANS) and contrast variation technique to characterize the behaviors of polymer ligands on the nanoparticle (NPs) surfaces. The Janus-type Au NPs were coated with a mixture of two different ligands, PMMA-SH and deuterated PS-SH, and the Au NPs coated only with P(MMA-r-dS)-SH were also prepared for the control case of NPs with homogeneous ligand. From the SANS analysis, it was observed that the Janus ligands become phase separated with increasing the molecular weight of ligands. Furthermore, computational simulation was performed to examine how ligands are phase separated on the curved NPs surfaces.

12:15PM T41.00006 Semi-crystalline polymer nanocomposites: interplay of matrix crystal-
lization and nanoparticle self-assembly. DAN ZHAO, JACQUES JESTIN, LONGXI ZHAO, SANAT K. KUMAR, Columbia University, MOHAMMAD MOHAMMADKHANI, BRIAN C. BENICEWICZ, University of South Carolina — We investigate a new class of nanocomposite materials made of semi-crystalline poly(ethylene oxide) and poly(methyl methacrylate) grafted silica nanoparticles (NPs). The results indicate that NPs do not act as nucleating agents as indicated from the lowering of the onset of crystallization temperature with addition of NPs. Although the crystal sizes and rate of crystallization are reduced in the presence of NPs, the equilibrium melting temperature seems to be unaffected. Furthermore, no remarkable change was observed in the spatial dispersion of NPs upon fast crystallization. However, for slow crystallization, both TEM and X-ray scattering reveal that the system starts to be organized in a “layer-by-layer” architecture, where the NPs are aligned in the amorphous phases intercalated by the crystalline lamellar phases.

12:27PM T41.00007 Chemically Designed Molecular Interfaces in Cross-Linked Poly(ethylene glycol)/Silica Nanocomposites Reveal Strong Size-Dependent Trends in Gas Permeability. NORMAN SU, Univ of California - Berkeley, JEFFREY URBAN, Lawrence Berkeley National Lab — Polymer nanocomposite membranes can exhibit gas separation performance that surpasses conventional polymeric membranes. While promising, the optimization of nanocomposite membranes requires a fundamental understanding of the transport mechanism and interfacial effects between the inorganic and polymer phase that is currently limited to empirical relationships. Synthesized nanocomposites often consist of poorly dispersed and polydisperse inorganic nanomaterials. It is known that polymer dynamics can change drastically upon introduction of an inorganic phase, which can dramatically alter polymer transport behavior. Here, we systematically explore the role of nanoparticle sizes from 12 to 130 nm on polymer dynamics and permeability in a series of cross-linked poly(ethylene glycol)/silica nanocomposite membranes. The nanocomposites are well-dispersed and display excellent homogeneity throughout. Size-dependent broadening of the Tg indicates strong attractive interactions especially at high surface area loadings, which lead to deviations in permeability not captured by Maxwell’s model. Chemical modifications of silica at this interface can yield significantly different polymer dynamics than previously observed with enhanced transport and mechanical properties.

12:39PM T41.00008 Interactions between Nanoparticles and Polymer Brushes: Molecular Dynamics Simulations and Self-consistent Field Theory Calculations1, SHENGFENG CHENG, CHENGYUAN WEN, Virginia Polytechnic Institute and State University, SERGEI EGOROV, University of Virginia — Molecular dynamics simulations and self-consistent field theory calculations are employed to study the interactions between a nanoparticle and a polymer brush at various densities of chains grafted to a plane. Simulations with both implicit and explicit solvent are performed. In either case the nanoparticle is loaded to the brush at a constant velocity. Then a series of simulations are performed to compute the force exerted on the nanoparticle that is fixed at various distances from the grafting plane. The potential of mean force is calculated and compared to the prediction based on a self-consistent field theory. Our simulations show that the explicit solvent leads to effects that are not captured in simulations with implicit solvent, indicating the importance of including explicit solvent in molecular simulations of such systems. Our results also demonstrate an interesting correlation between the force on the nanoparticle and the density profile of the brush.

1We gratefully acknowledge the support of NVIDIA Corporation with the donation of the Tesla K40 GPU used for this research.
12:51PM T41.00009 Dispersion/Aggregation of polymer grafted nanorods in a polymer matrix studied by Dissipative Particle Dynamics , JOAO MAIA, SHAGHAYEGH KHANI, Case Western Reserve University — Nanorods are incorporated into polymer matrices for fabricating composite materials with enhanced physical and mechanical properties. The final macroscopic properties of the composites are strongly related to the dispersion and organization of the nanoparticles in the matrix. For instance, a significant improvement in the mechanical properties of the nanorod-polymer composites is observed upon formation of a percolating network. One way of controlling the assembly of nanorods in the polymer medium is adjusting the chemical interactions which is done through grafting polymer chains on the surface of the rods. The recent developments in the computational techniques have paved the road for further understanding of the controlled dispersion and aggregation of nanorods in polymer matrices. In this study, Dissipative Particle Dynamics (DPD) is employed in order to investigate the effect of enthalpic and entropic variables on the phase behavior of the abovementioned nanocomposites. In DPD, the interaction parameter between the components of the systems can be mapped onto the Flory-Huggins \( \chi \)-parameter via well-known Groot-Warren expression. This work studies the effect of the enthalpic and entropic variables on phase transitions. The main goal is to provide a phase diagram that can be used to guide the experiments in designing new materials.

1:03PM T41.00010 Phase Behavior of Polymer-Grafted Nanoparticles in a Polymer Matrix , KATRINA IRENE MONGCPOA, University of Houston, RANA ASHKAR, PAUL BUTLER, National Institute of Standards and Technology, RAMANAN KRISHNAMOORTI, University of Houston — We examine the thermodynamic interactions of polystyrene (PS) grafted onto spherical silica nanoparticles blended with a poly(vinyl methyl ether) (PVME) matrix using light, x-ray and neutron scattering techniques. PS/PVME systems are known to exhibit a lower critical solution temperature, with blending thermodynamics greatly affected by the chain length of the components. Thus, we study how enthalpic and entropic effects play a role in the dispersion of PS-grafted nanoparticles in a chemically-distinct matrix, especially as the system approaches a phase boundary. Scattering techniques are used to examine the effect of molecular weight on the blend thermodynamics and concentration fluctuations for such strongly interacting polymer blends. x-ray scattering data and analysis of the structure factor reveal that for a grafted deuterated polystyrene brush (33,000 Da) in a PVME matrix (226,000 Da), an initial dispersion of nanoparticles occurs at low temperatures. The system then gradually transitions to an aggregated state as temperature is increased, suggesting the presence of strong inter-particle interactions that lead to fractal formation as the system approaches a phase boundary. Complementary neutron scattering experiments confirm this phenomenon.

1:15PM T41.00011 Study of Polymer/Graphene Nanocomposites through Atomistic Molecular Dynamics Simulations , ANASTASSIA RISSANOU, Institute of Applied and Computational Mathematics (IACM), Foundation for Research and Technology Hellas (FORTH), GR-71110 Heraklion, Crete, Greece, VAGELIS HARMANDARIS, Department of Applied Mathematics, University of Crete, GR-71409, Heraklion, Crete, Greece — Polymer/graphene nanostructured systems have attracted great attention the last years both for scientific and technological reasons. A main challenge in the study of graphene based polymer nanocomposites is to predict their properties at the molecular level. In the current study we focus on the effect of the weight fraction of graphene in a polymer matrix, as well as the size of the graphene sheet, on the properties of polymer chains are examined. Density profiles, structural and conformational characteristics as well as mobility aspects are studied. All the above properties are examined, as a function of the distance from the substrate. Results are compared with the interfacial properties of polymer chains confined between two periodic (i.e., "infinite") frozen graphene layers. In addition dynamical and conformational properties of the graphene sheet are studied as a function of the size and the weight fraction of the sheet in the polymer matrix. Furthermore, thermal as well as matrix induced fluctuations (i.e. wrinkling) of graphene sheets are examined. The extent of the fluctuations and the frequency of conformation interchange between crests and troughs are computed. All above properties are presented for different polymeric systems.

1:27PM T41.00012 Thermally Tunable Metallodielectric Photonic Crystals from Self-assembly of Brush Block Copolymers and Gold Nanoparticles, DONGPO SONG, CHENG LI, NICHOLAS COLELLA, XUEMIN LU, JAMES WATKINS, University of Massachusetts Amherst — Photonic crystals (PCs) based on the self-assembly of block copolymers (BCPs) are under intense investigations, providing a unique platform for the self-assembly of inorganic nanoparticles (NPs) into specific domains of the microphase separated BCPs, to tune the optical constant of the target domains and create hybrid materials with unique optical properties. In this work, we demonstrate a simple strategy for rapid fabrication of well-ordered metallodielectric 1-D PCs using PS-b-P2VP brush BCPs as the templates and H-bonding as the driving force for selective incorporation of phenol-coated gold nanoparticles (NPs) into PEO domains. By varying gold NP loading or molecular weight of the brush BCP, periodic layered metallodielectric structures with the domain spacing controlled from 120 nm to 261 nm were readily created resulting in reflection of light widely tunable from the visible to near IR regions (458-1010 nm). The control over size as well as the distribution of the gold NPs in the well-ordered structure was realized through simple thermal treatment, showing significant effects on the optical properties.

1:39PM T41.00013 Design and organization of nanoparticles in thin film copolymer/homopolymer hosts , JUNNAN ZHAO, PETER GREEN, University of Michigan, Ann Arbor — The organization of polystyrene (PS) grafted gold (Au) nanoparticles (NPs) in supported thin film mixtures of polystyrene-b-poly(2-vinylpyridine) (PS-b-P2VP) diblock copolymers (BCP) with PS homopolymers was examined. The copolymer chains formed micelles, composed of inner cores of P2VP blocks and outer coronae of PS blocks, within the PS hosts. The spatial distribution of nanoparticles within this thin film BCP/homopolymer system is characterized by a morphological diagram of the curvature of the Au cores, \( 1/R_C \), vs. the degree of polymerization \( N_c \) of the grafted PS-chains. The distribution is quantified by five basic regimes, largely dictated by competing entropic and enthalpic intermolecular interactions. The NP distributions range from predominantly residing at external interfaces (free surface and substrate) to primarily "decorating" the surface of micelles. The phase behavior of PS-Au/BCP/homopolymer (PS) systems is necessarily more intriguing than PS-Au/homopolymer (PS) systems, as the relative roles of specific intermolecular interactions on local NP distributions become more apparent.

1:51PM T41.00014 ABSTRACT WITHDRAWN —

2:03PM T41.00015 Directed Phase Separation of Brush-coated Nanoparticles in Miscible and Immiscible Polymeric Thin Films , REN ZHANG, Univ of Akron, BONGJOON LEE, Carnegie Mellon University, JACK DOUGLAS, National Institute of Standards and Technology, SANAT KUMAR, Columbia University, MICHAEL BOCKSTALL, Carnegie Mellon University, ALAMGIR KARIM, Univ of Akron — Fascinating as the combined properties of polymer/inorganic nanoparticle composite system, it is challenging to manipulate the distribution and assembly structures of the nanofilizers at nanoscale with high loading fraction. Inspired by polymer blend phase separation, we expect similar behavior for blend-brushed nanoparticles and a polymer matrix with unfavorable enthalpic interactions. We confirm this relationship in blend thin films of polystyrene (PS) grafted gold nanoparticles (AuPS) in immiscible poly (methyl methacrylate) (PMMA). We show that application of soft-shear dynamic thermal zone annealing (DZA-SS) generates tunable directional aligned anisotropic nanoparticle structures. Alternatively, the phase-separated nanoparticle domains can also be organized into periodic nanostructures with well-defined shape and order with a simple geometric patterned elastomer confinement. These simple yet powerful strategies to fabricate nanomembranes can be exploited for many nanotechnology applications.
11:15AM T42.00001 Dynamics and rheology of living polymers, SUBHAS DHAKAL, Department of Biomedical and Chemical Engineering, Syracuse University, RADHAKRISHNA SURESHKUMAR, Department of Biomedical and Chemical Engineering, and Department of Physics, Syracuse University — Molecular dynamics simulations are used to study the dynamics and stress relaxation in “living” polymers such as wormlike micelles (WLMs) of surfactants. These systems exhibit complex dynamical properties due to incessant chain scission and inter-chain recombination events over time scales that range from few ns to milliseconds. We study the structure and energetics of WLMs obtained from large-scale coarse-grained Molecular Dynamics simulations that consist of millions of atoms. Various dynamical properties such as the non-monotonic variation of the zero shear viscosity with salt concentration, as well as the recombination time and a possible reptation-based stress relaxation mechanism will be discussed.

1We acknowledge the computational resources provided by XSEDE which is supported by NSF grant number OCI-1053575 and the financial support by National Science Foundation under Grant No. 1049489 and 1049454.

11:27AM T42.00002 Extreme value statistics of work done in stretching a polymer in a gradient flow, MARIJA VUCELJA, Center for Studies in Physics and Biology, The Rockefeller University, 1230 York Avenue, New York, NY 10065, USA, KONSTANTIN TURYSYN, Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA, 02139, US, MICHAEL CHERTKOV, Theory Division & Center for Nonlinear Studies at LANL and with New Mexico Consortium, Los Alamos, NM 87545, US — We study the statistics of work on a finitely extensible polymer subjected to a gradient flow and thermal fluctuations. The flow breaks the detailed balance and stretches the polymer, the work to stretch the molecule is stored as elastic energy, which later dissipates with fluctuations of the molecule’s elongation. The whole system is in a non-equilibrium dynamical state, which is sustained by the energy flow into the molecule and back. We obtain the Large Deviation Function (LDF) of the work in the full range of appropriate flow, elasticity and thermal noise parameters by combining analytical and numerical tools. The LDF shows two distinct asymptotes: “near tails” are linear in work and dominated by coiled polymer configurations, while “far tails” are quadratic in work and correspond to preferentially fully stretched polymers. We find the extreme value statistics of work for several elastic potentials, as well as the mean and the dispersion of work near the coil-stretch transition. The dispersion shows a maximum at the transition. In our work, we use non-equilibrium work relations to study the extension of a polymer in a flow. Relations like these are becoming instrumental in studies of soft matter materials.

11:39AM T42.00003 Importance of chain tumbling and finite extension on the start-up and relaxation behavior of transient networks, MICHELLE SING, Massachusetts Inst of Tech-MIT, ZHEN-GANG WANG, California Institute of Technology, GARETH MCKINLEY, BRADLEY OLSEN, Massachusetts Inst of Tech-MIT — Associative polymer networks are ubiquitous in tissue and biomedical engineering. However, the particular molecular attributes that contribute to the macroscopic behavior like shear thinning, self-healing, and yield stress are less well known. Here we incorporate chemical kinetics in the Smoluchowski Equation capable of modeling the full network chain end-to-end distance distribution while tracking the fraction of looped, bridged, and dangling chains in the gel. In steady shear, we see the development of non-monotonic flow instabilities when the rate of chain association grows larger than the rate of chain relaxation. These instabilities arise due to a combination of chain finite extensibility and tumbling. During start-up of steady shear, the combination of these two phenomena also results in stress overshoots followed by multiple damped oscillations toward steady-state. The timescale of chain relaxation after the cessation of shear is dominated by the chain kinetics of association and dissociation as a function of the fraction of dangling chains present at any time post-shear.

1Institute for Soldier Nanotechnologies, Department of Defense National Defense Science and Engineering Fellowship Program

11:51AM T42.00004 Mesoscopic Simulation Methods for Polymer Dynamics, RONALD LARSON, University of Michigan, Ann Arbor, MI — We assess the accuracy and efficiency of mesoscopic simulation methods, namely Brownian Dynamics (BD), Stochastic Rotation Dynamics (SRD) and Dissipative Particle Dynamics (DPD), for polymers in solution at equilibrium and in flows in microfluidic geometries. Both SRD and DPD use solvent particles to carry momentum, and so account automatically for hydrodynamic interactions both within isolated polymer coils, and with other polymer molecules and with nearby solid boundaries. We assess quantitatively the effects of artificial particle inertia and fluid compressibility and show that they can be made small with appropriate choice of simulation parameters. We then use these methods to study flow-induced migration of polymer chains produced by: 1) hydrodynamic interactions, 2) streamline curvature or stress-gradients, and 3) convection of wall depletion zones. We show that large concentration gradients can be produced by these mechanisms in microfluidic geometries that can be exploited for separation of polymers by size in periodic contraction-expansion geometries. We also assess the range of conditions for which BD, SRD or DPD is preferable for mesoscopic simulations. Finally, we show how such methods can be used to simulate quantitatively the swimming of micro-organisms such as E. coli.

In collaboration with Lei Jiang and Tongyang Zhao, University of Michigan, Ann Arbor, MI.

12:27PM T42.00005 Multi-fluid simulations of polymer dynamics, DOUGLAS TREE, KRIS DELANEY, GLENN FREDRICKSON, Univ of California - Santa Barbara — In many industrially important polymeric materials, a discrepancy exists between the time scale intrinsic to the system and processing time scales. As a consequence, models which go beyond equilibrium thermodynamics are required to understand the evolution of the microstructure of such systems. Building a tractable model to address such a system becomes especially challenging when process dynamics coexist with complex flow-induced behaviors (e.g. chain association and dissociation schemes (e.g. Brownian or molecular dynamics or dynamic field theories), cost constraints become prohibitive for 3D dynamic simulations as length and time scales increase. To address such problems, we explore a framework of meso-scale dynamic phase field models originally proposed by Brochard and de Gennes. Expanding on the “two-fluid” formalism of Doi and Onuki, we find that such models are capable of incorporating many phenomena relevant for industrially important polymer materials, including phase separation dynamics and viscoelastic fluid flow. In addition, we explore numerical methods capable of solving such models, with the goal of developing a framework for inexpensive “multi-fluid” simulations of polymer dynamics.

12:39PM T42.00006 Tightening the noose on tube models: a priori determination of equilibration time and other tube model parameters for 1,4-polybutadiene, PRIYANKA DESAI, RONALD LARSON, University of Michigan, XUE CHEN, Dow Chemical Company, SEUNG JOON PARK, Korea Polytechnic University — Linear viscoelastic G’ and G” master curves for multiple linear, star, H, and comb 1,4-polybutadienes from the literature were compared and found with only one exception to agree well in the high deformation range, at 25°C, regardless of chain architecture. From a study by Carella et al. (Macromolecules 17:2775, 1984), the plateau modulus for 1,4-polybutadiene is expected to vary by only 2% for 1,2 content ranging from 0.06 to 0.10, and a similar variability of the entanglement molecular weight over this range can be inferred for this range of 1,2 content. Accordingly, for typical 1,4-polybutadienes, with 1,4 content ranging from 6-10%, all three canonical parameters of the tube model can be taken as fixed within a tight range, for 1,4-polybutadienes of any architecture, thus providing tight constraints on parameter adjustments that might be used to fit theories, such as tube theories, to rheological data.
1:03PM T42.00008 Entanglement effect in polymer melts by Dissipative Particle Dynamics (DPD). SHAHAYEGH KHANI, JOAO MAIA, Case Western Reserve University — Dissipative Particle Dynamics (DPD) is a mesoscale simulation method that has shown a very good potential in modeling different soft matter systems from colloidal suspensions to highly entangled polymers. Like any other simulation technique DPD is associated with some deficiencies, for instance in the case of entangled polymers soft repulsions used in DPD allow particle overlap which may result in topology violations that prevent the correct capturing of the entanglement effect. Therefore, in the present work in order to properly reproduce the dynamics and viscoelastic properties of polymers the soft repulsions between the particles are substituted with a repulsive potential between non-adjacent bonds of different FENE chains. Also, DPD is a coarse-grained simulation method that can be used to model time and length scales longer than atomistic models; however, due to the existence of an upper level limit for the level of coarse graining this method is not applicable for the whole mesoscopic range. Thus, this work represents a new approach for tuning the level of coarse-graining by adjusting the simulation parameters. The ability of the method in capturing the entanglement effects is validated by simulating dynamic and viscoelastic properties of polymers.

1:15PM T42.00009 Manipulating and Separating Polymers and Particles at the Microscale using Conformation-dependent Electrophoretic Mobility. PATRICK UNDERHILL, HARSH PANDEY, Rensselaer Polytech Inst — Many separation techniques rely on different physical or chemical characteristics of the objects being separated. This includes separations based on size, total charge, or strength of interaction with a substrate. Recently there are many contexts in which it is important to manipulate or separate objects with different deformabilities. The deformability of an object is also important because it is related to the rheological response. We have developed a coarse-grained Brownian dynamics simulation method that incorporates the change in electrophoretic mobility of rigid as well as flexible objects with conformation. The model incorporates the effect in a computationally efficient way, and has been validated by comparing with experiments with double-stranded DNA. In this talk, we will describe the results of computer simulations using the new model in which we quantify the stretch and residence time of polymers in a combination of electric field gradients and pressure-driven flow. The coupling of the stretch and mobility leads to a new way to trap and manipulate biomaterials. A comparison of the simulations with single molecule experiments will also be shown.

1:27PM T42.00010 Long-time diffusivity of DNA chains in nanochannels: A Brownian dynamics study. AASHISH JAIN, KEVIN DORFMAN, Univ of Minn - Minneapolis — The simplest approach to calculate the diffusivity of any polymer chain is to use the double sum Kirkwood formula, which is based on preaveraging approximation of diffusion tensor. The error due to the preaveraging approximation has been reported by a number of researchers in the context of free solution by computing both Kirkwood diffusivity $D^{(K)}$ (also known as short-time diffusivity) and long-time diffusivity $D_L$. In nanochannels, the main approach to compute the diffusivity is the Kirkwood formula. However, the error due to the preaveraging approximation is not known in a confined system. We use Brownian dynamics simulation algorithm with excluded volume and hydrodynamic interactions to calculate both short-time and long-time diffusivities of DNA chains in nanochannels, and compare them for a range of channel sizes and DNA chain sizes. Our results indicate that the long-time diffusivity is always smaller than the short-time diffusivity, which is consistent with the result obtained in free solution using linear response theory $D_L < D^{(K)}$ [M. Fixman, Macromolecules 14, 1710 (1981)]. We show that this preaveraging error decreases as channel size decreases. Even for weakly confined channels, errors are found to be about 1% for chains up to 40 nm.

1:39PM T42.00011 ABSTRACT WITHDRAWN —

1:51PM T42.00012 Nanovoid formation in cross-linked epoxy and poly(dicyclopentadiene) networks during high strain rate deformation. ROBERT M. ELDER, DANIEL B. KNORR, JR., JOSEPH L. LENHART, JAN W. ANDZELM, TIMOTHY W. SIRK, US Army Research Laboratory — Cross-linked polymer networks are widely used as structural and protective materials under extremes of temperature, pressure, or strain rate. In particular, substantial effort has been devoted to improving the high strain rate impact resistance of epoxy resins. Although epoxy resins are widely used in applications requiring impact resistance, epoxy resins with the strength and stiffness necessary in structural applications typically have poor toughness. Recent work showed that other chemistries in cross-linked polymers can overcome this trade-off between strength and toughness. Specifically, cross-linked poly(dicyclopentadiene) (pDCPD) was found to have exceptional performance compared to epoxy resins, which is related to the high toughness of pDCPD. Based on the physicochemical properties of epoxy and pDCPD, it was hypothesized that the excellent toughness of pDCPD was due to the formation and growth of nanovoids during impact events. Void growth dissipates energy that otherwise would contribute to failure. We use atomistic molecular dynamics simulations to quantify void formation in these cross-linked polymer networks and to examine the molecular-level properties of the voids. Our findings suggest methods to increase void formation and growth, which may improve toughness.

2:03PM T42.00013 Modelling poly(p-phenylene teraphthalamide) at Extreme Tensile Loading using Reactive Potentials1. DUNDAR YILMAZ, Zirve University — Aromatic polyamides classified as rigid-rod polymers due to orientation of their monomers. Because of their excellent mechanical and thermal properties, aramids are widely used in the industry. For example DuPont’s brand Kevlar, for its commercial aromatic polyamide polymer, due to wide usage of this polymer in ballistic applications, habitually used as a nickname for bulletproof vests. In order to engineer these ballistic fabrics, material properties of aramid fibers should be studied. In this work we focused on the poly(p-phenylene teraphthalamide) PPTA fiber, known as brand name Kevlar. We employed Reactive potentials to simulate PPTA polymer under tensile loading. We first simulated both amorphous and crystalline phases of PPTA. We also introduced defects with varying densities. We further analysed the recorded atomic positions data to understand how tensile load distributed and failure mechanisms at extreme tensile loads.

1This work supported by TUBITAK under grant no: 113F358

Thursday, March 5, 2015 11:15AM - 2:15PM —
Session T43 DPOLY: Focus Session: Dynamics of Glassy Polymers Under Confinement II 214C
- Rodney Priestley, Princeton University
11:15AM T43.00001 Cooperative Motion as a Unifying Principle to Understand Confinement Effects on Glass Formation, FRANCIS STARR, Wesleyan University — We examine how confinement scale and interfacial interactions affect glassy network formation, studied via molecular dynamics simulations. We consider both thin supported polymer films and polymer-nanoparticle composites. By varying the film thickness, nanoparticle loading fraction, or polymer-interfacial interactions, we can significantly alter both $T_g$ and the fragility of glass formation, leading to a seemingly intractable degree of complexity. However, we find that all our observations can be described in unified way by using the scale of collective motion as a measure of “cooperatively rearranging regions” in the Adam-Gibbs (AG) description of glass formation. For thin films, we show how the scale of cooperative motion relates to the scale of enhanced interfacial dynamics at the free surface, offering a promising route to experimentally determine the scale of cooperative motion. These string-like motions can further be described as a living polymerization. Combining polymerization theory with the AG approach, we theoretically predict the relaxation time at much lower $T$, which suggests a return to Arrhenius behavior that avoids a Kauzmann “entropy crisis.” Finally, we consider the applications of these ideas to ultra-stable polymer films formed by vapor deposition.

11:51AM T43.00002 Effects of Substrate Interaction on Slow Dynamics and Vitrification in Confined Thin Films, STEPHEN MIRIGIAN, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — The nanoscopic confinement of a glass-forming liquid can have major effects on its slow dynamics which depend on the nature of the confining surface in a nonuniversal manner. We generalize our force-level theory for free-standing films [1] to incorporate the effects of solid surfaces in supported and capped films. A solid surface is treated as locally modifying the liquid density as a consequence of packing-induced layering and/or physical adsorption. For films supported on a neutral surface where the former densification mechanism is dominant, the theory predicts that the physical behavior is akin to a free-standing film but with one interface behaving in a nearly unperturbed bulk manner, in agreement with experiment. With increasing interfacial attraction, the relaxation near the solid surface slows down dramatically and a very large local mobility gradient emerges. The competition between the dynamical effects of the adsorbed layer and the mobile layer near the vapor interface results in a rich behavior of an apparent vitrification temperature. Representative calculations of the full spatial gradient of the relaxation time as a function of temperature, film thickness, and interfacial densification will be presented.


12:03PM T43.00003 Slow Relaxation, Vitrification, and Mobility Gradients in Free Standing Thin Films, KENNETH SCHWEIZER, STEPHEN MIRIGIAN, University of Illinois at Urbana-Champaign — Glass forming molecular and polymeric liquids confined by free surfaces experience major changes of their slow dynamics beginning at relatively large film thickness. We have constructed a predictive, quantitative, force-field level theory of relaxation in free-standing films that addresses the nature of the spatial mobility gradient [1]. The theory predicts a generic speed up of relaxation near the free surface due to two coupled effects: a local, direct surface reduction of cages near the vapor interface, and a weakening of the spatially long ranged component of the activation barrier associated with collective elasticity. Effective vitrification temperatures, dynamic length scales and mobile layer thicknesses naturally follow. At low temperatures in the vicinity of the thickness-dependent $T_g$, highly mobile and immobile regions are predicted to coexist near the surface and in the film interior, respectively. The latter can result in mechanical stiffening which can commence at a large film thickness. Our results provide a theoretical basis for reconciling a variety of experimental results (e.g., probe mobility, dielectric relaxation, particle embedding, ellipsometry, creep) within a single framework.


12:15PM T43.00004 Fragility Nanoconfinement Effect in Thin Polymer Films: Novel Characterization by Ellipsometry, TIAN LAN, Department of Materials Science and Engineering, Northwestern University, JOHN TORKELSON, Department of Materials Science and Engineering, Department of Chemical and Biological Engineering, Northwestern University — A novel ellipsometry-based method was introduced to determine kinetic fragility in polymer films and to investigate the effect of nanoscale confinement on polymer fragility. Three systems were studied: polystyrene (PS), polycarbonate (PC), and PS doped with small molecule dilluents of 1,10-bis-(1-pyrene)decane (BPD). In bulk-like films, fragility index measured by ellipsometry agreed very well with that by differential scanning calorimetry. With confinement, a dramatic decrease in fragility was observed in highly fragile PS and PC. The fragility decreased by 58% from 166 to 69 in PS and by 65% from 214 to 75 in PC as film thickness decreased from bulk to 27-28 nm; a substantially muted response was observed in the strongest of the three: PS + 2 wt% BPD, where the fragility decreased only 21% from 134 to 106 from a bulk film to a 27-nm-thick film. The larger fragility-confinement effect in more fragile polymers strongly correlates with a previous discovery of the $T_g$-confinement effect: the strength of the $T_g$-confinement effect increases with increasing fragility of bulk polymers. It indicates that bulk fragility is associated with the susceptibility of polymers to effects of nanoscale confinement.

12:27PM T43.00005 Vitrification of thin polymer films: from linear chain to soft-colloid like behavior, EMMANOULIS GLYNOS, BRADLEY FRIEBERG, University of Michigan, GEORGIOS SAKELLARIOU, University of Athens, ALEXANDROS CHREMOS, Imperial University, PETER GREEN, University of Michigan — The glass transition temperature $T_g$ of sufficiently thin, supported polymer films is dependent on the film thickness. Based on the nature of the polymer substrate interactions $T_g$ may increase, $\Delta T_g > 0$, or decrease, $\Delta T_g < 0$, in relation to the bulk. We show that for star-shaped macromolecules the value of $\Delta T_g$ depends on the functionality $f$ of the molecule, for polymer films supported by the same substrate. Specifically in the case of polystyrene (PS) macromolecules, with arms of molecular weight $M_{arm} < 10$ kg./mol., supported by silicon oxide substrates, $\Delta T_g < 0$, when $f < 4$. For much higher functionalities, $f > 32$, where the polymer exhibits soft-colloid like behavior $\Delta T_g \sim 0$. For values of $4 < f < 32$, $\Delta T_g > 0$. The transition from the linear-chain to the soft-colloid behavior is gradual and occurs with increasing $f$ and/or decreasing $M_{arm}$. With the help of molecular dynamics simulations we rationalize this behavior in terms of competing entropic effects, associated with changes in $f$ and $M_{arm}$, which drives the stability of these molecules to efficiently pack at interfaces.

12:39PM T43.00006 Dynamics of Hyperbranched Polymers under Confinement1, KRYSTALLLENIA ANDROULAKI, KIRIAKI KRISSHOPPOULOU, SPIROS H. ANASTASIADIS, Foundation for Research and Technology-Hellas and Univ. of Crete, Greece, DANIELE PREVOSTO, MASSIMILIANO LABARDI, University of Pisa, Italy — The effect of severe confinement on the dynamics of three different generations of hyperbranched polymers (Boltorns) is investigated by Dielectric Spectroscopy. The polymers are intercalated within the galleries of natural Na+–MMT, thus, forming 1nm polymer films confined between solid walls. The $T_g$’s of the polymers determined by DSC show a clear dependence on the generation whereas the transition is completely suppressed when all the polymer chains are intercalated. Combining polymerization theory with the AG approach, we theoretically predict the relaxation time at much lower $T$, which suggests a return to Arrhenius behavior that avoids a Kauzmann “entropy crisis.” Finally, we consider the applications of these ideas to ultra-stable polymer films formed by vapor deposition.

1 Co-financed by the EU and Greek funds through the Operational Program ”Education and Lifelong Learning” of the NSRF-Research Funding Program: THALES-Investing in knowledge society through the Eur. Social Fund (MIS 377278) and COST Action MP0902-COINAPO
and thin films, as well as in a BLJ liquid that we have simulated. The glass-formation can equally well describe the relaxation data for a large range of fragility variations of glass-forming liquids, such as polymer nanocomposites, and the local volume accessible for particle motion, and the growth of the collective motion in supercooled liquids. Surprisingly, we find that each of these models of local dynamics can be used to understand such different perspectives. In this work, we find quantitative relations between emergent elasticity in terms of the average local dynamics of glass-forming liquids. Some of them emphasize the importance of a progressively growing cooperative motion which grows while the configuration changes from the two processes are different.

Thermodynamic theories have predicted that the observed Tg reduction in ultrathin polymer films may be tied to small shifts in the specific volume of the liquid-line above Tg. Here we use ellipsometry to investigate the temperature-dependent specific volume for supported polystyrene (PS) films of different thicknesses. Using the Lorentz-Lorenz parameter as a measure of the relative change in film density, we calculate the specific volume from temperature-dependent measurements of the index of refraction. While the slope of the liquid-line (thermal expansion coefficient) remains constant upon confinement, the Tg(h) decrease is accompanied with a broadening of the transition and a small increase in the glass-line thermal expansion, consistent with a larger fraction of the sample remaining liquid to lower temperatures. We find that both the liquid and glass specific volume lines shift together with decreasing thickness.

An open question at present is what material property changes correspond to the large shifts in film dynamics upon packing effects at the pore wall and the Tg depression arising from intrinsic size effects.

The effect of nanoconfinement on free radical equilibrium polymerization, HAOYU ZHAO, SINDEE SIMON, Texas Tech University — Free radical polymerization under nanoconfinement results in changes in reaction kinetics, reaction thermodynamics, and polymer properties. In this work, hydrophilic and hydrophobic nanoporous media (d < 13 nm) are employed as the nanoconfined matrix to perform polymerization of acrylate monomer. Differential scanning calorimetry (DSC) is used to study the reaction kinetics and thermodynamics, whereas gel permeation chromatography (GPC) is used to measure the molecular weight of the polymer produced. Although the polymerization is thermodynamically feasible at low temperature, as reaction temperatures increase, the depolymerization rates in acrylate polymerization become appreciable resulting in equilibrium polymerization at high temperature. For polymer synthesized in nanoconfined environment, the change in entropy upon propagation becomes a larger negative number resulting in a decrease in equilibrium conversion and a shift of the ceiling temperature to lower temperatures. The results are analyzed in the context of the scaling of the change in confinement entropy of chains on chain length.

The effect of film processes on the chain conformations of adsorbed polymer nanolayers, MANI SEN, MAYA K. ENDOH, TADANORI KOGA, Department of Materials, Stony Brook, NY 11794-2275, DAISUKE KAWAGUCHI, Education Center for Global Leaders in Molecular Systems for Devices, Kyushu University, Fukuoka 819-0395, Japan, KEIJI TANAKA, Department of Applied Chemistry, Faculty of Engineering, Kyushu University, Fukuoka 819-0395, Japan — Polymer chains adsorb even onto weakly attractive solid surfaces, resulting in the formation of adsorbed polymer nanolayers ("PNs")..

We report how film processing affects the chain conformations composed of PNs. 50 nm thick polystyrene (PS, Mw=290 kDa) thin films were prepared onto hydrogen-passivated silicon substrates by using two different processes (i.e., spin coating and dip coating). The PNs were then formed by high temperature thermal annealing and subsequent rinsing with a good solvent. We characterized the PNs using x-ray reflectivity (XR), atomic force microscopy (AFM), and sum-frequency generation spectroscopy. The XR and AFM data reveal that the homogenous PNs are composed of the two different architectures regardless of the film processing: flattened polymer chains that constitute the inner higher density region of PNs and loosely adsorbed polymer chains that form the outer bulk-like density region although adsorbed chain conformations from the two processes are different.

1:51PM T43.00007 Enhanced Tg-Confinement Effect in Crosslinked Polystyrene Characterized by Ellipsometry, KAILONG JIN, JOHN TORKELSON, Northwestern University — The effects of nanoscale confinement on the glass transition temperature, Tg, and related behavior are studied in crosslinked polystyrene (PS). Crosslinked PS films are achieved by thermally annealing the spin-cast linear precursor (polystyrene-vinylbenzocyclobutene) films with varying thicknesses at 250 °C. Tg reductions are observed with ellipsometry measurements of both supported linear and crosslinked PS films, with confinement effects being enhanced in crosslinked polystyrene compared to the linear precursor. The greater magnitude of Tg reduction observed in confined crosslinked PS films can be rationalized by the increased bulk fragility induced by crosslinking. Effects of confinement on fragility and physical aging in the crosslinked PS will also be discussed.

1:03PM T43.00008 Reaction Rate Acceleration and Tg Depression of Polycyanurate Under Nanopore Confinement, EVELYN LOPEZ, SINDEE L. SIMON, Texas Tech University — Material properties such as Tg and the reaction kinetics are known to deviate from the bulk when subjected to nano-sized confinement. Previous work from our laboratory on the trimerization of cyanoate esters found that the reaction kinetics were faster for a monofunctional reactant compared to a difunctional monomer, whereas the Tg depression was greater for the crosslinked product of the latter compared to the low molecular weight trimer of the former. The origin of the changes in nanoconfined reaction rates differs from those that govern changes in the Tg. The research objective is to further explore the effect that confinement has on reaction kinetics and Tg using a mixture consisting of mono- and di-cyanoate ester monomers. The product is an uncrosslinked polycyanurate with Mn = 5240 g/mol and PDI = 1.78. The confinement mediums are controlled pore glasses with diameters ranging from 8.1 to 111.1 nm. The nanopore-confined material was synthesized in-situ and the reaction kinetics are followed by DSC; after the reaction, the Tg values of the nanoconfined polymer where also measured by DSC. An acceleration factor of 13 and a Tg depression of 38 °C are observed for the material confined in the smallest 8.1 nm-diameter pores. The Tg depression is between those of the trimer and network previously studied, while the acceleration of the reaction rate is lower. Our results are consistent with the reaction acceleration arising from packing effects at the pore wall and the Tg depression arising from intrinsic size effects.

1:15PM T43.00009 The Effect of Nanoconfinement on Free Radical Equilibrium Polymerization, HAOYU ZHAO, SINDEE SIMON, Texas Tech University — Free radical polymerization under nanoconfinement results in changes in reaction kinetics, reaction thermodynamics, and polymer properties. In this work, hydrophilic and hydrophobic nanoporous media (d < 13 nm) are employed as the nanoconfined matrix to perform polymerization of acrylate monomer. Differential scanning calorimetry (DSC) is used to study the reaction kinetics and thermodynamics, whereas gel permeation chromatography (GPC) is used to measure the molecular weight of the polymer produced. Although the polymerization is thermodynamically feasible at low temperature, as reaction temperatures increase, the depolymerization rates in acrylate polymerization become appreciable resulting in equilibrium polymerization at high temperature. For polymer synthesized in nanoconfined environment, the change in entropy upon propagation becomes a larger negative number resulting in a decrease in equilibrium conversion and a shift of the ceiling temperature to lower temperatures. The results are analyzed in the context of the scaling of the change in confinement entropy of chains on chain length.

1:27PM T43.00010 Effect of film processes on the chain conformations of adsorbed polymer nanolayers, MANI SEN, MAYA K. ENDOH, TADANORI KOGA, Department of Materials, Stony Brook, NY 11794-2275, DAISUKE KAWAGUCHI, Education Center for Global Leaders in Molecular Systems for Devices, Kyushu University, Fukuoka 819-0395, Japan, KEIJI TANAKA, Department of Applied Chemistry, Faculty of Engineering, Kyushu University, Fukuoka 819-0395, Japan — Polymer chains adsorb even onto weakly attractive solid surfaces, resulting in the formation of adsorbed polymer nanolayers ("PNs"). We report how film processing affects the chain conformations composed of PNs. 50 nm thick polystyrene (PS, Mw=290 kDa) thin films were prepared onto hydrogen-passivated silicon substrates by using two different processes (i.e., spin coating and dip coating). The PNs were then formed by high temperature thermal annealing and subsequent rinsing with a good solvent. We characterized the PNs using x-ray reflectivity (XR), atomic force microscopy (AFM), and sum-frequency generation spectroscopy. The XR and AFM data reveal that the homogenous PNs are composed of the two different architectures regardless of the film processing: flattened polymer chains that constitute the inner higher density region of PNs and loosely adsorbed polymer chains that form the outer bulk-like density region although adsorbed chain conformations from the two processes are different.

1:39PM T43.00011 Investigation of the Temperature-Dependent Specific Volume of Supported Polystyrene Films Upon Confinement, XINRU HUANG, CONNIE ROTH, Dept. of Physics, Emory University — The experimentally observed large changes in the glass transition temperature Tg of ultrathin supported and free-standing polymer films with decreasing thickness h have puzzled the field for more than two decades. An open question at present is what material property changes correspond to the large shifts in film dynamics upon confinement. Thermodynamic theories have predicted that the observed Tg(h) decrease in ultrathin polymer films may be tied to small shifts in the specific volume of the liquid-line above Tg. Here we use ellipsometry to investigate the temperature-dependent specific volume for supported polystyrene (PS) films of different thicknesses. Using the Lorentz-Lorenz parameter as a measure of the relative change in film density, we calculate the specific volume from temperature-dependent measurements of the index of refraction. While the slope of the liquid-line (thermal expansion coefficient) remains constant upon confinement, the Tg(h) decrease is accompanied with a broadening of the transition and a small increase in the glass-line thermal expansion, consistent with a larger fraction of the sample remaining liquid to lower temperatures. We find that both the liquid and glass specific volume lines shift together with decreasing thickness indicative of small 0.5-1% changes in overall film density with decreasing thickness.

1:51PM T43.00012 Quantitative Relations Between Cooperative Motion and Emergent Elasticity in Model Glass-Forming Polymer Materials, BEATRIZ A PAZMINO BETANCOURT, Wesleyan/NIST, PAUL HANAKATA, FRANCIS W STARR, Wesleyan, JACK F. DOUGLAS, NIST — There are many semi-empirical models that allow us to understand the dynamics of glass-forming liquids. Some of them emphasize the importance of a progressively growing cooperative motion which grows while the configuration entropy of the liquid drops. Others from a solid-like nature of glass perspective look at the emergent elasticity. However, there has been limited success in finding a unified framework of understanding such different perspectives. In this work, we find quantitative relations between emergent elasticity in terms of the average local volume accessible for particle motion, and the growth of the collective motion in supercooled liquids. Surprisingly, we find that each of these models of glass-formation can equally well describe the relaxation data for a large range of fragility variations of glass-forming liquids, such as polymer nanocomposites, and thin films, as well as in a BLJ liquid that we have simulated.
2:03PM T43.00013 Molecular-weight Dependent $T_g$ Depression of Silica-supported Poly($\alpha$-methyl styrene) Films1, KUN GENG, FEI CHEN, Department of Physics, Boston University, OPHELIA K. C. TSUI, Department of Physics and Division of Materials Science and Engineering, Boston University — The glass transition temperature ($T_g$) of poly($\alpha$-methyl styrene) (P$\alpha$MS) films supported by silica is studied as a function of film thicknesses from 17 to 168 nm at three molecular weights of 1.3, 20 and 420 kg/mol. For the 20 and 420 kg/mol films, the glass transition temperature decreases with decreasing film thickness, consistent with previous results. But for the 1.3 kg/mol films, it becomes independent of the film thickness. We tentatively suggest the $T_g$ depression to be caused by free volume excess at the polymer-air interface and that its influence diminishes at low enough molecular weights because of a chain stiffness effect.

1Support from National Science Foundation (Award no. DMR-1310536) is gratefully acknowledged.

Thursday, March 5, 2015 11:15AM - 2:15PM – Session T44 GSNP GSOFT: Focus Session: Granular Materials and Continuum Descriptions of Discrete Media II

11:15AM T44.A00001 ABSTRACT WITHDRAWN –

11:27AM T44.A00002 ABSTRACT WITHDRAWN –

11:39AM T44.A00003 Shear of ordinary and elongated granular mixtures1, ALEXANDER HENSLEY, MATTHEW KERN, Rochester Institute of Technology, THEODORE MARCHALL, STEPHEN TEITEL, University of Rochester, SCOTT FRANKLIN, Rochester Institute of Technology — We present an experimental and computational study of a mixture of discs and moderate aspect-ratio ellipses under two-dimensional annular planar Couette shear. Experimental particles are cut from acrylic sheet, are essentially incompressible, and constrained in the thin gap between two concentric cylinders. The annular radius of curvature is much larger than the particles, and so the experiment is quasi-2d and allows for arbitrarily large pure-shear strains. Synchronized video cameras and software identify all particles and track them as they move from the field of view of one camera to another. We are particularly interested in the global and local properties as the mixture ratio of discs to ellipses varies. Global quantities include average shear rate and distribution of particle species as functions of height, while locally we investigate the orientation of the ellipses and non-affine events that can be characterized as shear transformational zones or possess a quadrupole signature observed previously in systems of purely circular particles. Discrete Element Method simulations on mixtures of circles and spherocylinders extend the study to the dynamics of the force network and energy dissipated as the system evolves.

1Supported by NSF CBET #1243571 and PRF #51438-UR10.

11:51AM T44.A00004 Maxwell Construction for a Nonequilibrium Steady-State Phase Separation in Granular Matter, MARCO G. MAZZA, JAMES CLEWETT, Max Planck Institute for Dynamics and Self-Organization, JACK WADE, ROGER BOWLEY, University of Nottingham, STEPHAN HERMINGHAUS, Max Planck Institute for Dynamics and Self-Organization, MICHAEL SWIFT, University of Nottingham — Experiments and computer simulations are carried out to investigate phase separation in a granular gas under external vibration in a large sample cell. The densities of the dilute and the dense phase are found to follow a lever rule, suggesting an equation of state. We show that this equation of state, which exhibits a non-monotonous pressure-volume characteristic, $P(v)$, can be obtained from simulations of a small cell. A Maxwell construction is found to predict both the coexisting pressure and binodal densities remarkably well, despite the fact that $P(v)$ is not an isotherm. Although the system is far from equilibrium and energy conservation is strongly violated, we can derive this finding from an energy minimization argument of fluctuating currents.

12:03PM T44.A00005 Electrical charging in shaken granular media1, FREJA NORDSIK, DANIEL LATHROP, University of Maryland College Park — Collisional electrification of granular particles and the resulting electric fields are seen but poorly understood in sand storms, volcanic ash clouds, thunderstorms, and thundersnow. We present results on the electrical charging of granular media (100 micron to 1 mm in size) shaken between two conducting plates. The voltage between the plates was measured. We saw particle electrification through capacitive coupling with the plates and electrical discharges for a diverse class of materials: polystyrene (polymer), soda-lime glass (glass), 69%:31% ZrO$_2$:SiO$_2$ (ceramic), and aluminum (metal). We found 1) a monotonic increase in charging with shaking strength, 2) a threshold in the number of particles to see charging of about the number of particles needed to form a monolayer on the plate, 3) material and diameter differences causing an order of magnitude spread in measured signal but little difference between mono-material sets with one size range and bi-material and/or bi-size range set combinations, and 4) long time scale transients. We argue that while two-body collisions and the physical properties of the particles (material and size) are relevant, collective phenomena are a necessary part of explaining natural charging of granular flows.

1We gratefully acknowledge funding from the Julien Schwinger Foundation.

12:15PM T44.A00006 Complex Kepler Orbits and Particle Aggregation in Charged Microscopic Grains, VICTOR LEE, Univ of Chicago, SCOTT WAIKUKAITIS, Leiden University, MARC MISKIN, Cornell University, HEINRICH JAEGER, Univ of Chicago — Kepler orbits are usually associated with the motion of astronomical objects such as planets or comets. Here we observe such orbits at the microscale in a system of charged, insulating grains. By letting the grains fall freely under vacuum, we eliminate the effects of air drag and gravity, and by imaging them with a co-falling high-speed camera we track the relative positions of individual particles with high spatial and temporal precision. This makes it possible to investigate the behaviors caused by the combination of long-range electrostatic interactions and short-range, dissipative, contact interactions in unprecedented detail. We make the first direct observations of microscopic elliptical and hyperbolic Kepler orbits, collide-and-capture events between pairs of charged grains, and particle-by-particle aggregation into larger clusters. Our findings provide experimental evidence for electrostatic mechanisms that have been suspected, but not previously observed at the single-event level, as driving the early stages of particle aggregation in systems ranging from fluidized particle bed reactors to interstellar protoplanetary disks. Furthermore, since particles of different net charge and size are seen to aggregate into characteristic spatial configurations, our results suggest new possibilities for the formation of charge-stabilized “granular molecules”. We can reproduce the observed molecule configurations by taking many-body, dielectric polarization effects into account.
A nonlinear feedback model for granular and surface charging. TROY SHIN-BROT, LEO KOZACHKOV, THEO SIU, Rutgers University — Independent laboratories have experimentally demonstrated that identical materials brought into symmetric contact generate contact charges. Even the most basic features of this odd behavior remain to be explained. In this talk, we provide a simple,· Ising-like, model that appears to account for many of the observed phenomena. We calculate the electric field acting on surface molecules in a lattice, and we show that if the molecules are polarizable, then infinitesimal random polarizations typically build exponentially rapidly in time. These polarizations self-assemble to produce surface patterns that come in two types, and we find that one of these types accounts for strong localized charging, while the other produces a weaker persistent surface charge pattern. We summarize predictions for both ideal surfaces and for defects in granular beds.

1:03PM T44.00010 Effect of system and particle properties on closure relations for granular segregation models. ABHINENDRA SINGH, D. R. TUNUGUNTALA, A. R. THORNTON, Univ of Twente, MULTI SCALE MECHANICS TEAM — In recent years, much effort has been made on developing valid constitutive laws for continuum models to describe kinetic sieving driven segregation in granular flows over inclined channels. Surprisingly, the existing closure relations for such continuum models have not considered factors such as particle contact stiffness, coefficient of restitution etc. Using Discrete Element method simulations, we investigate the effects of these factors on particle segregation and thereby manifest the grain-to-wall effective friction force is reached. This can be related to a theoretical model which treats the silo as a thin cylindrical shell subjected to an axial stress with the profile predicted by Janssen’s model for the stresses in a silo filled with a granular material. This model predicts correctly the experimental scaling of with various parameters of the system.

1:15PM T44.00011 Formation and properties of a dynamic suspension. TESS HOMAN, VALÉRIE VIDAL, SYLVAIN JOUBAUD, Laboratoire de Physique, Ecole Normale Supérieure de Lyon — We experimentally study the behaviour of an immersed granular bed in a Hele-Shaw cell when perturbed by an airflow from a single inlet at the bottom. When the particles are slightly heavier than the liquid, the competition between particles being dragged up into the liquid and particles settling due to gravity results in a dynamic suspension. In the stationary regime, part of the initial granular bed never moves, and forms a so-called “dead zone.” We investigate its shape and extent as a function of the parameters (air flow-rate, initial grains and liquid height). We also focus on the formation and properties of the dynamic suspension by optically recording the full particle density field in the Hele-Shaw cell. The mean density and density fluctuations of the dynamic suspension are studied as a function of the gas flow-rate and the ratio between the initial granular bed never moves, and forms a so-called “dead zone.” We investigate its shape and extent as a function of the parameters (air flow-rate, initial grains and liquid height). We also focus on the formation and properties of the dynamic suspension by optically recording the full particle density field in the Hele-Shaw cell. The mean density and density fluctuations of the dynamic suspension are studied as a function of the gas flow-rate and the ratio between the amount of grains and liquid.

1:27PM T44.00012 Raindrop impact on sand: dynamic and crater formation. SONG-CHUAN ZHAO, RIANNE DE JONG, DEVARAJ VAN DER MEER, Univ of Twente — Droplet impact on a granular bed is very common in nature, industry, and agriculture and extends from raindrops falling on earth to wet granulation in the production process of many pharmaceuticals. In contrast to more traditionally studied impact phenomena, such as a droplet impact on solid substrate and solid object impact on fluid-like substrate, raindrop impact on sand induces more complicated interactions. First, both the intruder and the target deform during impact; second, the liquid composing the droplet may penetrate into the substrate during the impact and may, in the end, completely merge with the grains. These complex interactions between the droplet intruder and the granular target create the very diverse crater morphologies that has been described in the literature. An appealing and natural question is how the craters are formed. To gain insight in the mechanism of crater formation, we resolve the dynamics with high-speed laser profilometry and study the dependence of the dynamics on impact speed and packing fraction of the granular substrate. Finally, we establish a dynamical model to explain the various crater morphologies.

1:39PM T44.00013 Granular impact cratering by liquid drops: Understanding raindrop imprints through an analogy to asteroid strikes. XIANG CHENG, RUNCHEN ZHAO, QIANYUN ZHANG, HENDRO TJUGITO, University of Minnesota — When a granular material is impacted by a sphere, its surface deforms like a liquid yet it preserves a circular crater like a solid. Although the mechanism of granular impact cratering by solid spheres is well explored, our knowledge on granular impact cratering by liquid drops is still very limited. Here, by combining high-speed photography with high-precision laser profilometry, we investigate liquid-drop impact dynamics on granular surface and monitor the morphology of resulting impact craters. Surprisingly, we find that, despite the enormous energy and length difference, granular impact cratering by liquid drops follows a similar energy scaling and reproduces the same crater morphology as that of asteroid impact craters. Inspired by this similarity, we propose a simple, theoretical model that quantitatively describes all the main features of liquid-drop imprints in granular media. Our study sheds light on the mechanisms governing raindrop impacts on granular surfaces and reveals a remarkable analogy between familiar phenomena of raining and catastrophic asteroid strikes.
1:51PM T44.00014 Kinetics of Gravity-Driven Water Channels under Steady Rain, REMI DREYFUS, CESARE CEJAS, REMI BARROIS, CNRS-Solvay-UPenn UM13254, Complex Assemblies of Soft Matter, COMPASS, Bristol, PA, USA 19007, YULLI WEI, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19014, CHRISTIAN FREITIGNY, CNRS UMR 7615 Sciences et Ingénierie de la Matière Molle (SIMM), ESPCI, Paris, France 75005, DOUGLAS DURIAN, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19014 — We investigate the physical mechanisms that govern the formation of water channels that develop from finger instabilities at the wetting front. Using controlled experiments in a quasi-2D cell and varying physical parameters (particle size, fluid viscosity, etc.), we simulate rainfall and characterize the homogeneous wetting front as well as channel size and estimate relevant time scales associated with the instability as well as channel velocity. We validate the results by developing a model based on linear-stability analysis with the addition of another term describing the homogenization of the wetting front. This shows that the way we introduce a fluid into a granular medium affects the formation of water channels. Results permit us to calculate the ideal flow rate for maximizing water distribution and minimizing runoffs using granular and fluid properties.

2:03PM T44.00015 Splash Suppression by Solvent Viscosity in Dense Suspension Impact, WENDY ZHANG, KEVIN DODGE, IVO PETERS, MARTIN KLEIN SCHAARSBERG1, HEINRICH JAEGGER, University of Chicago — When a dense suspension droplet impacts a hard surface, it will either break apart (“splash”) or remain in a compact configuration without ejecting any particles. We use experiments and discrete particle simulations in which relative particle motions are penalized by lubrication-flow drag to analyze the influence of solvent viscosity on splashing. We find that suspension splash is driven by particle inertia. It can be suppressed in 2 different ways. At low solvent viscosity, lubrication drag due to viscous flow has a negligible effect. Splash is suppressed by surface tension overcoming particle inertia. At high solvent viscosity, lubrication drag alone suppresses splashing. Because impact produces an expanding flow that stretches the suspension radially, suppression in the high-viscosity regime is largely accomplished by lubrication-flow drag preventing initially nearby particle pairs from separating fully. Energy dissipation by viscous flow during collisions plays a smaller role.

1Present Address: Physics of Fluids Group, University of Twente

Thursday, March 5, 2015 11:15AM - 2:15PM — Session T45 DPOLY: Transport in Polymer Membranes 216AB - Rajiv Taribagil, Infineum

11:15AM T45.00001 Three-Step Water Sorption of Thin Nafion Films, DAISUKE KAWAGUCHI, Education Center for Global Leaders in Molecular Systems for Devices, Kyushu University, YUDAI OGATA, Department of Applied Chemistry, Kyushu University, Japan, NORIFUMI YAMADA, Neutron Science Laboratory, High Energy Accelerator Research Organization, Japan, KELII TANAKA, Department of Applied Chemistry, Kyushu University, Japan — Nafion has been widely used as a proton exchange film in polymer electrolyte fuel cell (PEFC). Although downsizing PEFC is one of the interesting developments in the near future, it appears that most studies conducted so far are limited to bulk systems. Here we examined water sorption behavior in thin Nafion films based on optical and neutron reflectivity measurements. Nafion films were prepared on silver and silicon oxide substrates. It was found that the thicknesses of Nafion thin films increased with time after contacting water in three steps. The asymptotic swelling ratios in regimes I, II and III were 1.05, 1.26 and 1.41, respectively. These values were in-dependent of the substrate species, and were coincident with the transition points of different hydration states in the bulk Nafion; water binding to sulfonic acid groups, the formation of sphere-like ionic clusters, and bridge formation between clusters. The swelling was much slower in thin films than in the bulk due to the mobility restriction of Nafion near the substrate.

11:27AM T45.00002 Impact of Ageing on Properties of PFSA Ionomers1, AHMET KUSOGLU, MERON TESFAYIR, SHOUWEN SHI, WILL TONG, ADAM WEBER, Lawrence Berkeley National Laboratory — Perfluorosulfonic-acid (PFSA) ionomers are widely used as the solid-electrolyte in electrochemical energy applications due to their remarkable conductivity and chemical/mechanical stability. However, in various applications, it is not uncommon for the ionomer to be subjected to various operational environmental stressors that could impact their morphology and properties. In this talk, the impact of hygrothermal ageing on both bulk ionomer and ionomer thin films will be discussed. The intrinsic changes to the morphology and properties will be presented including water uptake and swelling behavior as well as nanostructure using both transmission and grazing-incidence small- and wide-angle x-ray scattering. It will be shown how ageing at intermediate humidities (50 to 70% relative humidity) induces higher mechanical properties and subsequently lower water uptake for both bulk and thin film ionomers due to a loss of accessible ionic sites, which are thought to form crosslinks. Ageing at higher and lower relative humidities shows a decrease in these changes. The ionomers to be studied include both Nafion and the short-side-chain analogue by 3M with higher ion-exchange capacity. Our findings provide new insights into how ageing alters the structure/function relationship of ionomers.

1Supported by U. S. Department of Energy under contract number DE-AC02-05CH11231 and Joint Center for Artificial Photosynthesis

11:39AM T45.00003 In-situ measurement of swelling induced stress of thin Nafion films during hydration cycles, BRADLEY FRIEBERG, KIRT PAGE, GERY STAFFORD, CHRISTOPHER SOLES, Natl Inst of Stds & Tech (NIST) — Perfluorinated ionomers, in particular Nafion, are a critical component in hydrogen fuel cells, as the binder within the membrane electrode assembly in which it can be confined to thicknesses on the order of ten nanometers. During normal operation of a hydrogen fuel cell the ionomer will progressively swell and de-swell in response to the changes in hydration, resulting in a mechanical fatigue and ultimately failure of the fuel cell with time. In this study we have developed and implemented a cantilever bending technique in order to investigate the swelling induced stresses in Nafion thin films. By monitoring the deflection of a cantilever beam coated with a polymer film as it is exposed to various humidity environments, the swelling induced stress-thickness of the polymer film can be measured. By combining the stress-thickness results with a measurement of the film thickness as a function of humidity, the swelling stress can be determined. Using this techniques we have measured the shear modulus and estimated the Young’s modulus of thin Nafion films as a function of film thickness (ranging from 30 nm to 200 nm), processing conditions and humidity.

11:51AM T45.00004 Elucidating the Role of Confinement on Structure and Water Transport in Nafion Thin Films, ERIC DAVIS, NICHOLE NADERMANN, EDWIN CHAN, CHRISTOPHER STAFFORD, KIRT PAGE, Materials Science and Engineering Division, National Institute of Standards and Technology, Gaithersburg, MD 20899 — Perfluorinated ionomers, specifically Nafion, are the most widely used polymer membranes for fuel cell applications. For these devices, Nafion is utilized in both a bulk (hundreds of microns) and confined (tens of nanometers) state. Therefore, a more complete understanding of the structure-processing-property relationships of these thin ionomer films, compared to the bulk membranes, is needed. In this study, water transport and structure of a series of Nafion thin film thicknesses were measured using a variety of experimental techniques. Water diffusion was measured via time-resolved in situ polarization modulation infrared reflection absorption spectroscopy (PM-IRRAS) and poroelastic relaxation indentation (PRI). The former probes through-thickness diffusion (direction of confinement), while the latter probes in-plane diffusion in the Nafion thin films. Suppressed water diffusion relative to the bulk was observed in both the through-thickness and in-plane directions of the thin film Nafion. Additionally, the structure of hydrated Nafion thin films was captured using small-angle neutron scattering (SANS). These results suggest that the nanostructure of the Nafion changes as the thickness of the film is decreased, resulting in a decrease in the effective water diffusivity of these thin ionomer films compared to the bulk membranes.
12:03PM T45.00005 Kinetics of swelling enhancement of polyelectrolyte brushes , XIAO CHU, JINGFA YANG, Institute of Chemistry, Chinese Academy of Sciences, GUANGMING LIU, University of Science and Technology of China, JIANG ZHAO, Institute of Chemistry, Chinese Academy of Sciences — The swelling of polystyrene sulfonate brushes is enhanced due to the break-up of the multiplets formed by dipole-dipole interactions inside, when external salt concentration is increased to moderate value. By quartz crystal balance with dissipation, the kinetics of this process is investigated and a systematic study on the effect of grafting density and salt concentration is conducted. The results demonstrate the effect of spatial hindrance due to uneven distribution of segments and osmotic pressure of the external ions.

12:15PM T45.00006 Nano Aggregation of Structured Ionic Copolymers: Molecular Dynamics Simulation Study1 , DIPAK ARYAL, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — Driven by mutual segregation, block copolymers exhibit a fascinating ability to self-assemble into a variety of ordered mesoscopic structures. Incorporating an ionizable block enhances incompatibility that together with tailoring blocks for specific functions presents an immense step towards engineering controlled transport systems. Here the interplay between the interactions of solvents with the specific blocks of a pentablock with a randomly sulfonated polystyrene center, tailored for transport, tethered to flexible poly(ethylene-r-propylene) end-capped with poly-(t-butyl styrene) is studied by fully atomistic molecular dynamics simulations. The assembly of 2 to 30 macromolecules, in water results in a spherical tightly packed aggregate in which the ionizable blocks dominates the water interface. Transferred to a cyclohexane-heptane mixture, the hydrophobic blocks migrate to the interface. Surprisingly however, the ion blocks form a nano-network rather than a corona. Further, this network also develops when assembled from hydrophobic solvents, where now the hydrophobic blocks dominate the interface. This network only slightly contracts or expands as the solvent is changed while concurrently the hydrophobic blocks migrate towards or away from the solvent interface.

12:27PM T45.00007 Cluster Morphology in Lightly Sulfonated Polystyrene1 , ANUPRIYA AGRAWAL, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — Aggregation of ionic groups into clusters in ionomers renders their unique properties that drive the use in energy applications. The ionic clusters however have a dramatic impact on the rheology of this polymer. Even small fractions of ionic groups (less than 5%), constrain their dynamics, making them difficult to process. Using molecular dynamics simulations, we show that in lightly sulfonated polystyrene melts, the ionic groups aggregate into ladder type clusters. These ladder morphologies prevail for a broad temperature range and degree of sulfonation, although with some variation due to steric effects of the chain. Reducing the electrostatic strength by tuning the dielectric constant changes the cluster morphology from ladder to spherical, which in turn, greatly increases the diffusion of the polymer. The effect of changing the electrostatic strength is comparable to the effect of addition of diluents to these melts. Enhancing the electrostatic screening results in breaking the clusters, whereas increasing temperature within the measured range, results in faster diffusion of the entire polymers while the clusters remain intact.

12:39PM T45.00008 Salt uptake and dynamics in thin, highly crosslinked polyamide membranes , KATHLEEN FELDMAN, EDWIN CHAN, CHRISTOPHER STAFFORD, National Institute of Standards and Technology — Water purification membranes have historically been developed through an Edsionian, trial and error approach. It has been challenging to establish fundamental structure-property-performance relationships, including salt/water permeability, in large part due to the typically rough and poorly-defined nature of the polyamide membrane active layer. By using molecular layer by layer (mLbL) deposition, we are able to produce thin, well-defined polyamide films with controlled chemistry analogous to commercial reverse osmosis and nanofiltration membranes. While water permeation in polyamide membranes is reasonably straightforward to measure, salt permeation is more challenging, particularly in ultrathin films. We measure both equilibrium salt uptake and dynamic behavior in nanofiltration-type membranes using x-ray photoelectron spectroscopy (XPS), electrochemical impedance spectroscopy (EIS), and quartz crystal microbalance (QCM). By connecting intrinsic material properties such as the salt permeability and permselectivity with macroscopic performance measures we can begin to establish design rules for improving membrane efficiency while lowering energy requirements.

12:51PM T45.00009 Fabrication of ultrafiltration membranes using dynamic thermal annealing of Block Copolymer films , ALAMGIR KARIM, YAN LUO, YAN SUN, The University of Akron — Block copolymer (BCP) thin films have attracted immense attention for fabrication of ultrafiltration membranes due to their potential to provide dense nanostructured pores giving high flux and good efficiency. We have demonstrated generation of well-ordered hexagonally packed perpendicular cylindrical BCP films with greater than 90 percent of perpendicular cylinder orientations over large areas with high cylinder density and desired porosity at the nanoscale via facile dynamic thermal annealing. The films are then transferred to a support membrane and subsequently the vertically oriented minority block is selectively etched to form a nanoporous membrane. The porosity of film and pore density is tuned by addition of selective homopolymer block component. The structure of nanoporous BCP membranes is characterized by Atomic Force Microscopy(AFM), Grazing Incidence Small Angle X-ray Scattering and Transmission Electron Microscopy(TEM). We further demonstrate the application of these membranes for separation of emulsions and correlate flux and efficiency to parameters such as porosity, membrane thickness and tortuosity.

1:03PM T45.00010 Super stretchy polymer multilayer thin films with tunable gas barrier , FANGMING XIANG, SARAH WARD, TARÁ GIVENS, JAIME GRUNLAN, Texas A&M Univ — Super stretchy multilayer thin film assemblies with tunable gas barrier were fabricated using layer-by-layer (LbL) assembly. Unlike ionically-bonded gas barrier coatings that exhibit mud-cracking after 10% strain, hydrogen-bonded polyethylene oxide (PEO) and polyacrylic acid (PAA) multilayer thin films show no cracking after 100% strain due to low modulus. It is believed that the exceptional elasticity of this thin film originates from the intrinsic elasticity of PEO and the moderate hydrogen bond strength between PEO and PAA. The oxygen transmission rate (OTR) of a 1.58 mm thick natural rubber sheet can be reduced 10 times with a 367-nm-thick PAA/PEO nanocoating. This gas barrier improvement is largely retained after 100% strain. The modulus and oxygen permeability of PAA/PEO assembly can be tailored through altering the barrier improvement is largely retained after 100% strain. The modulus and oxygen permeability of PAA/PEO assembly can be tailored through altering the modulus and oxygen permeability of PAA/PEO assembly can be tailored through altering the barrier properties such as the salt permeability and permselectivity with macroscopic performance measures we can begin to establish design rules for improving barrier properties such as the salt permeability and permselectivity with macroscopic performance measures we can begin to establish design rules for improving membrane efficiency while lowering energy requirements.

1:15PM T45.00011 A molecular study of gas solubility in nitrile rubber , MUSAB KHAWAJA, Imperial College London, London College of Drinking, London College of Materials and Physics, London College of Physics, London College of Physics, London SW7 2AZ, UK — One of the most important uses of elastomers in the oil industry is for seals to encase and protect sensitive monitoring equipment from contamination by gases and liquids at the high pressures and temperatures in the well. Failure of such seals sometimes occurs on decompression when they are returned to the surface. The conditions in the well lead to gases being absorbed by Nitrile rubber (NBR) seals. NBR exhibits a strong permselectivity towards CO2 compared to other gases; something attributed experimentally to the enhanced solubility of CO2. In this study an explanation is sought at the molecular level for this phenomenon. A series of molecular mechanics calculations are performed to compute solubilities of different gases in NBR. The effect of acrylonitrile content on their solubilities is studied for the first time by simulation, and we discuss the important issue of convergence with respect to the sampling of different elastomer configurations. It is observed that the presence of cyano groups has a marked impact on the solubility of CO2 and an explanation is offered.
1:27PM T45.00012 Liquid Crystalline Block Copolymers with Brush Type Architecture: Toward Functional Membranes by Magnetic Field Alignment1, YOUNGWOO CHOO, MANESH GOPINADHAN, Yale University, LALIT MAHAJAN, RAJESWARI KASI, University of Connecticut, CHINEDUM OSUJI, Yale University — We introduce a novel liquid crystalline block copolymer with brush type architecture for membrane applications by magnetic field directed self-assembly. Ring-opening metathesis of n-alkoxy cyanobiphenyl and poly lactide (PLA) functionalized norbornene monomers provides efficient polymerization yielding low polydispersity block copolymers. The molecular weight of the PLA side chains, spacer length of the cyanobiphenyl mesogens are systematically varied to form well-ordered BCP morphologies at varying volume fractions. Interestingly, the system features morphology dependent anchoring condition where mesogens adopt planar block interface while homeotropic anchoring was preferred on a planar block interface. The minority PLA domains from highly aligned materials can be readily degraded by hydrolysis to produce vertically aligned nanoporous polymer films which exhibit reversible thermal switching behavior. The polymers introduced here provide a versatile platform for scalable fabrication of aligned membranes and further functional materials based on such templates.

1This work was supported by NSF(CCFMI-1246804)

1:39PM T45.00013 Bubble Growth and Dynamics in a Strongly Superheated Electrolyte within a Solid-State Nanopore1, EDLYN LEVINE, GAKU NAGASHIMA, School of Engineering & Applied Sciences, Harvard University, MICHAEL BURNS, The Rowland Nanoscience Institute at Harvard, Harvard University, JENE GOLOVCHENKO, Dept. of Physics and School of Engineering & Applied Sciences, Harvard University — Extremely localized superheating and homogeneous vapor bubble nucleation have recently been demonstrated in a single nanopore in thin, solid state membranes. Aqueous electrolytic solution within the pore is superheated to well above its boiling point by Joule heating from ionic current driven through the pore. Continued heating of the metastable liquid leads to nucleation of a vapor bubble in the pore followed by explosive growth. Here we report on the growth dynamics of the vapor bubble after nucleation in the strongly superheated liquid. The process is modeled by numerically solving the Rayleigh-Plesset equation coupled with energy conservation and a Stefan boundary condition. The initial temperature distribution, peaked at the pore center, is taken to be radially symmetric. Energy conservation includes a Joule heating source term dependent on the bubble radius, which grows to constrict ionic current through the nanopore. Temperature-dependent properties of the electrolyte and the vapor are incorporated in the calculation. Comparison of the model to experimental results shows an initial bubble growth velocity of 50m/s and total bubble lifetime of 16ns.

1This work was supported by NIH Grant #5R01HG03703 to J.A. Golovchenko.

1:51PM T45.00014 Self-assembly of Spherical Macroions in Solution: A Coarse-grained Molecular Dynamics Study1, ZHUONAN LIU, TIANBO LIU, MESFIN TSIGE, University of Akron, Department of Polymer Science, Akron, Ohio — Macroions (such as poloxomelatates) in solution can form a stable hollow spherical super-molecular structure called blackberry when they have moderate surface charge density and size (< 10 nm). Depending on the surface charge density of macroions, the size of the blackberry can be from 20 to more than 100 nm. Other macroions such as dendrimers can also self-assemble into similar super-molecular structure in solution. Existing theories such as Deby-Hückel and DLVO theories cannot explain this phenomenon and we are not aware of any other theory that can explain this. Previous studies using all-atom Molecular Dynamics simulations have shown identical macroions forming oligomers mediated by counterions. Due to the limitations in all-atom simulation and available computational capabilities, these studies handled only small systems with simple macroions, leading to less conclusive but still relevant results on the self-assembly behavior. To overcome these limitations, in this work large-scale coarse-grained modeling of macroions in solution is used. In order to understand the origin of the attractive force that is responsible for the self-assembly of macroions, different types of macroions in different solution conditions are studied.

2:03PM T45.00015 Effects of polymer hydrophobicity on the diffusivity of water and ethanol in acrylate copolymer gels, FARID KHABAZ, SRIRAM VIGNESHWAR MANI, RAJESH KHARE, Texas Tech University — Pervaporation is an energy efficient process for separating dilute alcohol-water mixtures. The efficiency of the pervaporation process is governed by the solubility and diffusivity of the water and alcohol molecules in the polymer. Molecular simulations can be used to provide detailed insights on the dependence of the diffusivity on the molecular structure of the polymer. Polyacrylate systems with varying degree of hydrophobicity are built by changing the relative concentrations of butyl acrylate and 2-hydroxy ethyl acrylate monomers which are hydrophobic and hydrophilic, respectively. In order to create the membrane structure, a random copolymer of these monomers that is cross-linked with pentaerythritol tetracrylate, is obtained using the simulated annealing polymerization technique. The volumetric properties of the systems such as density and glass transition temperature (T_g), are compared with the experimental values to validate the model structures. The diffusivity of the water and ethanol molecules inside the membrane is characterized by determining their mean squared displacement (MSD) in systems with varying degrees of hydrophobicity and cross-linker concentration. The calculated diffusion coefficients of water and ethanol from simulations will be compared with available experimental diffusion data. The correlation between the diffusivities and the degree of hydrophobicity as well as the molecular packing in these systems will be identified.


11:15AM T46.00001 Cell size control in microorganisms, ARIEL AMIR, Harvard University — Organisms in all kingdoms of life face a challenge of regulating the size of their cells, control of which is essential for their viability. How do cells decide when to divide? For decades, a popular hypothesis has been that cells can measure their absolute size, and that reaching a critical size triggers the division process. This would imply that a cell that was born smaller than average will not be smaller than average when it divides - in contrast to experiments showing that such correlations exist, and that size is partly inherited. I will present a biophysical model that sheds new light on this problem, showing that a cell does not need to know its absolute size to regulate size robustly, quantitatively explaining the experimentally measured correlations in both E. coli and budding yeast, and predicting that such correlations degrade by hydrolysis to produce vertically aligned nanoporous polymer films which exhibit reversible thermal switching behavior. The polymers introduced here provide a versatile platform for scalable fabrication of aligned membranes and further functional materials based on such templates.

11:51AM T46.00002 Determinants of Bacterial Cell Shape, AARON DINNER, The University of Chicago — We determine intergenerational shape dynamics of single Caulobacter crescentus cells. We use imaging techniques that enable us to study ~100 cells across ~4,000 total generations to achieve high statistical precision. Our data show that constriction initiates early in the cell cycle and that its dynamics is controlled by the time scale of exponential longitudinal growth. Furthermore, we find that the division plane location is inherited from the previous generation. Based on our observations, we develop a minimal mechanical model that qualitatively accounts for the cell shape dynamics and suggests that the asymmetric location of the division plane reflects the distinct mechanical properties of the stalked and swarmer poles. Generalization of the model can provide a common framework for understanding bacterial cell shape.
Contact guidance efficiency depends on the spacing between adjacent ridges. The greatest guidance efficiency occurs on 1.5-µm-spaced ridges. A larger average velocity of cell motion and actin waves, we found that the nanoridges exert bidirectional guidance on migrating cells and actin wave propagation. More cells that gels formed at lower temperature are more inhomogeneous, anisotropic, and compliant than those formed at high temperature, and cellularized samples rather than confined directional propagation along the 1.5-µm-spaced ridges. A Lagrangian implementation of this model allows us to calculate the full deformation of an initially spherical cell, when it is subjected to a band of overactivity at the cell equator that mimics the RhoA signaling pattern. Our simulations reproduce the formation and ingestion the actomyosin ring, with cell shapes and dynamics mirroring those of embryos. This model predicts cytokinesis completion above a well-defined threshold of equatorial contractility excess, and simple scaling arguments unveil the key mechanism for this first-order transition: cytoplasmic incompressibility results in a competition between the furrow line tension and the cell poles surface tension. Our theory explains how cytokinesis duration may be independent on cell size in embryos and predicts a critical role for actin turnover on the rate and success of furrow constriction. We extend our theoretical approach to explore cell shape dynamics in other essential cellular processes, such as cell polarization or cell-cell adhesion.

In collaboration with Basile Audoly, Universite Pierre et Marie Curie; Jacques Prost, Institut Curie; and Jean-François Joanny, Institut Curie, ESPCI.

Thursday, March 5, 2015 11:15AM - 2:03PM
Session T47 DBIO: Focus Session: Mechanical Structure-Function Relations in Biological Matter II

11:15AM T47.00001 Heritable adhesion geometries and mechanosensing of surfaces by biofilm-forming bacteria, VERNITA GORDON, BENJAMIN COOLEY, CHRIS RODESNEY, NUMA DHAMANI, The University of Texas at Austin — Biofilms are dense, interacting communities of single-celled organisms that are bound to each other with a self-produced polymeric matrix. Biofilms have devastating clinical impact as they increase resistance to antibiotics and the immune system as well as the production of virulence factors that damage the host. Here we examine effects very early in biofilm development, when the infection is still in a stage of a few cells not yet characterized by high biofilm densities. *Pseudomonas aeruginosa*, an opportunistic human pathogen, produces multiple extracellular polysaccharides that form the biofilm's structuring matrix. We have recently shown that the two primary polysaccharides, Pel and Psl, have distinct roles in controlling the mechanics of single-cell adhesion to a surface – Psl dominates adhesion to the surface, and Pel impairs the bacterium lie down flat (Cooley et al., 2013 Soft Matter). Here, we show that expressing Pel alters the symmetry of Psl's distribution on the surface of rod-shaped *Pseudomonas*. We also show that expressing Pel decreases the work of detachment from the surface. It seems paradoxical that a biofilm-forming organism should pay the cost of maintaining and making a gene product that reduces the energy input required to detach it from a surface. Therefore, we probe the possibility that a flat-lying bacteria may better sense a solid surface and change its signaling state accordingly.

11:27AM T47.00002 How the velvet worm squirts slime, ANDRES CONCHA, PAULA MELLADO, Adolfo Ibañez University, BERNAL MORERA-BREÑES, Universidad Nacional de Costa Rica, CRISTIANO SAMPAIO, Universidade de Sao Paulo, L. MAHADEVAN, Harvard University, JULIÁN MONGE-NÁJERA, Universidad de Costa Rica — The rapid squirt of a proteinaceous slime jet endows the ancient velvet worms (*Onychophora*) with a unique mechanism for defense from predators and for capturing prey by entangling them in a disordered web that immobilizes their target. However, to date neither qualitative nor quantitative descriptions have been provided for this unique adaptation. Here we investigate the fast oscillatory motion of the oral papillae and the exiting liquid jet that oscillates with frequencies $f \sim \sim 30 - 60$ Hz. Using anatomical images, high speed videography, theoretical analysis and a physical simulacrum we show that this fast oscillatory motion is the result of an elastohydrodynamic instability driven by the interplay between the elasticity of oral papillae and the fast unsteady flow during squirting. Our results demonstrate how passive strategies can be cleverly harnessed by organisms, while suggesting future oscillating micro-fluidic devices as well as novel ways for micro and nano fiber production using bioinspired strategies.

11:39AM T47.00003 Micromechanics of cellularized collagen I networks, CHRISTOPHER JONES, MATT CIBULA, DAVID MINTYRE, BO SUN, Oregon State Univ — Collagen gels are commonly used in experiments on cell mechanics because collagen is the most abundant protein in the mammalian extracellular matrix. Collagen gels are often approximated as homogeneous elastic materials; however, variations in the collagen fiber microstructure and cell adhesion forces cause the mechanical properties to be inhomogeneous at the cellular scale. We study the mechanics of type I collagen on the scale of tens to hundreds of microns by using holographic optical tweezers (HOT) to apply pN forces to micron-sized particles embedded in the collagen fiber network. We calculate the local compliance and elastic modulus of the collagen network and find that particle displacements are inhomogeneous, anisotropic, and often have components perpendicular to the direction of the applied force. Confocal reflection microscopy (CRM) is used to reveal the local fiber structure and a simulation treating fibers as rigid rods is used for comparison to the HOT measurements. Collagen samples prepared at 21°C and 37°C show that gels formed at lower temperature are more inhomogeneous, anisotropic, and compliant than those formed at high temperature, and cellularized samples allow us to characterize the effects of cell adhesion forces on the network mechanics.

11:51AM T47.00004 Cellular Contact Guidance Through Dynamic Sensing of Nanotopography, XIAOYU SUN, SATARUPA DAS, CAN GUVEN, JOHN FOURKAS, WOLFGANG LOSERT, Univ of Maryland-College Park — We evaluated the contact guidance of nanoscale ridges on the cellular motion and actin waves in HL60 neutrophil-like cells, a model system for studying cell migration. By analyzing the velocity of cell motion and actin waves, we found that the nanoridges exert bidirectional guidance on migrating cells and actin wave propagation. More cells migrate parallel to the nanoridges than any other direction. Nanoridges nucleate actin polymerization waves which then proceed preferentially along the ridges. Contact guidance efficiency depends on the spacing between adjacent ridges. The greatest guidance efficiency occurs on 1.5-µm-spaced ridges. A larger average actin wave speed is observed on 5-µm-spaced than 1.5-µm-spaced ridges, which may arise from a larger portion of random propagation on 5-µm-spaced ridges rather than confined directional propagation along the 1.5-µm-spaced ridges.

1Work supported by the HHMI

212:27PM T46.00003 How do bacteria couple growth to division? MANUEL CAMPOS, Microbial Sciences Institute / Yale University — Cell size control is an intrinsic feature of the cell cycle. In bacteria, cell growth and division are thought to be coupled through a cell size threshold. Here, we provide direct experimental evidence disproving the critical size paradigm. Instead, we show through single-cell microscopy and modeling that the evolutionarily distant bacteria Escherichia coli and Caulobacter crescentus achieve cell size homeostasis by growing on average the same amount between divisions, irrespective of cell length at birth. This simple mechanism provides a remarkably robust cell size control without the need of being precise, abating size deviations exponentially within a few generations. This size homeostasis mechanism is broadly applicable for symmetric and asymmetric divisions as well as for different growth rates. Furthermore, our data suggest that constant size extension is implemented at or close to division, implying that the initiation of DNA replication or the formation of the FtsZ cytokinetic ring are unlikely to dictate the timing of division. Altogether, our findings provide fundamentally distinct governing principles for cell size and cell cycle control in bacteria.

3Work supported by the HHMI
12:03PM T47.00005 Cardiac tissue as a mechanically and electrically active medium. JASON ROCKS, KEVIN CHIOU, ANDREA LIU, University of Pennsylvania — The heart is an active solid in which energy is injected at the cell scale when cardiomyocytes contract. This energy is transmitted up to macroscopic scales, leading to a collective function—the pumping of the heart—where a wavefront of contraction propagates across the heart from one end to the other. We will present results for a model that couples a traditional model for electrical signaling to an overdamped biphasic model for tissue mechanics to look at the competition between mechanical and electrical signaling in the contractile wavefront in the embryonic heart. We speculate on the ramifications of our results for the adult heart, which is conventionally described exclusively in terms of electrical signaling.

12:15PM T47.00006 The dynamics of body elongation in vertebrate morphogenesis. IDO REGEV, Harvard School of Engineering and Applied Science, OLIVIER POURQUIÉ, Harvard Medical School/Brigham and Women’s Hospital, L. MAHADEVAN, Harvard School of Engineering and Applied Science — Vertebrate embryos have a body axis that grows by the addition of cells in a posterior growth zone in the embryo. Experiments show that these cells show a gradient in motility that decays towards the anterior of the embryo, consistent with a degradation of specific cellular signals (Fgf) that control cellular motility. However, this motility is primarily diffusive in nature, and converted into an advective gradient by virtue of inhomogeneous confinement. We use these observations to build a minimal mechanochemical model for tissue extension as a function of Fgf activity, cell motility and tissue rheology with results that allow us to explicitly test the model in a variety of in-vivo and ex-vivo situations, with implications for normal and pathological axis elongation.

12:27PM T47.00007 Quantitative analysis of actin monomer funneling: how capping protein enhances actin filament growth and nucleation on biomimetic beads1. RUIZHE WANG, ANDERS CARLSSON, Washington University — Capping protein (CP) caps the growing ends of actin filaments and thereby halts their polymerization. However, CP is required for actin-based motility, and experiments by Akin and Mullins [1] have shown that CP also enhances the rate of filament nucleation. Proposed explanations for these phenomena include the Actin Funneling Hypothesis (AFH) [1], in which the presence of CP increases the free-actin concentration, and structural changes of the actin networks induced by increasing CP [1]. In this article, we provide a quantitative analysis of the AFH based on rate equations including actin nucleation and branching, polymerization and capping, plus monomer depletion near the surface of the bead. With two adjustable parameters, our simulation results accurately match several aspects of the results of Akin and Mullins [1]. We find that CP increases the local monomer concentration at the bead surface, but has a much smaller effect on the global free-actin concentration. The increased local monomer concentration gives rise to an enhanced rate of branching events and thus a larger number of actin filaments. [1] O Akin and R. D. Mullins. Cell 133.5 (2008): 841-851. [2] M-F Carlier, and D. Pantaloni. Journal of molecular biology 269.4 (1997): 459-467.

1Supported by the National Institutes of Health under Grant GM107667.

12:39PM T47.00008 Measurement of DDR-Collagen interaction Forces with Atomic force Microscopy. ANWESA SARKAR, Department of Physics & Astronomy, Wayne State University, RAFAEL FRIDMAN, ANJUM SOHAIL, Department of Pathology, Wayne State University, PETER HOFFMANN, Department of Physics & Astronomy, Wayne State University, DEPARTMENT OF PATHOLOGY, WAYNE STATE UNIVERSITY AND KARMANOS CANCER INSTITUTE COLLABORATION — Discoid Domain Receptors (DDR) are membrane proteins of the tyrosine kinase receptor family. The binding of collagen to the extracellular domain of DDR stimulates activation of the tyrosine kinase inside the cell. Two types of DDR, DDR1 and DDR2, have been related to human cancers because of the discovery of alterations of DDR genes in several human cancers. However, not much is known about DDR behavior at the cell-collagen interface. We are combining biological information and force based microscopy to shed light on how DDRs function in physiological and pathological conditions. We have measured the kinetics, bond lengths and activation energy of DDR-collagen interactions at the single molecular level on live cells, including cells that are deficient in DDR and cells that overexpress DDR, as well as cancer cells. We have developed methods to take multiple attachments into account and obtain clean data. Interactions measured on live cells were compared to measurements between extracted extracellular domains of DDR and collagen plated on a substrate to determine how these interactions are altered by the microenvironment of the cell. The distribution of DDR receptors on live cells was determined by using a combination of fluorescence imaging and AFM-based adhesion mapping.

12:51PM T47.00009 Quantitative analysis of mass density fluctuation inside biological cells under the effect of alcohol using light localization properties1. HEMENDRA M. GHIMIRE, PEEYUSH SAHAY, HUDA ALMABADI, PRABHAKAR PRADHAN, Univ of Memphis — Light localization properties can be used to analyze the nanoscale level alterations inside the biological cells. We present study of mass density fluctuation in the nuclei of colon cells, under the effect of alcohol, by quantifying the degree of structural disorder, of nanoscale, from their transmission electron microscopy (TEM) images. The light localization properties of the disordered optical lattice system, created using the TEM image data, were studied by statistically analyzing the inverse participation ratio (IPR) of the localized eigenfunctions of the optical lattice. The study, conducted on rat model, shows that nanoscale morphology of the colon cells with symptoms of carcinogenesis increases further under the effect of alcohol (ethanol). The quantified structural disorder strength, measured in the length scale 12.5 – 75 nm, for the cells under the effect of ethanol was noted to be significantly higher in comparison to the cells not under the influence of ethanol. This study is first of its kind where the effect of alcohol on the biological cells has been studied by quantifying the nanoscale level of mass density fluctuation inside the cells, using the mesoscopic physics approach.

1NIH and University of Memphis

1:03PM T47.00010 Arterial mechanobiology: The interrelation of elastin, collagen, and GAGs1. KATHERINE ZHANG, Boston University — The complex network structure of elastin and collagen extracellular matrix (ECM) forms the primary load-bearing component in the arterial wall. Pathogenesis of many cardiovascular diseases is associated with loss of organization and function of the ECM. However the interrelation of the function of collagen and elastin and the effect of ECM structural changes on vascular mechanics are not well understood. This talk will focus on our recent study on the interrelations of ECM constituents and how they contribute to the mechanical function of the arterial wall. Our recent study coupling mechanical loading and multi-photon imaging demonstrates an interesting sequential engagement of elastin and collagen fibers in response to mechanical loading. Our study also suggests that the elastin fibers are under tension and impart an intrinsic compressive stress on collagen. Such delicate interrelation between elastin and collagen is essential for an artery to function normally. Studies of the structural components and mechanics of arterial ECM generally focus on elastin and collagen while glycosaminoglycans (GAGs) are often neglected, most likely because of the relatively low content in arterial tissue. Our study shows that GAGs play a role in engaging the elastin and collagen fibers in the arterial wall and thus indirectly affect the biomechanical function of arteries. Together these results provide a more comprehensive understanding of the mechanobiology of arteries with the goal of incorporating such information in understanding disease progressions and structurally based constitutive models.

1The author would like to acknowledge the funding support from NIH R01HL098028, NSF CMMI 1100791 and CMMI 0954825.
fitness of a multicellular aggregate in a young bacterial biofilm of sequences, and a simple mechanistic model for the origin of the observed scaling laws. Our results define collective mutational pathways used by HIV to population stores memories of host-pathogen combat won by the virus. We describe an exactly solvable model that captures the main features of the sets branches of inquiry, and dynamics reminiscent of neural networks are observed. Like neural networks that store memories of past stimulation, the circulating to host. We show that the interplay between the diversity of human immune responses and the ways that HIV mutates to evade them results in distinct sets of the circulating HIV population has thus occurred in response to diverse, ultimately ineffective, immune selection pressures that randomly change from host to host. We attribute this competition-dependent growth advantage to an interplay between a spatially-structured nutrient environment and the spatial distribution of cells in the aggregate. We find that fluid waves propagate through the cell layer over multicellular length scales, accommodating these collective cell volume fluctuations. 1:51PM T47.00012 The effect of antiarrhythmic drugs on rate-dependent cardiac behavior, HANA DOBROVOLNY, BINAYA TULADHAR, Texas Christian Univ — While there are many studies examining the biomolecular effects of antiarrhythmic drugs and many studies examining their clinical effect, their effect on cardiac dynamics at the cellular and tissue levels is not well understood. We use a mathematical model of a human ventricular cell to study the effect of antiarrhythmic drugs on the appearance of alternans and 2:1 behavior over a range of doses. We study three different classes of drugs, calcium channel blockers, potassium channel blockers and sodium channel blockers, and compare their effects on cellular dynamics.

Thursday, March 5, 2015 11:15AM - 2:03PM — Session T48 DBIO: Focus Session: Physics of Evolutionary and Population Dynamics II 217C - Uwe Tauber, Virginia Tech University

11:15AM T48.00001 Noise-Induced Homochirality in Spatially Extended Chemical and Biological Systems, FARSHID JAFARPOUR, TOMMASO BIANCALANI, NIGEL GOLDENFELD, Department of Physics and The Institute for Genomic Biology, University of Illinois at Urbana-Champaign — Autocatalysis has long been assumed to be the primary mechanism for homochirality in chemical and biological systems. However, chirality has not been studied in the context of spatially extended systems. Here we remove this extra reaction, so that at the mean field level the only fixed point is the racemic state. Nevertheless, solving the full stochastic theory in zero dimensions, we show that homochiral states can arise due to intrinsic noise. Finally we explore whether these homochiral states are stable in spatially-extended systems.


11:27AM T48.00002 Moment Closure Analysis of SIRS Disease Model on Heterogeneous Networks, DANIEL T. CITRON, CHRISTOPHER R. MYERS, Cornell University — We perform a moment closure analysis of the stochastic susceptible-infected-recovered-susceptible (SIRS) model of infectious disease dynamics on heterogeneous networks. The SIRS model, which returns previously infected individuals to a susceptible state, supports a nontrivial steady state representing persistent endemic disease. In the context of networks, the heterogeneous mean field (HMF) method can be used to predict how network structure affects the SIRS model by dividing the network into classes with degree-dependent mean field coupling strengths. To verify the accuracy of the HMF, we simulate the SIRS model on heterogeneous networks. In our simulations we find, in disagreement with the HMF, the survival probability of the steady state depends on system size. This discrepancy stems from the fluctuations present in the stochastic model that are ignored by the HMF. We extend the HMF results by applying moment closure to each degree class. Our moment closure analysis provides a probabilistic description of the steady state for each degree class, which can be used to show how stochastic fluctuations and extinction depend on the size of the full network. We suggest that this technique may be used to analyze other stochastic models of dynamical processes.

11:39AM T48.00003 Scaling laws describe memories of host-pathogen riposte in the HIV population, JOHN BARTON, MEHRAN KARDAR, ARUP CHAKRABORTY, Massachusetts Institute of Technology — The enormous genetic diversity and mutability of the human immunodeficiency virus (HIV) has prevented effective control of this virus by natural immune responses or vaccination. Evolution of the circulating HIV population has thus occurred in response to diverse, ultimately ineffective, immune selection pressures that randomly change from host to host. We show that the interplay between the diversity of human immune responses and the ways that HIV mutates to evade them results in distinct sets of sequences defined by similar collectively coupled mutations. Scaling laws that relate these sets of sequences resemble those observed in linguistics and other branches of inquiry, and dynamics reminiscent of neural networks are observed. Like neural networks that store memories of past stimulation, the circulating HIV population stores memories of host-pathogen combat won by the virus. We describe an exactly solvable model that captures the main features of the sets of sequences, and a simple mechanistic model for the origin of the observed scaling laws. Our results define collective mutational pathways used by HIV to evade human immune responses, which could guide vaccine design.

[2] This research was funded by the Ragon Institute of MGH, MIT, & Harvard.

11:51AM T48.00004 Environmental spatial structure and competition determine the relative fitness of a multicellular aggregate in a young bacterial biofilm, JAIME HUTCHISON, University of Texas at Austin, KASPER KRAGH, University of Copenhagen, GAVIN MELAUGH, University of Edinburgh, CHRISTOPHER RODESNY, University of Texas at Austin, YASUHIKO IRIE, University of Bath, ALED ROBERTS, STEVE DIGGLE, University of Nottingham, ROSALIND ALLEN, University of Edinburgh, VERNITA GORDON, University of Texas at Austin, THOMAS BJARNSHOLT, University of Copenhagen — The canonical description of biofilm development begins with free-swimming, single bacterial cells which land on and adhere to a surface, mature into three-dimensional structures, and eventually disperse to form new biofilms. However, the interplay between single cells and larger, three-dimensional structures in early biofilm development has not been studied. We use time-lapse confocal microscopy and quantitative measurements of biomass, combined with numerical, individual-based simulations to determine the relative fitness of single cells and preformed, multicellular aggregates. We find that the relative fitness of multicellular aggregates depends markedly on the density of surrounding single-cells. We attribute this competition-dependent growth advantage to an interplay between a spatially-structured nutrient environment and the spatial distribution of cells in the aggregate. Our findings suggest that when competition for resources is high and there is spatial structure in the distribution of resources, aggregates of cells can outperform single cells and may be a preferred way to seed new biofilms.
12:03PM T48.00005 Population Dynamics of Metastable Growth Rates1, LINDSAY MOORE, ELAD STOLOVICKI, EREZ BRAUN, Technion - Israel Institute of Technology — Neo-Darwinian evolution provides a paradigm for population dynamics built on random mutations and selection with a clear separation of time-scales between single-cell mutation rates and the rate of reproduction. By studying the adaptation dynamics of genetically rewired yeast cells adapting to a severe regulatory challenge, we have uncovered a novel type of population dynamics in which intracellular processes seem to play a role in shaping the population structure. Under constant environmental conditions, we measure a wide distribution of growth rates that persists even after both the population has been outgrown (10 generations). Remarkably, the fastest growing cell do not take over the population on the time-scale dictated by the width of the growth-rate distributions and simple selection. In fact, the population-average growth rate plateaux and even decreases over the course of the adaptation, on intermediate time-scales of tens of generations. Our data show that the phenotypic state of the cells in a constant environment is metastable and varies on time-scales that reflect the importance of long-term intracellular processes in shaping the population structure. 

1Israel Science Foundation (grant # 496/10)

12:15PM T48.00006 Steering antibody evolution to combat rapidly mutating pathogens, SHEN-WANG WANG, JORDI MATA-FINK, MIT, DENNIS BURTON, The Scripps Research Institute, DANE WITTRUP, MEHRAN KARDAR, ARUP CHAKRABORTY, MIT — The adaptive immune system houses amazingly efficient evolutionary processes coordinated across multiple length and time scales to protect higher organisms from diverse infectious pathogens. The optimization problem to be solved is often intrinsically constrained and highly dynamical. Failure of solving the problem timely leads to loss of protection. One such devastating situation is posed by rapidly mutating viruses (e.g. HIV which infects the immune system itself). One major challenge of designing an effective vaccine is to contain a diversifying mixture of antigen variants from evading recognition by antibodies. To confront this challenge, we develop a multi-scale computational model to simulate the stochastic evolutionary process of antibody affinity maturation against time varying antigen. The model provides an optimal vaccination strategy which has been shown in mouse experiment to be very effective in focusing antibody response to the vulnerable part of the virus.

12:27PM T48.00007 Balancing the evolution advantages and drawbacks of CRISPR, PU HAN2, MICHAEL DEEM2, Rice University — CRISPR/Cas (Cluster Regularly Interspaced Short Palindromic Repeats/CRISPR associated proteins) is an adaptive immune system of prokaryotes. It can protect bacteria against invading genetic material. Besides providing immunity against lytic phages, the CRISPR/Cas system can block the acquisition of beneficial mobile genes, such as plasmids carrying antibody resistant genes. We discuss how bacteria balance the advantages and the drawbacks of CRISPR in an environment that has both lytic phages and beneficial mobile genes. We show that in the absence of lytic phages, bacteria lose CRISPR/Cas rapidly to acquire the beneficial mobile genes. We also discuss how CRISPR/Cas establishes in the bacterial population in the presence of both lytic phages and beneficial mobile genes.

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12:39PM T48.00008 A Stochastic Cooperative Agent Model of Band-Pass Antibiotic Resistance1, LOUIS NEMZER, ROBERT SMITH, Nova Southeastern University — The recently described phenomenon of band-pass antibiotic resistance occurs when bacteria exposed to a periodic environment of oscillating antibiotic concentration grow fastest at intermediate period lengths. Previously, it has been shown that such behavior can arise from a non-linearity in individual fitness as a function of the initial colony density, called the “Allee effect,” as well as a fixed-point catastrophe that depends very strongly on the antibiotic concentration. Here, we present a new agent-based, in silico stochastic model of cooperative antibiotic resistance. This model attempts to capture the behavior of “cooperative” bacteria that, for example, expend resources to produce enzymes that break down β-lactam antibiotic molecules, but are subject to the problem of freeloadng by non-secretors that benefit but do not contribute. Colony survival can be threatened when exposed to a periodic antibiotic challenge. By creating a simulation in which the bacteria are modeled as stochastic agents, the effect of antibiotic concentration, period of antibiotic oscillation, and degree of cooperativity can be evaluated.

1Funding for this project was provided through the Nova Southeastern University President’s Faculty Research and Development Grant #335347.

12:51PM T48.00009 Flow-driven waves during pattern formation of Dictostelium discoideum, AZAM GHOLAMI, Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany, OLIVER STEINBOCK, Department of Chemistry and Biochemistry, Florida State University, Tallahassee, Florida, VLADIMIR ZYKOV, Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany, ERBERHARD BODENSCHATZ, Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — The slime mold Dictostelium discoideum (D.d.) is a well known model system for the study of biological pattern formation. In the natural environment, aggregating populations of starving Dictostelium cells may experience fluid flows that can profoundly change the underlying wave generation process. Recently we conducted experiments to study the effect of a differential flow in quasi one-dimensional colonies of the signaling D.d. cells. The external flow advects the signaling molecule CAMP downstream, while the chemotactic cells attached to the solid substrate and are not transported with flow. This transport anisotropy in the extracellular medium induced macroscopic wave trains that developed spontaneously, propagated with the velocity proportional to the imposed flow velocity with a unique period. In this work, we investigate the mechanism of flow-induced waves using the well-established Martiel-Goldbeter model. In the linear regime, our analytical calculations show that a convective transport of extracellular CAMP in a uniform field of signal-relaying cells leads to a flow-induced instability of the traveling-wave type. In the nonlinear regime, numerical simulations show a convective instability with propagating waves, in agreement with the predictions of linear analysis.

1:03PM T48.00010 Diffusion limited mutualism, KIRILL KOROLEV, Boston University — Microbes trade diffusible molecules to survive and maintain complex ecological functions. Physicists have substantially advanced our understanding of microbial populations, primarily relying on the evolutionary game theory. Game theory however was developed for higher organisms and cannot easily describe microbial cooperation, which involves the exchange of small, highly diffusible molecules. We formulated and solved a model that accurately represents the physics of diffusion in microbial colonies. In particular, we discovered a general approach that eliminates metabolite diffusion and recasts population dynamics in the traditional game theory framework, but with renormalized parameters. We applied this approach to the problem of two-way cross-feeding, a common interaction motif in the microbial world that is the subject of several experimental studies. Naively one would assume that nutrient diffusion should facilitate mutualistic interactions in microbial colonies. Indeed, because microbes are not completely mixed inside a colony, different species tend to form small domains, and diffusion should facilitate the exchange of the nutrients between the two cross-feeding species. We, however, find that nutrient diffusion reduces the strength of mutualism and leads to a phase transition that makes mutualism impossible. We analytically compute the critical diffusivity at which mutualism is lost and find the universality class of the phase transition. The distance to this phase transition controls the size of the domains formed by the species, a quantity of prime interest in empirical studies. Finally, we show that the differences in public good diffusivities affect mutualism only in the presence of nonlinearity in the public good dynamics. In particular, fitness nonlinearities suppress mutualism and favor the species producing nutrients that diffuse more slowly.
Coalescent theory analysis of phylogenetic trees in a model of evolutionary dynamics. DAWN KING, SONYA BAHAR, University of Missouri at St. Louis — Phylogenetic trees and the hierarchical, biological levels of organization that exist within them are of great importance to evolutionary theory. With a neutral, agent-based model of evolutionary dynamics, we have investigated the conditions under which organisms form clusters, analogous to species. Previous work has shown phase transition behavior as a function of the maximum mutation size ($\mu$) on a rugged landscape with assortative mating (Dees and Bahar, 2010), and, with the addition of bacterial fission, on a completely neutral landscape (Scott et al., 2013). The bacterial version was then classified as belonging to the directed percolation universality class (Scott, 2014). Here, we further investigate the emergent property of speciation by analyzing the genealogical tree structures created by the forward-in-time reaction-diffusion dynamics of the three mating types — assortative, bacterial, and random — as a function of the random death percentage. Specifically, we will use Kingman’s n-coalescent to investigate the distributions of the times to most recent common ancestor (TMRCA) and determine whether universal ratios exist.

1:39PM T48.00011 Coalescent theory analysis of phylogenetic trees in a model of evolutionary dynamics

11:39AM T49.00003 Shape evolution in blueprinted liquid crystal polymer films: topological defects and artificial iris

11:27AM T49.00002 Wrinkling in thin nematic elastomers

11:15AM T49.00001 Differential Geometry Approach to Liquid-Crystal Elastomers and Glasses

Thursday, March 5, 2015 11:15AM - 2:03PM — Session T49 GSOFT: Focus Session: Reconfiguring and Actuating Soft Matter III: Shape 217D

- Karen Daniels, North Carolina State University

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- Supported by NSF DMR-1409658 and NSF DMR-1106014.

1:51PM T48.00012 Influenza Evolution and Vaccine Effectiveness in 2014/2015

11:51AM T49.00004 Thickness Effects on Piezoelectric Unimorphs under Various Boundary Conditions

11:49AM T49.00003 Shape evolution in blueprinted liquid crystal polymer films: topological defects and artificial iris

11:39AM T49.00001 Differential Geometry Approach to Liquid-Crystal Elastomers and Glasses

11:27AM T49.00002 Wrinkling in thin nematic elastomers

11:15AM T49.00001 Differential Geometry Approach to Liquid-Crystal Elastomers and Glasses

- This work was supported by NSF Grant DMR-1409658.

- This work supported by NSF Grant DMR-1409658 and NSF DMR-1106014.

- Corresponding Author
12:03PM T49.00005 A Three-Dimensional Phase Diagram of Growth-Induced Surface Instabilities. QIMING WANG, XUANHE ZHAO, Massachusetts Institute of Technology — A variety of fascinating morphological patterns arise on surfaces of growing, developing or aging tissues, organs and microorganism colonies. These patterns can be classified into creases, wrinkles, folds, period-doubles, ridges and delaminated-ducts according to their distinctive topographical characteristics. One universal mechanism for the pattern formation has been long believed to be the mismatch strains between biological layers with different expanding or shrinking rates, which induce mechanical instabilities. However, a general model that accounts for the formation and evolution of these various surface-instability patterns still does not exist. Here, we take biological structures at their current states as thermodynamic systems, treat each instability-pattern as a thermodynamic phase, and construct a unified phase diagram that can quantitatively predict various types of growth-induced surface instabilities. We further validate the phase diagram with our experiments on surface instabilities induced by mismatch strains as well as data on growth-induced instabilities in various biological systems. It is expected that the unified phase diagram will not only advance the understanding of biological morphogenesis, but also significantly facilitate the design of new materials and structures by rationally harnessing surface instabilities.

12:15PM T49.00006 Mechanical Responses of a Polymer Graphene-sheet Nano-sandwich. XIGUANG LI, JULIUSZ WARZYWODA, GREGORY MCKENNA, Texas Tech University — The interfacial mechanics and reinforcement by graphene sheets in polymer matrix nanocomposites are important to their understanding. However, the methods available for their investigation remain a challenge. Here we report on a novel study in which the mechanical responses of a nano-sandwich model structure made of a single graphene sheet sandwiched between ultrathin polymer layers are determined using a nano-bubble inflation method. The stress-strain behavior of the graphene nano-sandwich shows that significant reinforcement is obtained at small strains and that the method also provides a measurement of the interfacial shear strength. In addition, the study provides data related to internal stresses that develop between the graphene layer and the polymer sandwich faces.

12:27PM T49.00007 Reconfiguring and Actuating Liquid Metals, Gels, and Polymers. MICHAEL DICKEY, NC State University — This talk will describe efforts in our research group to control the shape and function of soft materials (liquid metals, polymers and hydrogels) for applications that include reconfigurable electronics, soft robots, and self-folding origami. The research harnesses interfacial phenomena, micro fabrication, patterning, and thin films. The talk will discuss the underlying fundamental science that enables the following:
1. Shape reconfigurable liquid metal alloys based on gallium. The metal is a liquid at room-temperature with low-viscosity (water-like) and can be micromolded due to a thin, oxide skin that forms rapidly on its surface. The metal can be patterned in a number of ways including injection into microchannels or by direct-write 3D printing. Recently, we discovered that the oxide may be the best surfactant ever reported and can be removed or deposited using electrochemistry in electrolyte as a new method to control and reconfigure the shape of the metal.
2. Self-folding polymers sheets that change shape in response to light. These sheets are a form of shape memory polymers that are compatible with 2D patterning techniques including lithography, inkjet printing, and roll to roll processing. The appeal of this work is converting 2D patterns into 3D shapes in a hands free manner.
3. New methods for actuating hydrogels by patterning ions in these gels. This reversible process can imprint topography in the hydrogel using modest voltages, tune its local mechanical properties to create physically-reinforcing exoskeletons, and generate stresses sufficient to actuate or fold hydrogels over large distances within seconds.

1:03PM T49.00008 Osmotic robotics: Reversible shape change driven by local osmolarity gradients. TAO ZHANG, DUANDUAN WAN, J. M. SCHWARZ, MARK J. BOWICK, Syracuse University — Nature provides us with many examples of biomaterials that can change their shape in response to external stimuli and/or in response to varying internal stresses embedded within the structure of the biomaterial. Inspired by such biomaterials as well as recent experiments, we consider a three-dimensional network of aqueous droplets joined by single lipid bilayers to form a cohesive, tissue-like material. The droplets in these droplet networks can be programmed with different osmolarities. These osmolarity gradients generate internal stresses via local flows and the network then folds into designed structures. Using molecular dynamics simulations, we study the formation of shapes ranging from rings to spirals to tetrahedra and determine the optimal range of parameters for such structures. We also add an osmotic interaction with a dynamic environment, i.e. external stimuli, to realize a reversible folding-unfolding process. This finding contributes towards the development of osmotic robotics in bio-inspired materials.

1:15PM T49.00009 Free-Standing Temperature-Sensitive Hydrogel-Particle Membranes from Evaporating Drops. TIM STILL, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104, PETER YUNKER, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332, KEVIN APTOWICZ, Department of Physics, West Chester University, West Chester, PA 19383, KASEY HANSON, ZOEY DAVIDSON, MATTHEW LOHR, A.G. YODH, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104 — We demonstrate a simple method using evaporating colloidal drops to prepare temperature-sensitive membranes composed of micron-sized colloidal hydrogel particles that are up to a few particle diameters thick. Sessile droplets of hydrogel particle suspension were evaporated on silicon wafers. The radially outward flows that drive the common coffee-ring effect push hydrogel particles towards the drop edge wherein the particles attach to the air-water interface. Most of these microgel particles move radially inward along the interface and coat the drop surface. The particles are then cross-linked, forming a membrane. The resultant thin films exhibit a temperature-responsiveness characteristic of the individual particles, permitting modulations of membrane size, shape, and optical transmission. We understand the optical properties using a Mie scattering model and an assumed membrane structure.

1:27PM T49.00010 Growth morphologies in active elastic bilayers. DAVID MAYETT, Syracuse University, SHILADITYA BANERJEE, James Frank Institute, The University of Chicago, J. M. SCHWARZ, M. CRISTINA MARCHETTI, Syracuse University — Many biological systems exhibit elastic instabilities ranging from buckling to folding to wrinkling. Such instabilities are typically driven by growth of the system. We explore the deformation properties of a layer of growing elastic material resting on a passive elastic substrate of finite thickness. We first show that there exists a mapping between the well-known Rodriguez formulation of growth and an active model where growth is incorporated via a component of the stress tensor describing the proliferation of active units in the elastic medium. Motivated by such systems as the epithelial cells making up the lining of the small intestines and sitting on top of the elastic stroma and the cerebral cortex of the brain that rests on the underlying white matter, we then use analytical and numerical approaches to show how the morphologies observed in different systems can be accounted for by different functional forms of the activity. Our active model of growth in elastic bilayer systems provides a simple, unified framework to classify the zoo of morphologies observed across seemingly different biological systems.
Evolution to increase the matrix composition of clinical biofilm infections makes them stiffer, consistent with a mechanical fitness benefit. MEGAN DAVIS-FIELDS, KRISTIN KOVACH, VERNITA GORDON, University of Texas at Austin — Pseudomonas aeruginosa is an opportunistic, bacterial pathogen that forms biofilms in long-term infections. Biofilms are aggregates of bacteria in a matrix composed of extracellular polymeric substance (EPS). Biofilm P. aeruginosa infections in the lungs of cystic fibrosis patients can persist for decades, ample time for the infecting microbes to evolve. Evolutionary pressures include clearance by antibiotics and the immune system; being within a biofilm makes the bacteria more resistant to both of these. To date, most research has focused on chemical benefits conferred on the biofilm by the EPS matrix. Other researchers have recently found that long-term lung infections of P. aeruginosa increase production of Psl, one type of EPS polysaccharide. Increasing Psl must therefore confer some benefit to P. aeruginosa in the lung. We do bulk rheological measurements of biofilms grown from chronological clinical isolates from cystic fibrosis patients and find that strains that have evolved higher production of Psl have increased storage modulus — i.e., they are stiffer. From others’ estimates of the stresses that phagocytic cells can apply, we estimate that the stiffening we measure could provide a mechanical benefit to biofilms, helping them avoid immunological clearance.

Switchable and Tunable Aerodynamic Drag on Cylinders, MARK GUTTAG, PEDRO REIS, Massachusetts Institute of Technology — We report results on the performance of Smart Morphable Surfaces (Smorphs) that can be coated onto cylindrical structures to actively reduce their aerodynamic drag. Our system comprises of an elastomeric substrate that contains a series of optimally designed undersurface cavities that, once depressurized, lead to a dramatic deformation of the surface topography, on demand. Our design is inspired by the morphology of the giant cactus (Carnegia gigantea) which possesses an array of axial grooves, which are thought to help reduce aerodynamic drag, thereby enhancing the structural robustness of the plant under wind loading. We perform systematic wind tunnel tests on cylinders covered with our Smorphs and characterize their aerodynamic performance. The switchable and tunable nature of our system offers substantial advantages for aerodynamic performance when compared to static topographies, due to their operation over a wider range of flow conditions.

Chiral liquid crystal droplets near the isotropic phase. JOSE MARTINEZ-GONZALEZ, MOHAMMAD RAHIMI, YE ZHOU, JUAN DE PABLO, Univ of Chicago — Liquid crystalline blue phases (BPs) are found between the helical and the isotropic phase of highly chiral compounds. A common feature of BPs is that the local director field forms double twist cylinders leading to defects that form regular, periodic patterns. As a result of their physical properties, which include selective light reflection, high viscosity and a small elastic shear modulus, BPs could find intriguing potential applications in photonic materials, micro-lasers, electrically switchable colour displays and light filters, to name a few. In the bulk, BPs are only formed in a narrow range of temperature. In this work, we use theory and simulations to examine the phase behavior of chiral liquid crystal droplets with weak planar anchoring in the vicinity of the isotropic phase, with special emphasis on the effects of confining blue phase I and blue phase II. We identify several new morphologies, whose complexity increases with the chirality of the medium, and we find that confinement of blue phases in micro-droplets increases their range of stability.

Probing helical structures in liquid crystals with resonant soft x-ray scattering at carbon edge1. , CHENHUI ZHU, CHENG WANG, ANTHONY YOUNG, ILJA GUNKEL, ALEXANDER HEXEMER, ALS, Lawrence Berkeley National Lab, FENG LIU, MSD, Lawrence Berkeley National Lab, DONG CHEN, DAVID WALBA, NOEL CLARK, LCMRC, Uni. of Colorado Boulder, WIM BRAS, DUBBLE CRG, European Synchrotron Radiation Facility, France — We report the first in-situ measurement of the helical pitch in nanofilm B4 phase, using resonant soft x-ray scattering at carbon resonant edge. A strong scattering peak was observed corresponding to ~100 nm periodicity in layer orientation variation. The scattering is anisotropic due to the nano-filament helical structure and bond orientation sensitivity enabled by the linearly-polarized soft x-rays. In-situ measurements of the helical pitch as a function of temperature provide unique information on the B4 structure and the nature of the B2-B4 phase transition. This approach can be extended to other helical structures in liquid crystals and beyond.

Biosensing using smectic and cholesteric liquid crystals. PIOTR POPOV, ELIZABETH MANN, Kent State University, ANTLAL JAKLI, Liquid Crystal Institute — Liquid-crystal-based biosensors utilize liquid crystal alignment’s high sensitivity to the presence of lipids and proteins self-assembled at the liquid crystal/aqueous solution interface. The optical response of the bulk liquid crystal to the interface offers inexpensive, easy optical detection of such biologically relevant molecules. Present technique uses nematic liquid crystal phase state that typically has a planar-to-homeotropic response only. Here we show that smectic and cholesteric phase states of liquid crystals can be used as new sensing modes that can provide additional information or improve the characteristics of a potential biosensor device. Smectic-A phase extends the detection range both toward the lower and higher concentration. Cholesteric phase (nematic with a chiral dopant) may be sensitive to the chirality of biological surface-active molecules such as phospholipids. Additionally, the “finger-print” texture of a cholesteric phase may show the differences between biomolecule homologues, thus providing a promising way of distinguishing between subtle differences of hydrocarbon chain or head-group size and structure.
12:15PM T50.00006 Topological defects in cholesteric liquid crystal shells . ALEXANDRE DARMON, EC2M - UMR CNRS 7083 Gulliver - ESPCI ParisTech, MICHAEL BENZACUEN, PCT - UMR CNRS 7083 Gulliver - ESPCI ParisTech, OLIVIER DAUCHOT, TERESA LOPEZ-LEON, EC2M - UMR CNRS 7083 Gulliver - ESPCI ParisTech — Confining rod-like molecules, such as the nematogens of liquid crystals, on a curved surface inevitably yields topological defects. Remarkably, in the specific case of a nematic sphere, Poincaré stated that the sum of the topological charges of the defects is equal to \( q = \frac{1}{2} \). Recent studies have shown that, in the case of nematic shells, three kinds of configuration are possible. Each of these configurations correspond to different arrangements of defects that satisfy Poincaré’s theorem. But much richer scenarios appear when playing with the shell thickness, since bulk effects start competing with surface effects. In particular, we show that inducing chirality in the liquid crystal can have a dramatic effect in the defect structure of the shell, where the ratio \( q \) between the cholesteric pitch and the shell thickness becomes the control parameter. We also study in details the equilibrium configuration obtained for \( q > > 1 \), which corresponds to the structure with a single disclination line of charge \( \pm 2 \), also known as the Frank-Précig system. The strong electric fields, due to the permanent dipole moment of the FNPs, trapped some mobile ions, reducing the free ion concentration in the LC media.

12:27PM T50.00007 Geometry and topology of the cholesteric pitch axis: Which way is everything twisting?1, DANIEL BELLER, Harvard University, University of Pennsylvania, THOMAS MACHON, University of Warwick, SIMON COPAR, University of Ljubljana, Jozef Stefan Institute, University of Pennsylvania, DANIEL SUSSMAN, University of Pennsylvania, GARETH ALEXANDER, University of Warwick, RANDALL KAMIEN, University of Pennsylvania, RICARDO MOSNA, Universidade Estadual de Campinas, University of Pennsylvania — In a cholesteric with distortions and topological defects, it is not obvious how to even define the pitch axis and locate its singularities. We propose a construction of the cholesteric pitch axis for an arbitrary director field as an eigenvalue problem. With this tool we are able to compare the defects of the cholesteric phase with seemingly analogous defects in the biaxial nematic and smectic phases. Our results show the limitations of these analogies and indicate in what ways the cholesteric’s topology is intermediate between, and distinct from, the topologies of the biaxial nematic and smectic phases.

12:39PM T50.00008 Spontaneous Ferromagnetic Ordering of Nanoplatelets in Isotropic Solvent1. MIN SHUAI, ARTHUR KLITTNICK, MICHAEL TUCHBAND, MATTHEW GLASER, JOSEPH MACLENNAN, NOEL CLARK, Department of Physics and Liquid Crystal Materials Research Center, University of Colorado Boulder, ROLFE PETSCHEK, Physics Department, Case Western Reserve University, ALEKNA MERTELJ, DARJA LIŠIJAK, J. Stefan Institute, MARTIN COPIC, J. Stefan Institute, Faculty of Mathematics and Physics, University of Ljubljana — Room-temperature ferroelectric fluids were first experimentally demonstrated by Mertelj, et al (Nature, 504: 237–241, 2013), by suspending surfactant wrapped coated barium hexaferrite (BHF) nanoparticles in the liquid crystal 5CB. We have studied the liquid crystal phase behavior of BHMF magnetic platelets suspended in isotropic solvent (1-butanol) at high volume fraction, where simulations predict a N-I transition for monodisperse hard platelets. In these suspensions, the anisotropic particles can be aligned by magnetic fields as weak as 2 gauss, leading to a state with substantial birefringence and dichroism. When the volume fraction of the magnetic platelets is higher than 28%, we observe a phase coexistence, with an isotropic state at the top of a capillary and a birefringence phase at the bottom. In the lower phase, domains are found to have different magneto-optical response from each other and the response is dependent on the sign of the magnetic field, showing broken time-reversal symmetry and ferromagnetism. Spike structures are observed at the interface between the isotropic and ferromagnetic states.

1:03PM T50.00010 Smectic Liquid Crystals in the Immediate Vicinity of the Superstructure of a Nanoparticle in a Nanocomposite1. LUZ J. MARTINEZ-MIRANDA, University of Maryland, College Park, MD — We have studied how the nanoparticle (or the superstructure the nanoparticle forms) aligns the liquid crystal in smectic liquid crystal nanocomposites to determine how charges are transferred between the liquid crystal and the nanoparticle superstructure [1,2,3]. This superstructure depends on the density of aliphatic functionalizations at the surface of the nanoparticle [4]. We have found evidence that the asymmetry of the liquid crystal distorts those superstructures that belong to the cubic structure. In addition, we have observed some differences in how the smectic liquid crystal behaves depending on the nanoparticle used and how the nanoparticle (or the superstructure the nanoparticle forms) aligns the liquid crystal in smectic liquid crystal nanocomposites to determine how charges are transferred between the liquid crystal and the nanoparticle superstructure. Following the idea brought by the simulations of Sec et al. on cholesteric droplets, we show experimentally that this structure is not a pure \( \pm 2 \) line but is actually found to be two non-singular \( \pm 1 \) lines that are wound around each other.

1:27PM T50.00012 ABSTRACT WITHDRAWN —
1:39PM T50.00013 Nanoparticle interfacial assembly in liquid crystal droplets1, MOHAMMAD RAHIMI, TYLER ROBERTS, JULIO ARMAS-PEREZ, Institute for Molecular Engineering, University of Chicago, Chicago, Illinois 60637, USA, XIAOGLANG WANG, EMRE BUKUSOGLU, NICHOLAS L. ABBOTT, Department of Chemical Engineering, University of Wisconsin - Madison, Wisconsin 53706, USA, JUAN J. DE PABLO, Institute for Molecular Engineering, University of Chicago, Chicago, Illinois 60637. Controlled assembly of nanoparticles at liquid crystal interfaces could lead to easily manufacturable building blocks for assembly of materials with tunable mechanical, optical, and electronic properties. Past work has examined nanoparticle assembly at planar liquid crystal interfaces. In this work we show that nanoparticle assembly on curved interfaces is drastically different, and arises for conditions under which assembly is too weak to occur on planar interfaces. We also demonstrate that LC-mediated nanoparticle interactions are strong, are remarkably sensitive to surface anchoring, and lead to hexagonal arrangements that do not arise in bulk systems. All these elements form the basis for a highly tunable, predictable, and versatile platform for hierarchical materials assembly.

1National Science Foundation through the UW MRSEC

1:51PM T50.00014 Translational and Rotational Diffusion of Nanoparticle Aggregates of Irregular Shape in 2D Fluid Membranes1, KYLE MEIENBERG, JOHN PAPAIOANNOU, CHEOL PARK, MATT GLASER, JOE MACLENNAN, NOEL CLARK, Physics, University of Colorado, TATIANA KURIABOVA, Physics Department, California Polytechnic State University, THOMAS POWERS, School of Engineering and Department of Physics, Brown University — We observe directly the diffusion and aggregation of nanoparticles (buckyballs) embedded in thin, freely suspended smectic A liquid crystal films of 8CB using reflected light microscopy. Individual buckyballs, initially homogeneously dispersed in the film, are too small to see but after some hours form nanoscale clusters. These, in turn, aggregate to form extended, micron-scale objects which diffuse in the film, enabling the measurement of 2D rotational and translational mobilities of inclusions with a wide variety of different shapes. The experimental mobilities are compared with predictions of the extended Saffman-Delbrück (SD) model used successfully to describe the diffusion of micron-sized objects in thin fluid membranes in a variety of experimental systems.

1This work was supported by NASA Grant No. NNX-13AQ81G, NSF MRSEC Grant No. DMR-0820579, and by NSF Grant No. CBET-0854108.

2:03PM T50.00015 Towards 2D nanocomposites, HYUN-SOOK JANG, CHANGQIAN YU, ROBERT HAYES, STEVE GRANICK, Univ of Illinois - Urbana — Polymer vesicles (“polymersomes”) are an intriguing class of soft materials, commonly used to encapsulate small molecules or particles. Here we reveal they can also effectively incorporate nanoparticles inside their polymer membrane, leading to novel “2D nanocomposites.” The embedded nanoparticles alter the capacity of the polymersomes to bend and to stretch upon external stimuli.

Thursday, March 5, 2015 11:15AM - 2:15PM — Session T51 GSOFT DCMP: Invited Session: Soft Matter Nanophotonics: DNA-Directed Assemblies of Metal Clusters and Metal Nanoparticles — Grand Ballroom C1 - Elisabeth Gwinn, University of California, Santa Barbara

11:15AM T51.00001 DNA base pairing by noble metal cations: Structure and electronic properties from Density Functional Theory, OLGA LOPEZ-ACEVEDO, Aalto University — Metallo-base pair interactions are two to three times larger than the conventional hydrogen-bond pair interaction. Such high stability can drive the formation of helices and higher-order structures with the possibility to design novel DNA-based nanomaterials. Nucleobases and noble metal atoms (Au,Ag) have wide range of possible interacting sites depending on both the metal charge (ion, cation or neutral) and chemical nature. I will overview the electronic properties, both ground state and optical, of metallo-DNA structures obtained by global optimization and Density Functional Theory, discussing the effect of pairing and inclusion of backbone on the metal-base elementary unit.

1T. Biver Coordination Chemistry Reviews 257 (2013) 27-65
2L. Espinosa Leal and O. Lopez-Acevedo, Nanotechnology Reviews to appear 2015, arXiv.1403.3494

11:51AM T51.00002 DNA templates silver clusters with magic sizes and colors for multi-cluster fluorescent assemblies, STACY COPP, University of California, Santa Barbara — The natural inclusion of information in DNA, a vital part of life’s rich complexity, can also be exploited to create diverse structures with multiple scales of complexity. Now emerging in novel photonic applications, DNA-stabilized silver clusters (AgN-DNA) are compelling examples of multi-scale DNA-directed assembly: individual fluorescent clusters, each templated by specific DNA base motifs, can then be arranged together in DNA-mediated multi-cluster assemblies with nanoscale precision. We discuss how DNA imbues AgN-DNA with unique features. Our optical data on pure AgN-DNA show that DNA base-cationic silver ligands impose rod-like shapes for neutral silver clusters, whose length primarily determines fluorescence color [1]. This shape anisotropy leads to the aspherical AgN-DNA magic number cluster sizes and “magic color” groupings [2]. We exploit DNA’s sequence properties to extract multi-base motifs that select certain magic cluster sizes, using machine learning algorithms applied to large data sets [3]. With these base motifs, we design DNA scaffolds to arrange multiple atomically precise AgN together in nanoscale proximity. We demonstrate that clusters are stable when held at separations below 10 nm, both in bicolor, dual cluster DNA clamp assemblies [4] and in one-dimensional assemblies of atomically precise clusters arrayed on DNA nanotubes.


1Supported by NSF-CHE-1213895 and NSF-DMR-1309410. SMC acknowledges NSF-DGE-1144085, a NSF GRFP.
12:27PM T51.00003 Plasmonic Enhancement of Raman Signal using Complex Metallic Nanostructures based on DNA Origami. GLEB FINKELSTEIN, Duke University — DNA-based nanostructures, such as “DNA origami,” have recently emerged as one of the leading techniques for precise positioning of nanoscale materials in fields ranging from computer science to biomedical engineering. The origami is composed of a single scaffold DNA strand to which smaller “staple” strands are attached through DNA complementarity. The staples help to fold the scaffold strand into the desired structure of a predetermined shape. The resulting templates are highly addressable and have proven to be versatile tools for site-specific placement of various nanomaterials, such as metallic nanoparticles, quantum dots, fluorophores, etc. Building upon massively parallelized assembly mechanism of the origami and its ability to position nanomaterials, one may hope to utilize it for biosensing purposes. One attractive goal is the Raman spectroscopy, which provides a highly specific chemical fingerprint. Unfortunately, the Raman scattering cross section is small; Surface Enhanced Raman Spectroscopy (SERS) enhances the otherwise weak Raman signal by trapping the analyte molecules in the regions of intense electric field produced near rough metallic surfaces. These “hot spots” can be understood as resulting from localized surface plasmon modes resonantly exited by the incident laser excitation. We have earlier shown that metallic nanoparticles controllably attached to DNA origami can be further enlarged via an in-solution metallization; this technique allowed us to build metallic structures of complex topology. Recently, we have performed Raman spectroscopy of molecules attached to these metallic assemblies. Specifically, DNA origina is first used to organize the metallic structures, followed by a covalent attachment of Raman-active molecules to the metal. We found that the substrates with four nanoparticles per origami produce a strongly enhanced Raman signal compared to the control samples with only one nanoparticle per origami for the same particle density. Furthermore, in the samples with four particles per origami the Raman signal systematically decayed as a function of the laser exposure time. Similar behavior has been previously reported and attributed to photo-damaging effects of the high intensity fields at the “hot spots.” In the samples with four nanoparticles per origami, the hot spots are located between the pairs of NPs; the one-particle control samples lacking the inter-particle hot spots showed no decay of the Raman signal, confirming our conclusion.

1:03PM T51.00004 DNA-bridged Chiroplasmonic Assemblies of Nanoparticles. NICHOLAS KOTOV, University of Michigan — Chirality at nanoscale attracts a lot of attention during the last decade. A number of chiral nanoscale systems had been discovered ranging from individual nanoparticles to helical nanowires and from lithographically defined substrates. DNA bridges make possible in-silico engineering and practical construction of complex assemblies of nanoparticles with of both plasmonic and excitonic nature. In this presentation, expected and unexpected optical effects that we observed in chiral plasmonic and excitonic systems will be demonstrated. Special effort will be placed on the transitioning of theoretical and experimental knowledge about chiral nanoscale systems to applications. The most obvious direction for practical targets was so far, the design of metamaterials for negative refractive index optics. The results describing the 3D materials with the highest experimentally observed chiral anisotropy factor will be presented. It will be followed by the discussion of the recent developments in analytical application of chiral assemblies for detection of cancer and bacterial contamination.

1:39PM T51.00005 DNA-mediated self-assembly of polyhedral plasmonic clusters. VINOTHAN N. MANOHARAN, Harvard University — A metafluid is a collection of electromagnetic resonators that have an isotropic response to incoming light. Because the resonators need not be oriented in any particular direction, metalfluids are perhaps the simplest metamaterial to fabricate – if one can first design resonators with an isotropic response. Such structures can in principle be self-assembled from metallic colloidal particles. The challenge is to organize these 100-nm-scale metallic particles into high-symmetry clusters, such as tetrahedra, that have very little variability between structures, so that the electric and magnetic resonances of all the clusters are at the same frequency. I will discuss how DNA can be used to assemble bulk suspensions of polyhedral colloidal clusters, using both equilibrium and non-equilibrium methods. I will also discuss how the yield of the structures is related to statistical mechanical and geometrical considerations.
12:27PM T52.00003 Ultrahigh mobility and giant magnetoresistance in the Dirac Semimetals Cd$_3$As$_2$ and Na$_3$Bi$^1$, N. PHUAN ONG, Dept of Physics, Princeton University — Dirac semimetals and Weyl semimetals are 3D analogs of graphene in which crystalline symmetry protects the nodes against gap formation. Na$_3$Bi and Cd$_3$As$_2$ were predicted to be Dirac semimetals, and recently confirmed to be so by photoemission. Several novel transport properties in a magnetic field $H$ have been proposed for Dirac semimetals. Here we report an interesting property in Cd$_3$As$_2$ that was unpredicted, namely a remarkable protection mechanism that strongly suppresses backscattering in zero $H$. In single crystals, the protection results in a very high mobility, $10^7$ cm$^2$/Vs at 5 K. Suppression of backscattering results in a transport lifetime 10$^4$ longer than the quantum lifetime. The lifting of this protection by $H$ leads to very large magnetoresistance with a striking $H$-linear profile. I will also report transport results on Na$_3$Bi and compare them with results in Cd$_3$As$_2$. I discuss how this may relate to changes to the Fermi surface induced by $H$.

Coauthors: Tian Liang, Jun Xiong, Quinn Gibson, Minhao Liu, Satya Kushwaha, Jason Krizan Maz Ali, and R. J. Cava

$^1$Research supported by the Army Research Office (W911NF-11-1-0379), MURI grant (ARO W911NF-12-1-0461) and NSF (DMR 0819860).

1:03PM T52.00004 Valley-Polarized Interlayer Conduction of Anisotropic Dirac Fermions in SrMnBi$_2$, JUN SUNG KIM, Department of Physics, POSTECH — We report anisotropic Dirac fermions in a Bi square net of SrMnBi$_2$ and their valley-selective interlayer conduction under in-plane magnetic fields. In contrast to the commonly-observed isotropic Dirac Fermi surfaces, the Dirac Fermi surface in SrMnBi$_2$ is highly anisotropic with strong momentum-dependence of Fermi velocity as well as interlayer coupling. The resulting $c$-axis resistivity exhibits clear angular magnetoresistance oscillations indicating coherent interlayer conduction. Strong fourfold variation of the coherent peak in the $c$-axis resistivity reveals that the contribution of each Dirac valley is significantly modulated by the in-plane field orientation. Furthermore, we found a signature of broken valley symmetry at high magnetic fields. These findings demonstrate that a quasi-two-dimensional anisotropic Dirac system can host a valley-polarized interlayer current through magnetic valley control.

Thursday, March 5, 2015 11:15AM - 2:15PM –
Session T53 DMP: Invited Session: DMP Prize Session Grand Ballroom C3 - John Mitchell, Argonne National Laboratory

11:15AM T53.00001 James C. McGroddy Prize Lecture: Iron-Based Superconductors: Discovery and Progress, HIDEO HOSONO, Tokyo Institute of Technology — The largest breakthrough in the history is the discovery of high $T_c$ Cuprates by G.Bednorz and A.Muller in 1986 and the maximum $T_c$ exceeded 77K, boiling temperature of liquid nitrogen in 1987. However, no new superconductors with high $T_c$ had been reported since then except MgB$_2$ ($T_c=39K$) discovered by J.Akimitsu in 2001. We found LaFePO superconductor with $T_c=3K$ in 2006 and LaFeAsO$_1$-F$_x$ with $T_c=56K$ (42K at under high pressure of 5GPa) in early 2008. The latter discovery rekindled the extensive superconductivity research globally, and more than 10,000 papers have been published to now. This excitement originates from disprovement of a widely accepted belief that iron with a large magnetic moment is harmful for emergence of superconductivity and relatively high $T_c$. Extensive research on iron-based superconductors pushed up the maximal $T_c$ to 58K, which is next to high $T_c$ cuprates and has led to the discovery of more than 50 new iron-based superconducting materials to date. Seen are so many advances in elucidation of superconducting properties and pairing mechanism. In this talk, I introduce a tale to the discovery and show the current status by reviewing progresses in materials, properties, mechanism and the application covering the recent hot topics. Emphases are placed on the unique characteristics arising from multi-orbital nature which totally differs from high $T_c$ cuprates.

11:51AM T53.00002 David Adler Lectureship Award Talk: Friction and energy dissipation mechanisms in adsorbed molecules and molecularly thin films$^1$, JACQUELINE KRIM, North Carolina State University — Studies of the fundamental origins of friction have undergone rapid progress in recent years, with the development of new experimental and computational techniques for measuring and simulating friction at atomic length and time scales [1]. The increased interest has sparked a variety of discussions and debates concerning the nature of the atomic-scale and quantum mechanisms that dominate the dissipative process by which mechanical energy is transformed into heat. Measurements of the sliding friction of physisorbed monolayers and bilayers can provide information on the relative contributions of these various dissipative mechanisms. Adsorbed films, whether intentionally applied or present as trace levels of physisorbed contaminants, moreover are ubiquitous at virtually all surfaces. As such, they impact a wide range of applications whose progress depends on precise control and/or knowledge of surface diffusion processes. Examples include nanoscale assembly, directed transport of Brownian particles, material flow through restricted geometries such as graphene membranes and molecular sieves, passivation and edge effects in carbon-based lubricants, and the stability of granular materials associated with frictional and frictionless contacts.


$^1$Work supported by NSFDMR1310456

12:27PM T53.00003 Nanoscale Impedance Imaging of Novel Quantum Materials, KEJI LAI, University of Texas at Austin — The research of complex quantum materials, in which a dazzling number of emergent phenomena take place in the nanoscale, is a major theme in modern condensed matter physics. For real-space mapping of complex systems, electrical impedance microscopy fills an important void that is not well represented by the existing local probes. Using shielded cantilever probes and sensitive microwave electronics, we can now perform non-invasive electrical imaging with unprecedented resolution (10-100nm) and sensitivity (sub-aF). To date, this powerful technique has enabled us to visualize the electronic inhomogeneity in colossal magnetoresistance manganites, spatially resolve the topological edge channels, image the metal-insulator transition in novel field-effect transistors, and probe the anomalous conduction in multiferroic domain walls. The sub-surface imaging capability is also ideal for understanding the evolution of chemical reaction involving low-dimensional layered materials. Further development of the technique will allow us to perform local dielectric spectroscopy across a large frequency span, explore the localized microwave magnetic resonance, and study the nanoscale nonlinear electromagnetic response in complex materials.
Magnetostructural coupling in spinel oxides

M. C. Kemei, J. K. Harada, M. R. Suchomel, and R. Seshadri


Schlumberger Foundation Faculty for the Future fellowship, MRL Facilities funded by the NSF under Award No. DMR 1121053, and the Advanced Photon Source supported by the DOE, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

Entanglement and Quantum Error Correction with Superconducting Qubits

Matthew Reed, Yale University — Quantum information science seeks to take advantage of the properties of quantum mechanics to manipulate information in ways that are not otherwise possible. Quantum computation, for example, promises to solve certain problems in days that would take a conventional supercomputer the age of the universe to decipher. This power does not come without a cost however, as quantum bits are inherently more susceptible to errors than their classical counterparts. Fortunately, it is possible to redundantly encode information in several entangled qubits, making it robust to decoherence and control imprecision with quantum error correction. I studied one possible physical implementation for quantum computing, employing the ground and first excited quantum states of a superconducting electrical circuit as a quantum bit. These transmon- qubits are dispersively coupled to a superconducting resonator used for readout, control, and qubit-qubit coupling in the cavity quantum electrodynamics (cQED) architecture. In this talk I will give an general introduction to quantum computation and the superconducting technology that seeks to achieve it before explaining some of the specific results reported in my thesis. One major component is that of the first realization of three-qubit quantum error correction in a solid state device, where we encode one logical quantum bit in three entangled physical qubits and detect and correct phase- or bit-flip errors using a three-qubit Toffoli gate. My thesis is available at arXiv:1311.6759.

Single crystal growth and magnetic excitations of transition metal oxide CoV$_2$O$_6$

Christopher Stockdale, F. Wallington, Univ of Edinburgh, J. W. Taylor, V. Garcia-Sakai, Rutherford Appleton Laboratory, A.M. Arevalo-Lopez, P. Attfield, C. Stock, Univ of Edinburgh — Low-dimensional magnetic materials are an area of interest due to their unusual properties such as metamagnetism and magnetization plateaus [1]. Solid state synthesis has produced polycrystalline CoV$_2$O$_6$ which exists in two polymorphs: one with a monoclinic structure, and the other with a triclinic structure [2]. Single crystals have been grown from polycrystalline CoV$_2$O$_6$ using the flux method under vacuum and are large enough to aid in single crystal neutron diffraction [3]. Magnetic excitations have been measured using powder neutron diffraction in the low temperatures regime with variable energies. The magnetic excitations have been compared between the two phases. The energy of the system has been modelled in terms of the spin-orbit coupling, structural distortions, and the crystal field and compared to neutron data.

V1.00004 Atomic Processes and Diagnostics of Low Pressure Krypton Plasma 1, RAJESH SRIVASTAVA, DIPTI GOYAL, DIPTI GOYAL, R. Gangwar, L. Sharma, R. Srivastava and A. D. Stauffer, Université de Montréal — Optical emission spectroscopy along with suitable collisional-radiative (CR) model is used in plasma diagnostics. Importance of reliable cross-sections for various atomic processes is shown for low pressure argon plasma [1,2]. In the present work, radially-averaged Kr emission lines from the $2p_i \rightarrow 1s_j$ were recorded as a function of pressure from 1 to 50mTorr. We have developed a CR model using our fine-structure relativistic-distorted wave cross sections [3].


1Work is supported by IAEA Vienna, DAE-BRNS Mumbai and CSIR, New Delhi.

V1.00005 Effect of nonlinear nonlinear coupling to a pure dephasing model, LI GE, NAN ZHAO, Beijing Computational Science Research Center, Beijing 100084, China — We investigate the influence of the nonlinear coupling to the coherence of a pure dephasing model. The total system consists of a qubit and a Bosonic bath, which are coupled by an interaction $H_i = g_1 \sigma_x \otimes 1 + g_2 \sigma_z \otimes x^2$ with $x = \frac{1}{\sqrt{2}} (a + a^\dagger)$. It’s shown that no matter how small $g_2$ is, the long time behavior of the coherence is significantly changed by the nonlinear coupling for free induction decay (FID), while the effect of $g_1$ can be neglected as long as $g_1$ is much smaller than the energy splitting of the qubit. In the case that many-pulse dynamical decoupling control is exerted on the qubit, $g_2$ also modulates the oscillation of the coherence. Our results indicate that the nonlinear coupling must be taken into account for long time dynamics.

V1.00006 Hartree-Fock Theory of a Harmonically Trapped Dirty Bose-Einstein Condensate via the Replica Method, T. KHELLIL, Department of Physics, Freie Universität Berlin, Germany, A. PELSTER, Technische Universität Kaiserslautern, Germany — A recent non-perturbative approach towards the dirty boson problem relies on the Hartree-Fock theory which is worked out on the basis of the replica method [1]. Here we extend this approach for a weakly interacting Bose-gas at finite temperature in a quenched delta-correlated disorder potential from the homogeneous case to an anisotropic harmonic confinement within the Thomas-Fermi approximation. In this way we obtain and solve coupled self-consistency equations, which relies on a decomposition of the particle density into the condensate density, the thermal density as well as the density of fragmented local Bose-Einstein condensates within the respective minima of the random potential landscape. Although we reproduce for weak disorder and at zero temperature the seminal results of Huang and Meng from a Bogoliubov theory [2,3] only qualitatively, we yield for strong enough disorder a quantum phase transition to a Bose-glass phase [4].


V1.00007 Formation and dynamics of anti-ferromagnetic correlations of ultracold fermions in tunable lattices, RÉMI DESBUQUOIS, DANIEL GREIF, GREGOR JOTZU, MICHAEL MESSER, FREDERIK GÖRG, TILMAN ESSLINGER, ETH Zürich, Switzerland — The observation of anti-ferromagnetic spin correlations of ultracold fermions in optical lattices is an important milestone towards an experimental study of the Hubbard model. In this model many questions on the low-temperature phase diagram still remain open, both for simple cubic and square configurations, as well as for more complex lattice geometries. Additionally, for creating an equilibrated low-temperature state and a successful implementation of advanced cooling schemes based on entropy redistribution, an understanding of the formation time for spin correlations is of paramount importance. In our experiment we load a two-component, repulsively interacting fermionic quantum gas into an optical lattice of tunable geometry. For very low temperatures we observe anti-ferromagnetic correlations on neighbouring sites in both isotropic 3D cubic and 2D square lattices. We also study the strength of the spin correlations in more complex lattice geometries, such as honeycomb, 1D-dimerized and spin-ladder lattice configurations. Furthermore, we investigate the characteristic formation time of spin correlations in optical lattices by changing the lattice geometry on variable timescales.

V1.00008 Direct probe of topological order for cold atoms, DON-LONG DENG, SHENG-TAO WANG, LU-MING DUAN, Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA — Cold-atom experiments in optical lattices offer a versatile platform to realize various topological quantum phases. A key challenge in those experiments is to unambiguously probe the topological order. We propose a method to directly measure the characteristic topological invariants (order) based on the time-of-flight imaging of cold atoms. The method is generally applicable to detection of topological band insulators in one, two, or three dimensions characterized by integer topological invariants. Using detection of the Chern number for the two-dimensional anomalous quantum Hall states and the Chern-Simons term for the three-dimensional chiral topological insulators as examples, we show that the proposed detection method is practical, and robust to typical experimental imperfections such as limited imaging resolution, inhomogeneous trapping potential, and disorder in the system.

3We thank S.-L. Zhu for discussions. This work was supported by the NBRPC (973 Program) Grants No. 2011CBA00302, the IARPA MUSIQC program, the ARO, and the AFOSR MURI program.

V1.00009 Collisional Microscopy and Generation of Entanglement with Ultracold Quantum Gases, QI LIU, CRAIG PRICE, NATHAN GEMELKE, The Pennsylvania State University — We describe an apparatus for cold collisional microscopy of quantum gases, in which pairwise entanglement is produced between a many-body gas and an optical-lattice-bound array of secondary atoms used as quantum-non-destructive probes. We discuss detailed implementation of collisional entanglement schemes based on Ramsey-style interferometer sequences, as well as tunnel-assist and -inhibit schemes, in which probe atoms are conditionally shuffled according to the presence or state of a sample atom. The technical implementation for precise manipulation of multichromatic optical lattices is discussed, including achromatic holographic projection microscopy at high numerical aperture and methods for achieving sufficient quantum state control within a lattice site. Applications of collisional microscopy will also be discussed, ranging from imaging of dynamical and non-equilibrium quantum many-body systems, to characterization of strongly entangled gases through extraction of entanglement entropy, to algorithmic cooling of quantum critical gases.
V1.00010 Cutoff frequency of sound velocities for a multi-slab Bose-Einstein condensate\footnote{We acknowledge partial support from PAPIIT IN111613.}, O.A. RODRÍGUEZ, Posgrado en Ciencias Físicas, UNAM, M.A. SOLÍS, Instituto de Física, UNAM — An inhomogeneous multi-slab 3D Bose gas is produced by applying to the gas a Kronig-Penney potential in one direction, while the bosons are free to move in the other two directions. The variable density produces a dispersive effect over the sound waves, making the phase and group sound velocities frequency dependent. Below the critical temperature the dispersion relation between wavenumber and frequency \( \omega(k) \) is determined by a constant factor called the curvature of the density, within the Klein-Gordon equation which describes the sound wave propagation in the condensate. Since the curvature of the density profiles between and inside the barriers are completely different, the sound velocities are distinct too. More importantly, in the region occupied by the slabs waves propagate only if their frequencies are greater than a cutoff frequency, otherwise evanescent waves arise. We show the density profile, the phase and group sound velocities and we give the curvature dependent cutoff frequency as obtained from the group velocity equation for the region occupied by the barriers. For high frequencies both phase and group velocities approach to that of a homogeneous gas at the same temperature.

V1.00011 Bose gas in disordered, finite-layered systems\footnote{We acknowledge support from grant UNAM-PAPIIT IN111613.}, Mauricio Fortes\footnote{Instituto de Física}, V.E. Barragán\footnote{Posgrado en Ciencia e Ingeniería de Materiales}, M.A. Solís\footnote{Instituto de Física}, Instituto de Física, UNAM — We report the isocoric specific heat for an ideal Bose gas confined in a periodic array of filaments with finite rectangular cross section and infinite length, set together to form a cable. The filament structure is created by applying to the gas two, mutually perpendicular, Kronig-Penney delta-potentials, while the bosons are free to move along the third direction. The energy spectrum accessible to the particles is obtained and introduced into the grand potential to calculate the specific heat of the system as a function of temperature for different values of the periodic structure parameters such as: the number, the area of the cross section and wall permeability, of the filaments. The specific heat shows a dimensional crossover from 3D to 1D, in temperature regions where the de Broglie wavelength of the bosons is comparable to twice the separation between the walls of the filaments. Furthermore, we provide and discuss a criterion for identifying the critical temperature based on the behavior of the chemical potential and its first derivatives, as well as the population of the ground state.

V1.00012 Specific heat for boson matter in multifilament cables\footnote{We acknowledge partial support from PAPIIT IN111613 and CONACYT 221030.}, Grecia Gujarró, Posgrado en Ciencias Físicas, UNAM, M.A. Solís, Instituto de Física, UNAM — We report the isocoric specific heat for an ideal Bose gas confined in a periodic array of filaments with finite rectangular cross section and infinite length, set together to form a cable. The filament structure is created by applying to the gas two, mutually perpendicular, Kronig-Penney delta-potentials, while the bosons are free to move along the third direction. The energy spectrum accessible to the particles is obtained and introduced into the grand potential to calculate the specific heat of the system as a function of temperature for different values of the periodic structure parameters such as: the number, the area of the cross section and wall permeability, of the filaments. The specific heat shows a dimensional crossover from 3D to 1D, in temperature regions where the de Broglie wavelength of the bosons is comparable to twice the separation between the walls of the filaments. Furthermore, we provide and discuss a criterion for identifying the critical temperature based on the behavior of the chemical potential and its first derivatives, as well as the population of the ground state.

V1.00013 Intrinsic Versus Extrinsic Which-Way Information and the Use of Extrinsic WW Information in a Delayed Choice Experiment to Send Information Immediately Between 2 Paired Particles, Douglas Snyder\footnote{None — Intrinsic states characterize a quantity inherent in the particle itself, such as spin. Extrinsic states characterize a quantity that is not in the particle itself but that describes the particle. An example is the specific path a particle is taking through an interferometer. Extrinsic states such as the specific path of a particle can be eliminated before a measurement is made. An experiment is described to show the impact that this ability to eliminate extrinsic states can make. This experiment relies on a delayed choice for an idler photon that immediately affects the signal photon with which it is entangled. The delayed choice concerns whether to maintain or eliminate the entanglement before any measurements are made. The idler photon can essentially be lost before any measurements are made because the states of the idler photon that enters the optical microcavity related to its entanglement are eliminated when the idler photon enters the optical microcavity. One of the reasons is that the states of the idler photon are extrinsic to the particle itself (they characterize the particular path of the particle, a characteristic not inherent to the particle itself) where the information underlying the entropic state is eliminated when the particle enters the cavity situated at the confluence of the two possible particle paths. Over a number of runs with this choice, the resulting distribution of the paired signal photons shows interference. If the entanglement is instead maintained, the resulting distribution of the paired signal photons shows WW information.}, None — Intrinsic states characterize a quantity inherent in the particle itself, such as spin. Extrinsic states characterize a quantity that is not in the particle itself but that describes the particle. An example is the specific path a particle is taking through an interferometer. Extrinsic states such as the specific path of a particle can be eliminated before a measurement is made. An experiment is described to show the impact that this ability to eliminate extrinsic states can make. This experiment relies on a delayed choice for an idler photon that immediately affects the signal photon with which it is entangled. The delayed choice concerns whether to maintain or eliminate the entanglement before any measurements are made. The idler photon can essentially be lost before any measurements are made because the states of the idler photon that enters the optical microcavity related to its entanglement are eliminated when the idler photon enters the optical microcavity. One of the reasons is that the states of the idler photon are extrinsic to the particle itself (they characterize the particular path of the particle, a characteristic not inherent to the particle itself) where the information underlying the entropic state is eliminated when the particle enters the cavity situated at the confluence of the two possible particle paths. Over a number of runs with this choice, the resulting distribution of the paired signal photons shows interference. If the entanglement is instead maintained, the resulting distribution of the paired signal photons shows WW information.

V1.00014 The Immediate Affect of Information in a Delayed Choice on a Distant Distribution as Seen in Different Inertial Reference Frames: The “Effect” May Occur Before the “Cause”, Douglas Snyder. None — An experiment is described in the laboratory reference frame that relies on delayed choices for idler photons that immediately affects the distribution of signal photons with which the idler photons are initially entangled. The delayed choices on the idler photons concern whether to maintain or instead eliminate the entanglement between the paired idler and signal photons before any measurements are made. Eliminating the entanglement is done through eliminating the which-way information carried by the idler photon. If the entanglement is maintained, the result is which-way information in the distribution of the signal photons. If the entanglement is instead eliminated, the result is the elimination of which-way information and the presence of interference in the distribution of the signal photons. In other inertial reference frames, the change in state in the signal photon may occur before the delayed choice on the paired idler photon is made. A Minkowski diagram depicts the situation for the laboratory reference frame and another inertial reference frame where the change in state in the signal photon occurs before the delayed choice on the paired idler photon.

V1.00015 FDTD study of the formation of optical vortices associated with core-shell nanoparticle cluster\footnote{The authors would like to acknowledge the valuable support from Masdar Institute and Massachusetts Institute of Technology for the solar thermal project grant.}, Md Mahfuzur Rahman, Jin You Lu, Masdar Institute of Science and Technology, George Ni, Nicholas Xuanlai Fang, Massachusetts Institute of Technology, Tiejun Zhang, Amal Al Ghaferi, Masdar Institute of Science and Technology — Light absorbing plasmonic metal-dielectric nanoparticles suspended in water, or nanofluids have recently been experimentally demonstrated to produce steam at high efficiencies upon solar illumination. This approach localizes high temperatures to the interior of the liquid through efficient trapping of incoming light via scattering and absorption mechanisms. In suspensions, nanoparticles may form clusters due to surface wetting properties, and little work has focused on understanding the optical properties of clusters. In this work, we use the FDTD method to accurately visualize the optical power flow through various plasmonic metal-silica core-shell nanoparticle pairs at different inter-particle separations (10-100 nm). At these separations phase singularities of the power flow can occur, such as vortices of light inside the dielectric core which can enhance the absorption cross-section of the cluster. We study the conditions required to form these vortices. We also consider titanium nitride as shell, other than the widely studied noble metals to visualize the extinction cross-section of a cluster which depends on the separation, and the permittivity of the dielectric core.
V1.00016 Nanometer Scale Microscopy via Graphene Plasmons, XIAODONG ZENG, MOHAMMAD AL-AMRI, MOHAMMAD SUHAIR ZUBAIRY, Institute for Quantum Studies and Department of Physics and Astronomy, Texas A&M University — Using graphene plasmons (GPs), we can realize a nanometer scale microscopy. Our scheme takes advantage of the extremely large wave number of GPs and the low loss of graphene. Comparing with conventional nonlinear structured illumination microscopy basing on high order nonlinearity associated with high intensity light, our proposal only requires linear response. Consequently we need very weak field, which means less damage to the sample and may play a significantly important role in imaging of the biological systems. 

V1.00017 Efficient Non-Resonant Absorption in Thin Cylindrical Targets: Experimental Evidence, ANDREY AKHMETELI, LTASolid Inc., Houston, Texas, USA, NIKOLAY KOKODY, BORIS SAFRONOV, VALERY BALKASHIN, IVAN PRIZ, V. N. Karazin Kharkiv National University, Kharkiv, Ukraine, ALEXANDER TARASEVITCH, University of Duisburg-Essen, Institute of Experimental Physics, Duisburg, Germany — A theoretical possibility of non-resonant, fast, and efficient (up to 40 percent) heating of very thin conducting cylindrical targets by broad electromagnetic beams was predicted in [Akhmeteli, arXiv:physics/0405091 and 0611169] based on rigorous solution of the diffraction problem. The diameter of the cylinder can be orders of magnitude smaller than the wavelength (for the transverse geometry) or the beam waist (for the longitudinal geometry) of the electromagnetic radiation. This can be used for numerous applications, such as pumping of active media of short-wavelength lasers, e.g., through efficient heating of nanotubes with laser radiation. Experimental confirmation of the above results is presented [Akhmeteli, Kokody, Safrovnov, Balkashin, Priz, Tarasevitch, arXiv:1109.1626 and 1208.0066]. Significant (up to 6%) absorption of microwave power focused on a thin fiber (the diameter is three orders of magnitude less than the wavelength) by an ellipsoidal reflector is demonstrated experimentally. For the longitudinal geometry, experiments provide a confirmation of significant absorption (up to 35%) of the power of a wide CO2 laser beam propagating along a thin wire (the diameter of the wire can be orders of magnitude less than the beam waist width).

V1.00018 Scattering of near-zero-energy positronium by H2, JUN-YI ZHANG, Division of Physical Science & Engineering, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia, YING QIAN, Department of Computer Science and Technology, East China Normal University, Shanghai 200241, China, YU-JUN YANG, Institute of Atomic and Molecular Physics, Jilin University, Changchun 130012, China, ZONG-CHAO YAN, Department of Physics, University of New Brunswick, Fredericton E3B 5A3, Canada, UDO SCHWINGENSCHLÖGL, Division of Physical Science & Engineering, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia — The scattering length and pick-off annihilation probability for the S-wave scattering of zero-energy positroniums (Ps) by H2 are calculated by the stabilization method using explicitly correlated Gaussians. The confined variational method is used to optimize the Gaussians in order to describe the short-range interaction of the incident Ps with H2 in the fixed nucleus approximation. By applying a confining potential to the center-of-mass of Ps, the problem of continuum states can be converted to a problem of discrete energy levels. For scattering at very low energies, the convergence of the scattering parameters can be improved by including exterior basis functions to describe the asymptotic region, which are given by products of Gaussians with H2 wave function and Ps wave function. In addition, the effect of van der Waals interaction between the Ps and H2 on scattering parameters will be taken into account.

V1.00019 Experimental and theoretical studies of excited-state angular-momentum alignment and orientation signals in atomic rubidium in the presence of an external magnetic field, MARCIS AUZINS, ANDRIS BERNIS, RUVIN FERBER, FLOURIAN GAHSAUER, LINARIS KALVANS, ARTHURS MOZERS, AGNIS SPIESS, Laser Centre, University of Latvia, Rainis Blvd. 19 LV-1586, Riga, Latvia — We present level-crossing signals for the hyperfine transitions of the D2 line of rubidium and show that these signals can be described very precisely by a theoretical model that is based on optical Bloch equations. The crossings occur when the levels are shifted by the nonlinear Zeeman effect in an external magnetic field B, whose direction defines the quantization axis z. A coherent state is said to be aligned if the population of atoms varies as a function of mF, the projection of the total atomic angular momentum F on the quantization axis z, but is equal for +mF and −mF. When the energies of two magnetic sublevels for which ΔmF = 2 cross, an aligned state can be created by excitation with coherent radiation. An oriented state can be created for crossings with ΔmF = 1. Because the theoretical model has been extended to include the hyperfine structure of the atomic levels, strong magnetic sublevel mixing in an external magnetic field, and the Doppler effect, precise agreement between theory and experiment is possible even at excitation power densities where optical pumping plays a role. We present experimental results and theoretical calculations, showing their dependence on laser power density and frequency.

1 We thank Latvian Council of Science project 119/2012 for financial support.

V1.00020 Stimulated and coherent Raman spectroscopy with 0? pulses, SUMAN DHAYAL, YURI ROS-TOVTSEV, University of North Texas — We developed a new variant of stimulated and coherent Raman spectroscopy with shaped short pulses, applicable to multi-scattering media. The technique is based on the spectral modulation of the laser pulse due to the Raman scattering. Using discrete dipole approximation we modeled the scattering from nanoparticles and calculated response from molecules in vicinity of nanoparticles to demonstrate the effects of 0?-short laser pulses. The obtained results may have a broad range of applications from spectroscopy and pathogen detection to microscopy.

V1.00021 Second quantization of squeezed light through non-linear medium, ZHIHIAO XIAO, R. NICHOLAS LANNING, Department of Physics and Astronomy, Louisiana State University, MI ZHANG, IRINA NOVIKOVA, EUGENIY E. MIKHAILOV, Department of Physics, College of William & Mary, JONATHON P. DOWLING, Department of Physics and Astronomy, Louisiana State University — We investigated the interaction of Rb atoms and squeezed light which is treated quantum mechanically. We establish the model of Gaussian beam propagating through the non-linear medium. The spatial modes of the output beam include high order Laguerre-Gaussian (LG) modes. We find the differential equation describing the second-quantized input-output relations. Since the spatial LG modes of the output beam are entangled with the squeezed states, we apply various schemes of spatial selection in order to produce the squeezed states which can lead to various applications. We also explain the result of the experiment where a Gaussian pump field is put through a Rb cell and a sub-shot noise is found.

V1.00022 Possibility of vibrationally resolved cross section measurements for low energy charge transfer in H + H2, C.I. GUILLEN, R.A. STROM, J.A. TOBAR, D.I. PANCHENKO, V.M. ANDRIANARIJAONA, Department of Physics, Pacific Union College, Angwin, CA 94508 — Charge transfer (CT) in H + H2 → H+ + H2 has fundamental implications because it involves the smallest atomic ion, atom, molecular ion, and molecule possible. The current merged-beam apparatus at Oak Ridge National Laboratory (ORNL) in Oak Ridge, Tennessee, can reliably create and access low collision energies; the existing ion-atom merged beams apparatus there is the only apparatus currently able to benchmark the CT of these fundamental systems at energies below 0.1eV/u (Phys. Rev. A 84, 062716, 2011). However, the data analysis suffers from the lack of information on the initial states of H2, which makes comparison to state-to-state calculations (PRA 67 022708 (2003) impossible without educated guesses. We are exploring the possibility of inserting a three-dimensional imaging technique at the end station of the ORNL apparatus in order to measure the vibrational state distribution of H2 that are produced by the electron cyclotron resonance ion source. Our initial design for the insertion of this technique in the aforementioned system will be presented here.

1 Work supported by the National Science Foundation under Grant No. PHY-1068877
V1.00023 The Utilization of Chloroform Post-Treatment to Improve the Adhesion of Au Thin Films onto PMMA. KATHLEEN KRIST, CHRIS HUGHES, XIAOFENG HU, James Madison University, BRIAN AUGUSTINE, High Point University — The metallization of Au onto plastics is an important processing step in the fabrication of microfluidic devices. While its corrosion resistance and excellent electrical and thermal conductivity make Au a good choice, its inertness results in poor adhesion to polymer surfaces. Previous studies have indicated that exposing commercially available Poly(methyl methacrylate) (PMMA) sheets to chloroform vapor following Au deposition significantly improves adhesion.

In this study, we deposited 6 nm of Au onto 1.50 mm thick PMMA and exposed the samples to vapor released from chloroform heated on a hot plate set at 70°C. The force required to remove the Au thin films was determined by placing samples on a polisher spinning at 150 rpm and utilizing UV-VIS spectroscopy to measure the transmittance of 700 nm light through the films to quantify their removal as a function of applied polishing force. The Au thin films were also characterized using AFM. AFM images demonstrated a progressive roughening of the surface corresponding to an increase in applied force. Additionally, these images support a model in which the chloroform treatment softens the PMMA surface, producing a softened layer that the polisher removes simultaneously with the Au thin film.

1Undergraduate

V1.00024 Spatial Modes of a Squeezed Vacuum Field1. MI ZHANG, College of William & Mary, R. NICHOLAS LANNING, ZHIHAO XIAO, JONATHAN P. DOWLING, Louisiana State University, IRINA NOVIKOVA, EUGENII E. MIKAHLIOV, College of William & Mary. We prepared a quantum noise suppressed squeezed vacuum field by propagating a beam with a wavelength of 795nm through a hot Rb cell. Observation of the quadrature noise showed that we achieved a noise suppression of -2.0 dB below the quantum noise limit. When a spatial mask was applied to the beam after its interaction with atoms, we observed that the detected quantum noise suppression strongly depended on the shape of the mask. An exploration of the spatial distribution of noise in the squeezed field illustrated that the squeezed field was in a different spatial mode from the pump field used as a local oscillator. Our research showed that the squeezed field consisted of several spatial modes with various squeezing parameters. If a pure squeezed mode could be extracted, it would enhance the signal to noise ratio, which would impact precision metrology and quantum memory applications.

1This project is supported by AFOSR grant FA9550-13-1-0098.

V1.00026 Experimental apparatus for quantum simulation with two-dimensional 9Be+ Coulomb crystals . KARSTEN PYKA, HARRISON BALL, TERRY MCRAE, CLAIRE EDMUNDS, MICHAEL W. LEE, SAMUEL HENDERSON, MICHAEL J. BIERCUK, The University of Sydney, QUANTUM CONTROL LAB TEAM — We report on the development of a new experimental setup designed for Quantum Simulation studies at a computationally relevant scale using laser-cooled 9Be+ ion-crystals in a Penning trap. The trap geometry is optimized using numerical calculations for trapping large ion crystals with enhanced optical access and reduced anharmonic perturbations. Separate loading and spectroscopy zones prevent long term drifts of the trapping parameters due to contamination of the trap electrodes with Be deposits. Our customized superconducting magnet provides a homogenous (dB/B < 10-6) magnetic field at 3T required for ion trapping. Laser frequencies required for cooling/detection and spin-motion entanglement are generated from telecom wavelength fiber laser systems in the IR via nonlinear conversion. Our new approach employs high-efficiency telecom modulators and mode-selecting cavities to generate multiple beamslines from a single Sum-frequency-Generation step. Ultimately, this newly developed setup will allow for studies of many-body spin systems with tunable interaction strength from infinite-range to nearest-neighbour type interaction.

V1.00027 Complete and Partial Transfer of Energy in Bremsstrahlung Should Include Rotational and Vibrational Kinetic Energies . STEWART BREKKE, Northeastern Illinois University (former grad student) — In complete braking achievement the rotational and vibrational as well as the linear kinetic energies of the charged particle results in a photon: \( h\nu = \frac{1}{2m^2} + \frac{1}{2I\omega^2} + \frac{1}{2k^2} \). In partial transfer of kinetic energies of the decelerating particle the resulting photon is \( h\nu = \left[\frac{1}{2m^2} + \frac{1}{2I\omega^2}\right] + \frac{1}{2k^2} \). The linear kinetic energy of the charged particle is \( \frac{1}{2m^2} \), the rotational kinetic energy is \( \frac{1}{2I\omega^2} \) and the vibrational kinetic energy is given by \( \frac{1}{2k^2} \).

V1.00028 Evolution of quantum wave packets in the presence of time-dependent absorption . MAXIMILIEN BARBIER, Northumbria University, MATHIEU BEAU, School of Theoretical Physics, Dublin Institute for Advanced Studies, ARSENI GOUSSEV, Northumbria University — The dynamics of a quantum particle submitted to a barrier is strongly influenced by the wave nature of matter, and may for instance lead to the classically forbidden phenomenon of tunneling. While the case of a real potential barrier is a standard problem in quantum mechanics, different approaches are possible to model an absorbing barrier. Here we present a quantitative comparison between two such approaches. The first one describes an absorbing point-like barrier by means of certain time-dependent boundary conditions of Kottler’s type, while the second approach treats the wave function of the moving particle as a component of a spinor evolving under the action of a matrix Hamilton operator.

V1.00029 Magneto-optical resonances and relaxation mechanisms in an extremely thin cell: experiment and theory for the cesium D1 line1. MARCIS AIZINSH, ANDRIS BERZINS, RUVIN FERBER, FLORIAN GAHBHAER, ULDIS KALNINS, LINARDS KALVANS, RONALDS RUNDANS, Laser Centre, University of Latvia, Rainis Blvd. 19 LV-1586, Riga, Latvia, DAVID SARKISYAN, Institute for Physical Research, NAS of Armenia, Ashtarak-0203, Armenia — Magneto-optical resonances are a sensitive effect that allows to make stringent tests for theoretical models, which in turn, can help to improve devices that measure magnetic field. The experiments were carried out with an extremely thin cell (ETC) that provides high spatial resolution and allows sub-Doppler spectroscopy. At the same time the theoretical description of the signal requires delicate treatment of effects peculiar to thin cells. The cell, manufactured in Armenia, consists of two YAG glass windows separated by a distance of less than one micrometer. The experimental measurements of magneto-optical resonances were done using LIF signals of a cesium atomic vapor layer with a thickness varying from about 350 nm to of about 900 nm. In this study we obtained an accurate theoretical description of magneto-optical resonances using a theoretical model based on the optical Bloch equations that is an expanded version of earlier models and now includes a more detailed treatment of relaxation processes and the saturation of the atom-laser interaction in the high-intensity areas of the beam.

1The Riga group gratefully acknowledges financial support from the Latvian State Research Programme (VPP) project IMIS²

V1.00030 Efficiency of multi-wave mixing in a sphere . SUMAN DHAYAL, YURI ROSTOVTSVE, University of North Texas — We consider nonlinear multi-wave mixing in a sphere. We compare the efficiency of wave mixing in a sphere with the efficiency in a bulk or in the slab where, as well-known, the phase-matching plays an important role. We have found the optimal conditions for nonlinear generation in a sphere. The obtained results can be applied to coherent Raman microscopy and allow us to maximize the signal for arbitrary shape of nanoparticles.

V1.00031 Efficiency of multi-wave mixing in a sphere . SUMAN DHAYAL, YURI ROSTOVTSVE, University of North Texas — We consider nonlinear multi-wave mixing in a sphere. We compare the efficiency of wave mixing in a sphere with the efficiency in a bulk or in the slab where, as well-known, the phase-matching plays an important role. We have found the optimal conditions for nonlinear generation in a sphere. The obtained results can be applied to coherent Raman microscopy and allow us to maximize the signal for arbitrary shape of nanoparticles.
V1.00031 Modelling Spatial Modes of Squeezed Vacuum – When it Comes to Squeezing, Plane Waves Are Just Too Plan, R. NICHOLAS LANNING, ZHIHAO XIAO, Louisiana State University, MI ZHANG, IRINA NOVIKOVA, EUGENIY E. MIKHAILOV, College of William and Mary, JONATHAN P. DOWLING, Louisiana State University — Recent research relying on the polarization self-rotation (PSR) effect in Rb$^8$ has revealed a squeezed vacuum field consisting of several spatial modes with various squeezing parameters [Mi Zhang, Spatial Modes of a Squeezed Vacuum Field, 2015 APS March Meeting]. In order to explain these results, we re-derive the beam propagation model describing the creation of squeezed vacuum via PSR and incorporate more realistic multimode input-output relations in the paraxial approximation. We solve the propagation equation and use it to predict the spatial distribution of squeezed vacuum via the proper Laguerre-Gauss modal structure. This modal structure is instrumental in the development of a complete second quantized beam propagation formalism also being reported at this meeting [Zhihao Xiao, Second quantization of squeezed light through non-linear medium, 2015 APS March Meeting].

V1.00032 Photoionization of Fe$^{7+}$ from the ground and metastable states1, SWARAJ TAYAL, Clark Atlanta University, OLEG ZATSARINNY, Drake University — The B-spline Breit-Pauli $R$-matrix method is used to investigate the photoionization of Fe$^{7+}$ from the ground and metastable states in the energy region from ionization thresholds to 172 eV. The present calculations were designed to resolve the large discrepancies between the recent measurements and available theoretical results. The multiconfiguration Hartree-Fock method in connection with B-spline expansions is employed for an accurate representation of the initial and final states wavefunctions. The close-coupling expansion includes 99 fine-structure levels of Fe$^{7+}$ in energy region up to $3s^23p^54s^4$ states. It includes levels of the $3s^23p^5$, $3s^23p^53d$, $3s^23p^54s$, and $3s^23p^53d$ configurations which lie in the energy region under investigation. The present photoionization cross sections agree well with the Breit-Pauli $R$-matrix calculation of Sossah et al. and is governed by the configuration of the background cross sections, but show new rich structure which qualitatively agree with the measurements. The calculated cross sections, however, are several times lower than the measured cross sections depending upon photon energy. The cross sections for photoionization of metastable states

1This work was supported by NASA under grant NNX11AB62G from the Solar and Heliophysics program.

V1.00033 Two-color x-ray pump x-ray probe study of the core-hole decay dynamics in XeF2, ANTONIO PICON, C. STEFAN LEHMANN, STEPHEN SOUTHWORTH, PHAY HO, GILLES DOUMY, ELLIOT KANTER, BERTOLD KRAESSIG, ANNE MARIE MARSH, DOOSHAYE MOONSHIRAM, LINDA WONG, STEVE PRATT, Argonne National Laboratory, DIPANWITA RAY, Lawrence Berkeley National Laboratory, DANIEL ROLLES, BENJAMIN ERK, CEDRIC BOMME, CFEL, DESY, ARTEM RUDENKO, Kansas State University, TIMUR OSIPOV, NORA BERRAH, Department of Physics, UCONN, LAN CHENG, JOHN STANTON, University of Texas — To resolve the femtosecond inner-shell dynamics and the subsequent induced electron transfer in a molecule, the core-hole decay dynamics in XeF2 have been directly studied using femtosecond time-resolved x-ray pump x-ray probe coincidence imaging. The study of XeF2 molecule allows us to compare the molecular core-hole decay with the atomic case, Xe atom. To study these processes, the recently developed capability at LCLS was used to generate two-color x-ray pulses with variable delay. A time and position sensitive detector has been used to record the ion fragments in coincidence. The correlated ion kinetic energies make it possible to select and assign different excitation pathways, being able to track the atomic and the molecular core-hole decay dynamics.

V1.00034 Electron Impact Inner-shell Ionization of Ions1, A.K.F. HAQUE, M.A.R. PATOARY, M.A. UDDIN, A.K. BASAK, Department of Physics, University of Rajshahi, Rajshahi-6205, Bangladesh, B.C. SAHA, Department of Physics, Florida A&M University, Tallahassee, FL-32307. — Electron impact ionization cross-sections (EIICS) for H to Sc isoelectronic series over incident energies ranging from threshold to 10 keV have been measured. Recent work and theoretical results are described. The experiment is based on the electron impact ionization of the K-, L- and M-shell ions, "Physica Scripta, 81, 045301 (2010)."

1Work is partially supported by DOE project (NNSA)

V1.00035 Absorption spectra of monolayer MoS2 in high magnetic field, HUNG-DUEN YANG, Natl Sun Yat Sen Univ, JIN-MONG HER, Chang Gung University, SHOJOIRO TAKEYAMA, YASUHIRO MATSUDA, The University of Tokyo, The Institute for Solid State Physics Kashiwano 5-1-5, Kashiwa, Chiba #277-8581 Japan, KAI-HSUAN WANG, Natl Sun Yat Sen Univ — We have measured the absorption spectra of monolayer MoS2 at several temperatures in pulsed high magnetic fields up to 52 T. At room temperature, the observed spectrum dominated by two peaks, which are located at 660 nm and 606 nm. These peaks are ascribed to excitation and trion absorption peaks respectively [1]. At low temperature (4.2 K), two peaks show the blue shift to 633 nm and 588 nm, respectively. Irrespective of the temperature, applying magnetic field does not show pronounced influence on the peaks even in 52 T.

V1.00036 Measuring the conductivity dependence of the Casimir force1, JUN XU, ROBERT SCHAFFER, ALEXANDR BANISHEV, UMAR MOHIDEEEN, University of California, Riverside, CA 92521 — The strength and distance dependence of the Casimir force can be controlled through the conductivity of the material bodies, with lower conductivity in general leading to lower Casimir forces. However low conductivity, large bandgap materials which are insulating, have drawbacks as any surface electrostatic charges cannot be easily compensated. This restricts experiments to metallic or highly doped semiconductor materials. We will report on measurements of the Casimir force gradient using the frequency shift technique. Improvements in the measurement technique will be discussed. Measurements of the Casimir force gradient using low and high conductivity silicon surfaces will be reported.

1The authors thank G.L. Klimchitskaya and V.M. Mostepanenko for help with the theory and the US National Science Foundation for funding the research.

V1.00037 Nonlinear dynamical phase diagram of ultra-cold atoms in periodic lattices, WAKUN LAM, GIL SUMMY, MARIO BORUNDÁ, Oklahoma State Univ — We study the dynamics of ultra-cold bosonic gases in periodic deep optical potential by incorporating the nonlinear inter-site coupling into the discrete nonlinear Schrödinger equation (DNLS). We numerically solve the DNLS to analyze and compare the evolution of Gaussian wave packets reported in [Phys. Rev. Lett., 86, 11(2001)]. Our result corroborates the validity of the phase diagram calculated by the variational method within a certain range of parameters of the initial wave packets. We calculate the long-term evolution of solutions of DNLS to generate a fine phase diagram to elaborate the transitions between different dynamic modes. We propose an experimental scheme to verify the phase diagram based on the Bose-Einstein condensates in optical traps.
V1.00038 Superfluidity and Chaos, GEVA ARWAS, AMICHAY YARDI, DORON COHEN, Ben-Gurion University — The hallmark of superfluidity is the appearance of a quantized metastable circulating current. The Landau criterion links the metastability of a vortex state to its spectral stability, i.e., to the inaccessibility of elementary excitations connecting it to other states with the same energy. In low dimensional systems, superfluid vortex states can exist due to their dynamical stability even if they are spectrally unstable. This traditional paradigm associate superfluid vortex states with stationary fixed points in phase space. Hence, Bogoliubov de Gennes (BdG) stability analysis is normally used to determine the feasibility of such states. In this work we challenge this traditional criterion and highlight the role of chaos in the analysis, thus explaining the existence of current carrying eigenstates which are neither spectrally-stable nor dynamically-stable.

V1.00039 Interaction and Disorder Effects across BCS-BEC Crossover in Two-Dimensional Fermi Gases, B. TANATAR, A. KHAN, Bilkent University — We investigate the effect of static impurities in two-dimensional ultracold atomic Fermi gases. We incorporate disorder from impurities through fluctuations and study its effects on the BCS-BEC crossover. We analyze the effect of quenched disorder for various physical quantities such as chemical potential, pairing gap, density of states, spectral function, and ground-state energy. We extend our study further towards the experimentally viable quantities such as condensate fraction, sound velocity and Landau critical velocity. The results are presented as a function of binding energy and scattering length. We observe negligible effect of disorder in 2D for BCS Cooper pairs and considerable amount of depletion in the BEC regime but intriguingly the results also reveal that disorder effect is masked at the crossover region.

V1.00040 Direct laser cooling of the BH molecule, DARREN HOLLAND, STEFAN TRUPPE, RICHARD HENDRICKS, BEN SAUER, MICHAEL TARBUtT, Imperial College London — Ultracold polar molecules are of interest for a variety of applications, including tests of fundamental physics, ultracold chemistry, and simulation of many-body quantum systems. The laser cooling techniques that have been so successful in producing ultracold atoms are difficult to apply to molecules. Recently however, laser cooling has been applied successfully to a few molecular species, and a magneto-optical trap of SrF molecules has now been demonstrated. We have investigated the BH molecule as a candidate for laser cooling. We have produced a molecular beam of BH and have measured the branching ratios for the excited electronic state, \( \Lambda^1\Sigma^+(v'=0) \), to decay to the various vibrational states of the ground electronic state, \( \Sigma^1\Sigma^- \). We verify that the branching ratio for the spin-forbidden transition to an intermediate triplet state is inconsequentially small. We measure the frequency of the lowest rotational transition of the X state, and the hyperfine structure in the relevant levels of both the X and A states, and determine the nuclear electric quadrupole and magnetic dipole coupling constants. Our results show that a relatively simple laser cooling scheme can be used to cool, slow and trap BH molecules.

V1.00041 Trapping effect on the sound velocity of a multilayer Fermi gas\(^1\), PATRICIA SALAS, M. A. SOLiS, Instituto de Física, UNAM — We present the trapping effect on the behavior of the isothermal compressibility and sound velocity for an interactionless Fermi gas immersed in a periodic interconnected multilayer structure created by an external Dirac comb potential which can vary both in spacing and in the intensity that controls the impenetrability of the layer edge (the wall) \([1]\). At \( T = 0 \), for a given layer width and respect to the free ideal Fermi gas values, the isothermal compressibility as a function of the impenetrability starts in one and then monotonically increases to reach a larger constant value which is width dependent. The sound velocity as a function of impenetrability starts in one and for a range of impenetrabilities shows a bump which suggests that the presence of the structure increases the sound velocity. For a finite temperature, given a separation between the walls and several values of their impenetrabilities, both properties start their evolution in temperature from the ideal Fermi gas value, unfold at temperatures near and under \( T^\gamma \), and then recover the behavior of a classical gas at higher temperatures.

\(^1\)We acknowledge partial support from PAPIIT IN111613 and CONACyT 221030.

V1.00042 Superfluidity in 1D and 3D Spin-Imbalanced Fermi Gases\(^1\), BEN A. OLSEN, MELISSA REVELLE, JACOB A. FRY, RANDALL G. HULET, Department of Physics & Astronomy and Rice Quantum Institute, Rice University, Houston, TX 77005 — The phase separation between superfluid and normal phases (both polarized and unpolarized) in trapped Fermi gases in the BEC-BEC crossover reveals the interplay between superfluid pairing, interactions, and dimensionality. We measure density profiles of both spins of a two-component, spin-polarized fermions cooled to \( \sim 100 \) nK. In a 3D gas, an unpolarized superfluid core is surrounded by a polarized shell. We observe gradual suppression of this core as interactions are weakened from unitarity. For a 1D gas in an optical lattice, the phase separation matches 1D models, where the central phase is partially polarized, and is predicted to exhibit FFLO correlations\(^2\). By increasing the inter-tube tunneling rate, we investigate the dimensional crossover between 1D and 3D Fermi gases. In this regime, the FFLO order parameter is predicted to be correlated between tubes\(^3\) and its modulation length constant over larger regions of the trap.\(^4\) These features are predicted to enhance the observable signatures of FFLO correlations; we report progress towards such measurements.

\(^1\)Supported by DARPA, NSF, ARO, and ONR
\(^3\)K. Sun, and C. J. Bolech, PRA 87, 053622 (2013)

V1.00043 APPLICATONs —

V1.00044 Feature Selection via Modified Gravitational Optimization Algorithm, NOOSHIN NABIZADEH, NIGEL JOHN, University of Miami — Feature selection is the process of selecting a subset of relevant and most informative features, which efficiently represents the input data. We proposed a feature selection algorithm based on \( n \)-dimensional gravitational optimization algorithm (NGOA), which is based on the principle of gravitational fields. The objective function of optimization algorithm is a non-linear function of variables, which are called masses and defined based on extracted features. The forces between the masses as well as their new locations are calculated using the value of the objective function and the values of masses. We extracted variety of features applying different wavelet transforms and statistical methods on FLAIR and T1-weighted MR brain images. There are two classes of normal and abnormal tissues. Extracted features are divided into groups of five features. The best feature is selected in each group using \( n \)-dimensional gravitational optimization algorithm and support vector machine classifier. Then the selected features from each group make several groups of five features again and so on till desired number of features is selected. The advantage of NGOA algorithm is that the possibility of being drawn into a local optimal solution is very low. The experimental results show that our method outperforms some standard feature selection algorithms on both real-data and simulated brain tumor data.
V1.00045 Optically Pumped NMR Studies of Mechanically Induced Strain in GaAs Films . CLIFFORD BOWERS, RYAN WOOD, JOHN TOKARSKI III, LAUREN MCCARTHY, DIPTA SAHA, CHRISTOPHER STANTON, Univ. of Florida - Gainesville, JESUS MORENO, MIT — We present a new methodology for measuring strain in semiconductor films based on optically pumped NMR (OPNMR). Single crystals of GaAs were epoxy bonded to Si wafers at 100 °C. The GaAs is then thinly thinned by selective chemical etching. Upon cooling, biaxial tensile strains are induced in the GaAs films since the coefficient of thermal expansion in GaAs is different than in the Si support. OPNMR experiments were carried out at 6-10 K. The OPNMR spectra are sensitive to nuclei within a phonon coherence depth from the surface. When illuminated with a 0.635 μm thick Si support, the strain, which is proportional to the observed quadrupole splitting, is found to decrease with increasing thickness of the GaAs films and appears to approach a residual value. When the same GaAs film is mounted on a thicker 5mm Si block, the strain increased. To explain the observations, we consider effects of dislocation relaxation of strain and bending of the composite. The interface strain extracted from the measurements is 5.5 × 10^{-4}, in good agreement with the value estimated using the differential thermal contraction of Si and GaAs. The strain resolution of the technique is about 10^{-5} in GaAs.

V1.00046 Theoretical study of the structural, vibrational and dielectric properties of PbSnTe alloys . HORACIO W. LEITE ALVES, ANTONIO R.R. NETO, Univ. Fed. de Sao Joao del Rei, JOHN E. PETERSEN, Texas State University, PAULO D. BORGES, Univ. Fed. de Viçosa, LUISA M.R. SCOLFARO, Texas State University — Thermoelastic devices have promise in dealing with the challenges of the growing demand for alternative clean energy and Te-based materials well-known candidates for them. Recently [1], we have shown that the high values for the dielectric constant, together with anharmonic LA-TO coupling, reduces the lattice thermal conductivity and enhances the electronic conductivity in PbTe. Also, it was shown that by alloying this material with Se, the electronic conductivity of the alloys is also enhanced [2]. But, it is not clear if the same occurs when alloying with Sn. We show, in this work, our ab initio results for the structural, vibrational and dielectric properties of Pb_{1-x}Sn_xTe alloys. The calculations were carried out by using the Density Functional Theory, and the alloys were described by the Virtual Crystal Approximation. Our results show that their structural properties do not obey the Vegard rule. However, we have detected that the anharmonic LA-TO coupling still exists and the obtained values for the dielectric constant show higher values than that obtained for PbTe.


V1.00047 Experimental observation of amplification death via asymmetric gain . MAHBOOBEH CHITSAZI, SAMUEL FACTOR, JOSEPH SCHINDLER, HAMIDREZA RAMÉZANI, FRED ELLIS, TSAMPIKOS KÖTTOS, Department of Physics, Wesleyan University, Middletown CT-06459, USA — The amplification action of a photon coupled RLC circuit is experimentally controlled via a spatially inhomogeneous gain. Specifically we have demonstrated that the overall gain of this uneasy RLC circuit can result in its stabilization. This counterintuitive phenomenon has its roots in managing impedance matching and thus can be applicable to a variety of wave systems.

V1.00048 Laser Induced Breakdown Spectroscopy of Glass and Crystal Samples . PRAKASH SHARMA, ALEJANDRA SANDOVAL, MICHAEL CARTER, AKSHAYA KUMAR, Department of Physics, Tuskegee University, Tuskegee, Alabama — Different types of quartz crystals and rare earth ions doped glasses have been identified using the laser induced breakdown spectroscopy (LIBS) technique. LIBS is a real time technique, can be used to identify samples in solid, liquid and gas phases. The advantage of LIBS technique is that no sample preparation is required and laser causes extremely minimal damage to the sample surface. The LIBS spectrum of silicate glasses, prepared by sol-gel method and doped with different concentration of rare earth ions, has been recorded. The limit of detection of rare earth ions in glass samples has been calculated. Total 10 spectra of each sample were recorded and then averaged to get a final spectrum. The ocean optics LIBS2500 plus spectrometer along with a Q-switched Nd:YAG laser (Quantel, Big Sky) were used to record the LIBS spectrum. This spectrometer can analyze the sample in the spectral range of 200 nm to 980 nm. The spectrum was processed by OOI LIBS-plus(v1.0) software. This study has application in the industry where different crystals can be easily identified before they go for shaping and polishing. Also, concentration of rare earth ions in glass can be monitored in real time for quality control.

V1.00049 Optical spectrum measurement of a cell-adhered microcavity for the cell-cycle analysis applications . RYUSUKE SAITO, MITSUHIRO TERAKAWA, TAKASUMI TANABE, Department of Electronics and Electrical Engineering, Keio University — We build a setup and demonstrate successful measurement of the transmittance spectrum of a whispering gallery mode silica optical microcavity in which NIH 3T3 cells adhered on the top surface to achieve real-time and label-free measurement of the cell cycle. Label-free measurement is expected to prevent the cells to exhibit secondary effect. We build a system that enables the control of the gap distance between the microcavity and the tapered fiber, both of which are placed in the cell culture medium. The optimization of the tapered fiber diameter is the key to measure the spectrum of a microcavity in liquid. A swept wavelength laser light at a wavelength of 766 to 780 nm is used for the measurement. The cavity exhibit a Q of 1.0 × 10^{10} in air, where the value is 1.0 × 10^{10} in the medium and drops to 3.1 × 10^{4} after the cell-adhesion. Still the Q of the microcavity is sufficiently high to detect the change at the cavity surface. Indeed we observe slight spectrum shift toward a longer wavelength, which we believe is due to the adherence of NIH 3T3 cells on the silica microcavity. The successful measurement of the transmittance spectrum of a microcavity in cell culture medium is the first step to realize the analysis of the cell-cycle based on microcavity system.

V1.00050 Laser performance at 1064 nm in Nd^{3+} doped oxi-tellurite glasses . MARIA JOSE BELL, VIRGILIO ANJOS, LYANE MOREIRA, RODRIGO FALCI, Federal University of Juiz de Fora, LUCIANA KASSAB, Faculdade de Tecnologia de Sao Paulo, D. SILVA, Escola Politécnica da USP, JEAN LOUIS DOULAN, PATRICE CAMY, RICHARD MONCORGE, Université de Caen, France — The search for Nd^{3+} doped new solid-state laser hosts having specific thermo-mechanical and optical properties is very active. Among tellurites, the TeO_2-ZnO glass combines good mechanical stability, chemical durability, high linear and nonlinear refractive indices, low phonon energies (~750 cm^{-1}) and a wide transmission window (0.4-6 μm). Their high nonlinear optical properties can be used for the development of Kerr-lens mode-locked subpicosecond lasers. The present work concentrates on the luminescence properties and the laser performance of a TeO_2-ZnO tellurite glasses doped with Nd^{3+}. True continuous-wave laser action is achieved by pumping the sample with a CW Ti:Sapphire laser inside a standard two-mirror laser cavity. A low laser threshold of 8 mW and a laser slope efficiency of 21% could be obtained for an output coupler transmission of 2.7%, which is an encouraging improvement compared to what was reported in the past with other Nd-doped tellurite bulk glasses.

3 Authors acknowledge the support of agencies CAPES, FAPEMIG National Institute of Photonics (INCT Project/CNPQ) and COFECUB.

V1.00051 Mie plasmon-polariton modes in two-dimensional metallic photonic crystals . BRAYAN DIAZ, Universidad del Valle, RICARDO MEJIA, Ciudad Universitaria, Maceió, NELSON PORRAS, Universidad del Valle — We have studied the Mie plasmon-polariton resonances in cylindrical metallic hollow rods by calculating the scattering (Q_{scat}), extinction (Q_{ext}) and absorption (Q_{abs}) coefficients, which were compared with results for the photonic band structure (PBS) of the corresponding periodic 2D system, showing that Bloch plasmon-polariton modes in the periodic system shift toward a longer wavelength, which is due to the relaxation of the resonances in both cases, we show that the symmetry properties remain similar, indicating a robustness of these localized plasmon modes.
V1.00052 Optical “Bernoulli” forces\(^1\). RAMIS MOVASSAGH, Massachusetts Institute of Technology and Northeastern University, STEVEN JOHNSON, Massachusetts Institute of Technology — By Bernoulli’s law, an increase in the relative speed of a fluid around a body is accompanied by a decrease in the pressure. Therefore, a rotating body in a fluid stream experiences a force perpendicular to the motion of the fluid because of the unequal relative speed of the fluid across its surface. It is well known that light has a constant speed irrespective of the relative motion. Does a rotating body immersed in a stream of photons experience a Bernoulli-like force? We show that, indeed, a rotating dielectric cylinder experiences such a lateral force from an electromagnetic wave. In fact, the sign of the lateral force is the same as that of the fluid-mechanical analogue as long as the electric susceptibility is positive (\(\epsilon > 0\)), but for negative-susceptibility materials (e.g. metals) we show that the lateral force is in the opposite direction. Because these results are derived from a classical electromagnetic scattering problem, Mie-resonance enhancements that occur in other scattering phenomena also enhance the lateral force. [This talk is based on Phys. Rev. A 88, 023829 (2013).]

\(^1\)Supported in part by the U.S. Army Research Office under contract W911NF-13-D-0001.

V1.00053 Extraordinary transverse magneto-optical Kerr effect in a superlens. EDWIN MONCADA, Universidade del Valle, ANTONIO GARCIA; Instituto de Microelectronicas de Madrid, JUAN CARLOS CUEVAS, Universidad Autonoma de Madrid — It has been shown that a slab of a negative index material can behave as a superlens enhancing the imaging resolution beyond the wavelength limit. We show here that if such a slab possesses in addition some magneto-optical activity, it could act as an ideal optical filter and exhibit an extraordinary transverse magneto-optical Kerr effect. Moreover, we show that losses, which spoil the imaging resolution of these lenses, are a necessary ingredient to observe this effect.

V1.00054 Characterization/Selection of a Continuous Wave Laser for RIMS Analysis in Nuclear Forensics. SUNNY LAU, F. ALVES, G. KARUNASIRI, C. SMITH, Naval Postgraduate School, B. ISSELHARDT, Lawrence Livermore Laboratory — The effort to implement the technology of resonance ionization mass spectroscopy (RIMS) to problems of nuclear forensics involves the use of multiple lasers to selectively ionize the elements of concern. While current systems incorporate pulsed lasers, we present the results of a feasibility study to determine alternative (Continuous Wave) laser technologies to be employed for analysis of the actinides and fission products of debris from a nuclear detonation. RIMS has the potential to provide rapid isotope ratio quantification of the actinides and important fission products for post detonation nuclear forensics. The current approach to ionize uranium and plutonium uses three Ti-Sapphire pulsed lasers capable of a fundamental wavelength range of 700-1000 nm. In this work, we describe the use of a COTS CW laser to replace one of the pulsed lasers used for the second resonance excitation step of plutonium near 847.282 nm. We characterize the critical laser parameters necessary to achieve high precision isotope ratio measurements including the stability over time of the mean wavelength, bandwidth and spectral mode purity. This far narrower bandwidth laser provides a simpler setup, more robust hardware (greater mobility), and more efficient use of laser irradiance.

V1.00055 Multi-level Capacitive Memory Effect in Metal/Oxide/Floating-Schottky Junction\(^1\), GAHYUN CHOI, SUNGCHUL JUNG, HOON HAHN YOON, YOUNGEUN JEON, KIBOG PARK*, Ulsan National Institute of Science and Technology — A memory computing (memcomputing) system can store and process information at the same physical location simultaneously. The essential components of memcomputing are passive devices with memory functionality, such as memristor, memcapacitor, and meminductor. We report the realization of a Schottky contact memcapacitor compatible with the current Si CMOS technology. Our memcapacitor is formed by depositing a stack of metal and oxide thin films on top of a Schottky contact. Here, the metal electrode of the Schottky contact is floating. The working principle of our memcapacitor is based on the fact that the depletion width of the Schottky contact varies according to the amount of charge stored in the floating metal electrode. The voltage pulse applied across the Metal/Oxide/Floating-Schottky junction controls charge flow in the Schottky contact and determines the amount of charge stored eventually. It is demonstrated experimentally that our memcapacitor exhibits hysteresis behaviors in capacitance-voltage curves and possesses multiple capacitance values that are switchable by the applied voltage pulse.

\(^1\)Supported by NRF in South Korea (2013R1A1A2007070).

V1.00056 High mobility field effect transistors of SnO\(_x\) on glass substrates made by reactive sputtering of Sn metal. CHANJONG JU, CHULWON PARK, HYEONSEOK YANG, USEONG KIM, YOUNG MO KIM, KOOKRIN CHAR, Seoul National University — We report on the electrical properties of SnO\(_x\) thin films and the performance of their field effect transistors on glass substrates made by reactive sputtering of a Sn metal target. We investigated the electrical properties of SnO\(_x\) films as a function of the oxygen pressure. The mobility of the SnO\(_x\) films on glass substrates after post-deposition annealing at 400 C was as high as 15.3 cm\(^2\)V\(^{-1}\)s\(^{-1}\) while its carrier density was 4.42 \(\times\) 10\(^{18}\) cm\(^{-3}\). By x-ray diffraction, we have found that the films are mixture of SnO and SnO\(_2\) phases, suggesting possibility of further enhancement of the electrical properties if the phase can be controlled. Nevertheless, we will report on the performance of thin film transistors using polycrystalline SnO\(_x\) as the channel layer and the atomic-layer-deposited AlO\(_x\) and HfO\(_x\) as the gate oxide.

V1.00057 Integrated silicon nanophotonics: structure and electro-optic properties of BaTiO\(_3\) on Si(001). KRISTY KORMONDY, University of Texas at Austin, FLORIAN FALLEGGER, STEFAN ABEL, YOUI POPOFF, IBM Research - Zurich, PATRICK PONATH, AGHAM POSADAS, University of Texas at Austin, MARYLINE SOUSA, DANIELE CAIMI, HEINZ SIEGWART, EMANUELE UCCELLI, LUKAS CZORNOMAZ, CHIARA MARCHIORI, JEAN FOMPEYRINE, IBM Research - Zurich, ALEXANDER DEMKOV, University of Texas at Austin — High-quality epitaxial BaTiO\(_3\) (BTO) on Si has emerged as a promising material for future electro-optic (EO) devices based on BTO’s large effective Pockels coefficient. In order to achieve strong EO coupling, a film must have (1) correct crystallographic orientation with respect to the applied electric field, and (2) low leakage current in the film to sustain a strong electric field. We report on the EO response of BTO films deposited on Si by molecular beam epitaxy. \(\alpha\) \(_2\) rapid thermal anneal at 600C for 30 min ensures full oxidation of BTO for minimal leakage current with minor change in crystalline structure. EO characterization was performed by analyzing changes of the polarization of a laser beam transmitted through pairs of lithographically defined electrodes. The EO response shows signatures of ferroelectric domains with in-plane polarization. Comparison with normalized responses of c-axis and a-axis films illustrate that a strong EO response is observed even for a mixed film. These results quantify the relationship between BTO structure and EO properties, an important step towards future silicon photonic devices based on ferroelectric oxides.

V1.00058 ABSTRACT WITHDRAWN —
V1.00059 Optimizing Energy Conversion: Magnetic Nanomaterials1, DYLAN MCINTYRE, MARTIN DANN, CAROLINA C. ILIE, State University of New York at Oswego — We present herein the work started at SUNY Oswego as a part of a SUNY 4E grant. The SUNY 4E Network of Excellence has awarded SUNY Oswego and collaborators a grant to carry out extensive studies on magnetic nanoparticles. The focus of the study is to develop cost effective rare-earth-free magnetic materials that will enhance energy transmission performance of various electrical devices (solar cells, electric cars, hard drives, etc.). The SUNY Oswego team has started the preliminary work for the project and graduate students from the rest of the SUNY 4E team (UB, Alfred College, Albany) will continue the project. The preliminary work concentrates on analyzing the properties of magnetic nanoparticle candidates, calculating molecular orbitals and band gap, and the fabrication of thin films.

1SUNY 4E Network of Excellence Grant

V1.00060 Prevention of Initial Defect of Low-Noise Solid-State-Nanopore Device, KAZUMA MATSUI, ITARU YANAGI, KENICHI TAKEDA, Hitachi Ltd — To achieve DNA sequencing using solid-state-nanopore, it is necessary to reduce an electric noise current. In this study, the noise was decreased by reducing the capacitance(C) of the nanopore device. We coated an insulating material near a nanopore on a membrane of the device, and confirmed that the capacitance of the device needs to be decreased down to 100 pF in order to reduce the noise. However, electric-charge difference (∆Q) between electrolyte in the one and the other chamber occurred high voltage (∆V = ∆Q/C) to the membrane because the capacitance(C) was reduced. The electric-charge difference defected the membrane when pouring the electrolyte onto the both sides of the membrane. In order to prevent the initial defects, we established new procedures to reduce the electric-charge difference using electric bypass between the one and the other chamber. Then, we confirmed that there were no defects on the membrane with this procedure.

V1.00061 Development of Multifunctional Luminomagnetic Nanoparticles as Bioimaging Contrast Agents1, LAWRENCE C. MIMUN, CHRIS RIGHTSSELL, G.A. KUMAR, FRANCISCO PEDRAZA, SERGIO A. MONTELONGO, TEJA GUDA, University of Texas at San Antonio, VINAYAK P. DRAVID, Northwestern University, DHIRAJ K. SARDAR, University of Texas at San Antonio — Trivalent rare earth doped nanocrystalline materials with multiple functionalities have drawn special attention in biomedical industry. Current research is focused on the use of various materials with dual functionality for potential multifunctional applications. In this project, we are developing near infrared(NIR) based nanocrystals (NCs) as contrast agents with multimodal features comprising of strong NIR fluorescence, X-ray fluorescence and magnetic properties by utilizing the super-paramagnetic features of Gd3+, the high X-ray excitation cross section of Lu3+, and the NIR fluorescence of Nd3+. Halides, such as MgGdLuF7 (M=K,Na), were doped with NIR active rare earth ions, Nd3+, where synthesis conditions have been optimized to obtain the brightest phosphor with a size of sub-50 nm. Characterization of the NCs were performed to explore the excitation and emission properties, crystal structure, morphology, magnetization properties, and X-ray fluorescence properties. The potential use of these NCs can be utilized as contrast agents for medical imaging application such as optical imaging, magnetic resonance (MRI) and X-ray imaging.

1This research was, in part, funded by NIGMS MBRs-RISE GM060655 and from the National Science Foundation Partnerships for Research and Education in Materials (NSF-PREM) grant N0-DMR-0934218

V1.00062 Intracellular Imaging Applications of Rare Earth doped Multifunctional Metal Oxy-sulphide Nanomaterials1, JULIO C. AVALOS, C. MIMUN, G.A. KUMAR, D.K. SARDAR, Univ of Texas, San Antonio — Nanomaterials with multiple imaging features have a lot of attention in the medical industry where there is always a high demand for contrast agents that can give more information about the intracellular level mechanisms. Nanomaterials with specific size, shapes, surface functionalities, and properties are needed for intracellular level optical imaging. Rare-earth doped inorganic nanophosphors are the best choice for these applications due to their several advantages such as excellent optical properties, size and composition control, etc. Though there are several efficient rare earth based halide nanophosphors, an efficient halide free nanophosphor is still lacking. In this work we are presenting a series of rare earth doped metal oxysulphide host, M2O2S:Re (M=Ca,Gd, La, Re=Yb,Er,Tb), as an alternate host with fluorescence efficiency equal or even higher than that of halides. Following a detailed study on the optical and magnetic properties we evaluated the potentiality of this material as nanoscale multifunctional contrast agents by in vitro and in vivo animal experiments. Our experimental results show that by adjusting the dopant concentrations and host structures the material property can be tuned over a wide range for multimodal imaging applications and optimized compositions can be achieved for high contrast intracellular imaging.

1This research was funded by the National Science Foundation Partnerships for Research and Education in Materials (NSF-PREM) grant N0-DMR-0934218 and partially funded by NIH/NIGMS MARC U*STAR GM07717.

V1.00063 MP04: Nd3+ (M=Ca, Gd), Luminomagnetic Nanophosphors with Optical and Magnetic Features for Multimodal Imaging Applications1, CHRIS RIGHTSSELL, LAWRENCE C. MIMUN, AJITH G. KUMAR, DHIRAJ K. SARDAR, Univ of Texas, San Antonio — Nanomaterials with multiple functionalities play a very important role in several high technology applications. A major area of such applications is the biomedical industry, where contrast agents with multiple imaging modalities can provide better results than conventional materials. Many of the contrast agents available now have drawbacks such as toxicity, photobleaching, low contrast, size restrictions, and overall cost of the imaging system. Rare-earth doped inorganic nanophosphors are alternatives to circumvent several of these issues, together with the added advantage of super high resolution imaging due to the excellent near infrared sensitivity of the phosphors. In addition to optical imaging features, by adding a magnetic ion such as Gd3+ at suitable lattice positions, the phosphor can be made magnetic, yielding dual imaging functionalities. In this research, we are presenting the optical and magnetic imaging features of sub-nanometer size MP04:Nd3+ (M=Ca, Gd) phosphors for the potential application of these nanophosphors as multimodal contrast agents. Cytotoxicity, in vitro and in vivo imaging, penetration depth etc. are studied for various phosphor compositions, and optimized compositions are explored.

1This research was funded by the National Science Foundation Partnerships for Research and Education in Materials (NSF-PREM) grant N0-DMR-0934218.

V1.00064 Measurement of Quantum Yield and Upconversion Brightness in Red, Blue and Green on NIR Excited M2O2S:Yb/Er/Ho/Tm Phosphors1, IVAN BEEKS, AJITH G. KUMAR, DHIRAJ K. SARDAR, Univ of Texas, San Antonio — A series of broadly color tunable upconversion phosphors were synthesized from M2O2S (M=Y,Gd,La) using a flux fusion method. We investigate their upconversion properties as a function of the dopant concentrations and excitation power density. The phosphor compositions were determined for their upconversion characteristics under 800, 980 and 1550 nm excitations. By measuring the quantum yield and luminous brightness, we investigate their potential applications in biomedical imaging as well as NIR display applications. Results are compared with the well-known upconversion phosphor NaYF4:Yb/Er/Ho/Tm and found that the M2O2S phosphor systems are more efficient compared to NaYF4. By adopting various synthesis protocols, we were able to examine M2O2S in the size range of 10 nm to 10 µm.

1This research is supported by the National Science Foundation Partnerships for Research and Education in Materials (NSF-PREM) grant N0-DMR-0934218.
V1.00065 Synthesis and Characterization of Down-converting $\text{Ca}_9(\text{PO}_4)_6\text{Nd}^{3+}$ Nanocrystals for Biomedical Imaging Applications, NICOLAS BALLI, LAWRENCE MIMUM, FRANCISCO PEDRAZA, AJITH KUMAR, DIRAJ SARDAR, University of Texas at San Antonio — Currently, fluorescent probes (FPs), such as organic dyes and fluorescent proteins, are widely used for biomedical imaging, but exhibit undesirable characteristics such as small Stokes shifts, large spectral overlaps, short fluorescence lifetimes, and photobleaching. In recent years rare earth doped nanoparticles (NPs) have shown promising results for use as FPs with properties that overcome the limitations of traditional fluorophores. Our current work utilizes the rare-earth ion, Nd$^{3+}$, which exhibits NIR-NIR excitation and emission wavelengths that are within the low absorption and scattering region for biological tissues. Calcium phosphate was chosen as the host crystal because of its biocompatibility. The nanocrystals were then characterized by X-ray diffraction and TEM imaging. Spectroscopic studies were done to determine the emission and absorption intensity, quantum yield, and fluorescence lifetime. Analysis of the data was performed and the NPs were shown to possess superior properties when compared to those of traditional fluorophores.

V1.00066 Novel conduction behavior in nanopores coated with hydrophobic molecules, VENKAT BALAGURUSAMY, GUSTAVO STOLOVITZKY, ALI AZZALI-ARDAKANI, IBM T.J. Watson Research Center, Yorktown Heights, NY — Nanopores that are hydrophilic either by the nature of their pore surface or after suitable treatment are well studied in the context of solid-state nanopores. The ionic conduction in these nanopores typically exhibit a near no-concentration-dependence region low concentrations of salt (<1 mM salt concentrations), followed by the high concentration region where it is proportional to the concentration. A simple cylindrical model for pore conduction can explain these behaviors based on surface and bulk conduction of the ions in the buffer solution [Smeets et al 2006 Nano Letters 6, 89]. However, in nanopores coated with hydrophobic pores we find that the pore conductance is $c^3$ (c: concentration). This behavior is in stark contrast with the behavior of hydrophilic pores. We will present these results for different hydrophilic molecular coatings that exhibit this behavior.

V1.00067 Mechanical Properties of Pentaerythritoltetranitrate (PETN) Single Crystals from nano-indentation: Depth Dependent Response at the Nano Meter Scale, MEIYU ZHAI, GREGORY MCKENNA, Texas Tech Univ — This paper presents the investigation of the mechanical behaviors of the energetic material pentaerythritol tetranitrate (PETN) single crystals using a nanoindentation technique. The indentation tests have been performed on the (110) crystal face, using both spherical and wedge-shaped tips. The load displacement curves along with analysis has been used to extract the mechanical properties and to identify the anisotropic indentation elastic constants for the PETN. The calculated indentation moduli of the PETN single crystal were found to decrease as indentation depth increases and become displacement independent when the indentation depth is higher than 200nm. The indentation modulus obtained from spherical tip indentation is compared with results calculated by using literature values of the anisotropic elastic constants. The wedge indenter tip measurements at various tip orientations are different due to the anisotropy of the PETN. The yield behaviors of the PETN single crystal were also explored using both spherical and wedge tip indentation and differences are discussed. Key Words: PETN, nano-indentation, anisotropic elastic constants, single crystal, plastic yield

1The authors thank the John R. Bradford Endowment at Texas Tech University and the Office of Naval Research under Project N00014-11-1-0424, each for partial support of this work.

V1.00068 All-optical near-field self-alignment in sub-nanoscale induced by Fano-resonance, HUI DONG, ZHENG WANG, University of Texas at Austin, UNIVERSITY OF TEXAS AT AUSTIN TEAM — Fano-resonance of photonic crystal (PC) slabs generally possesses extremely high quality-factor (Q-factor) which indicates large optical force produced via radiation pressure with low input power. Unlike atoms, nano- and micro-particles, periodicity of PC slab creates identical force field in every unit cell, which enables the manipulation of much wider area in millimeter scale. Here we developed a novel mechanism to construct a conservative optical force field to automatically align PC slabs with sub-nanometer resolution, a technique has a potential application in 3D photonic crystal fabrication. The phase response of our system can be predicted after the features of PC slab are precisely depicted using temporal coupled-mode theory. The conservation of optical force is then theoretically demonstrated based on Response Theory of Optical Force (RTOF) which has a perfect agreement with numerical simulation results of Maxwell Stress Tensor (MST) and Kelvin Force. In the end, we show no non-conservative component exists in the force field from Finite-element Method (FEM) simulation after applying Helmholtz-Hodge decomposition to it.

V1.00069 Effects of Metal Nanoparticles on Optical Behavior Tunability of Multi-layer MoS$_2$, SHERMIN ARAB, STEPHEN CRONIN, University of Southern California — We investigate the effects of metal nanoparticles (NP) on tunability of the optical response from relatively thick MoS$_2$ flakes. The plasmonic interactions and charge transfer at the metal-semiconductor interface is studied through metal NP deposition on mechanically exfoliated MoS$_2$. The optical quenching effect of metal NP capping is observed. Our photoluminescence results show that the surface charge transfer at the metal-semiconductor interface and creation of possible defect points at the semiconductor surface can lead to quenching of the photoluminescence response. Our optical observation of thicker MoS$_2$ flakes shows that, by using a metal NP capping layer, one can selectively exclude photoluminescence response from the peak due to indirect transition. This approach provides a controlled method for tuning the optical response of relatively thick MoS$_2$ flakes. In this study the effects of Au, Cu and Ag NPs are investigated. Micro-PL spectroscopy of the MoS$_2$ flakes is performed; where, PL spectra are collected in the 1.2 eV to 2.3 eV energy range and a 532 nm CW laser is used for excitation. X-ray photoelectron spectroscopy (XPS) is performed to investigate the nature of the metal-semiconductor interface.

V1.00070 Metrology for Nanoscale Manufacturing, ALEXANDER MUNOZ, Arizona State Univ — The extension of optical techniques to the nanoscale is increasingly powerful because manufacturing requires fast, in-line, non-destructive metrology. As part of the NASCENT NSF Engineering Research Center led by the University of Texas at Austin, the focus of the effort is on the tools necessary for establishing manufacturing infrastructure required for process control of nanoscale printing. The initial exploration of scatterometry involved the use of a 244 nm laser to evaluate the zero-order reflectivity as a function of angle of incidence for two polarizations. Measurements of the wire-grid polarizer were then repeated with 405 nm to investigate the extensibility of scatterometry. In conjunction with the scatterometry data, rigorous coupled wave analysis simulations were used to determine the behavior of the reflectivity as a function of five critical dimensions. Varying the parameters led to the ability to fit the simulation curves to the experimental data, thus revealing the dimensions of the wire-grid polarizer. Grating profiles are established continuously allowing for the implementation of roll-to-roll manufacturing as envisioned by NASCENT. Scatterometry is a workhorse of Si lithography because of its fast, non-contact measurements at extreme sub-wavelength scales.

1 This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science by Los Alamos National Laboratory (Contract DE-AC52-06NA25396) and Sand.

V1.00071 SEMICONDUCTORS —
V1.00072 Spin-valley coupling study in transition metal dichalcogenides. LU XIE, the University of Hong Kong — A single layer (monolayer) of transition metal dichalcogenide (TMD), a two-dimensional (2D) crystal with a Honeycomb lattice structure, has attracted tremendous interests thanks to its unique optical and electronic properties. Unlike graphene, TMD monolayer is a direct-gap semiconductor with interband transition in the visible energy range. The direct gap is located at the corners of the 2D hexagonal Brillouin zone which are technologically called valleys. The two degenerate but inequivalent valleys (denoted by ±k) constitute a binary degree of freedom, which is potentially treated as a new kind of information carrier just like the traditional charges and spin. In TMD monolayer, the inversion symmetry is originally broken. This leads to valley-selective circular dichroism meaning that the ±k valleys can only be exclusively excited by right-(r+) or left-circularly (l-) polarized light, which enables optical manipulation of the valley pseudospin. Besides, the strong spin-orbital coupling (SOC) mainly stemming from the transition metal atoms gives a remarkable valence band splitting ranging from 0.1 eV to 0.5 eV for different TMDs. Together with the above mentioned inversion symmetry breaking, this leads to strong coupled spin and valley which makes the valley and spin robust against scattering by smooth deformations and long wavelength phonons. As a result, the valley-dependent optical selection rule is often accompanied by a spin-dependent optical selection rule. Here, we will present the experimental demonstration of the spin-valley locking in TMD monolayer. The spin polarization is realized by the circular polarized optical fields and is electrically detected.

V1.00073 Coherent Manipulation of a Single Magnetic Atom Using Polarized Single Electron Transport in a Double Quantum Dot. WENXI LAI, Dr, WEN YANG, collaboration tutor — We consider theoretically a magnetic impurity spin driven by polarized electron tunneling in a double quantum dot transport. Spin blockade effect and spin conservation in the system make the magnetic impurity to sufficiently interact with each transported electron. This effect yields the nanomagnet coherently driven by a single electron which carries information about the magnetic impurity spin. The present scheme may develop all electrical manipulation of manomagnets by means of single electrons, which is significant for the implementation of scalable logical systems in information processing.

V1.00074 Spin textures for surface states with non-Rashba-type spin-orbit interaction. KOKIN NAKAJIN, SHUICHI MURAKAMI, Tokyo Institute of Technology — Surface states in Ti/Si and Bi/Si surfaces show non-Rashba-type spin splitting due to spin-orbit interaction (SOI). We construct effective tight-binding models on the triangular lattice for the surface states of B/Si and Ti/Si surfaces with spin-orbit interaction, respecting the crystal symmetries. Consequently, band structures and spin textures calculated from these models qualitatively agree with the experimental results. We find a new term in the Ti/Si model, which does not exist in Rashba systems. In addition, we numerically find bound states at the junction between two surface regions which have different signs of the SOI parameters in the Bi/Si system and in the Ti/Si system. Interestingly, the spin direction of the bound states is perpendicular to the crystal surface, whereas the spins of the bulk states are in-plane in the Bi/Si junction model. We compare the results with calculations using continuum models in two junction models. We also discuss physical realizations of such junctions.

V1.00075 A comparative analysis of deposition methods for nickel contacts onto CZT. JONATHAN LASSITER, SAMUEL UBA, MAXX JACKSON, SATILMIS BUDAK, Alabama A&M Univ, CLAUDIU MUNTELE, Cygnus Scientific Services, STEPHEN BABALOLA, TRENT MONTGOMERY, Alabama A&M Univ — Our studies have demonstrated quality of material surface, interface and interface contacts must be considered in fabrication of an optimally functioning radiation detector. Dangling bonds, poor surface processing, contamination of the surface and the quality of the contacts negatively contribute to detector energy resolution, and increased leakage currents. A Cadmium Zinc Telluride (CZT) crystal had nickel contacts deposited and characterized for these three cases: a) PVD, b) sputter cleaned plus PVD, and c) Ion Beam Assisted Deposition. In each of these cases the materials were characterized through use of current voltage (IV) measurements, Gamma Ray response and Scanning Electron Microscopy. The IV curves, resistivities, gamma responses, and surface features of the sample have been analyzed and compared. These results elucidate the influence of surface processing on quality of contacts and interfaces in optimizing the fabrication of a functioning radiation detector.

V1.00076 Characterization of deposited nickel contacts for CZT. JONATHAN LASSITER, SAMUEL UBA, MAXX JACKSON, SATILMIS BUDAK, Alabama A&M Univ, CLAUDIU MUNTELE, Cygnus Scientific Services, STEPHEN BABALOLA, TRENT MONTGOMERY, Alabama A&M Univ — Cadmium Zinc Telluride (CZT), a material used in room temperature radiation detectors, has many surface features which contribute to suboptimal functioning as a radiation detector. Dangling bonds, quality of polished surface, and the contacts are contributing factors to reduced detector energy resolution, and increased leakage currents. Nickel contacts were deposited, characterized and compared to the gold chloride electroless contact, and deposited gold. We took current voltage (IV) characteristics of CZT-based detectors and obtained their Gamma response spectra. These measurements enabled us to determine an optimal metal contact deposition process and material with improved detector performance as measured by leakage current and charge collection efficiency. The work functions of the contacts were chosen to work well with CZT. Quality surfaces, and contacts may serve as a means to improve the functioning of CZT in detector applications.

V1.00077 Effects of annealing conditions on the structural and electrical properties of a-oriented ZnO thin films. C.W. CHANG, Q.Y. CHEN, National Sun Yat-Sen University, Taiwan, P.V. WADEKAR, University of Liverpool, UK, H.C. HUANG, C.F. CHANG, H.H. KO, W.C. HSEIH, National Sun Yat-Sen University, Taiwan, C.H. LIAO, ROC Military Academy, Taiwan, H.W. SEO, University of Arkansas, Little Rock, Arkansas, USA, W.K. CHU, University of Houston, Houston, Texas, USA, H.H. LIAO, Enli Technology Inc., Taiwan — We studied the structural and optical properties of non-polar a-plane ZnO films grown on r-plane Al2O3 substrates by RF-spattering with different annealing conditions and oxygen partial pressure. Epitaxial relationships between the ZnO films and Al2O3 substrates was determined by ϕ-scan to be ZnO[0001]//[Al2O3][10-1], ZnO[1-100]//[Al2O3][1-101], and ZnO[1-210]//[Al2O3][1-210]. Photoluminescence spectra showed that band gap depended on annealing times, which is sensitive to intrinsic emission and surface defects in the a-plane ZnO. Hall Effect was measured on all samples by a PPMS system to find the relations amount annealing times, carrier concentrations and mobilities.

V1.00078 Enhancement of UV upconversion emission under near infrared excitation from NaYF4 nanocrystals doped with different lanthanide dopants. CAROLINA VALDES, MADHAB POKHREL, YUANBING MAO, None — Lanthanide doped nanocrystals have been attracted intensive attentions recently due to their interesting photoluminescence properties. Each lanthanide exhibits its own unique optical property, allowing for emission of light at different wavelengths. Consequently, different dopants can be used at varying concentrations to fine-tune desired emission wavelengths. The hexagonal crystal structure with low phonon energy and high photon efficiency has made NaYF4 a very efficient host for lanthanide dopants. Excitation of this material occurs at low energy in the near infrared (NIR) region and through energy transfer between dopants, emission at higher energy in visible regions is observed. A lot of work has been reported on upconversion to visible light; however, there is limited work on UV upconversion and enhancement of emission. Our current work focused on synthesizing a pure crystalline phase of NaYF4 and doping these nanocrystals with different lanthanides, including Tm, Nd and Gd using various concentrations. These nanocrystals have been systematically characterized by X-ray diffraction (XRD), scanning electron microscope (SEM), and photoluminescence (PL).
V1.00079 Transition Dynamics for Muonium in Silicon Germanium Alloys, GANGA JAYARATHNA, ROGER LICHTI, PATRICK MENGYAN, Texas Tech University, YASAR CELEBI, Istanbul University, BRITTANY BAKER, Texas Tech University — We use a longitudinal field muon spin relaxation technique to observe charge-state and site-change transitions of muonium in Si_{1-x}Ge_{x} samples (x = 0.45, 0.77, 0.81, 0.84, and 0.94). We primarily focus on modeling the temperature and field dependence of the relaxation data to investigate the donor and acceptor ionization energies, paramagnetic hyperfine frequencies and charge-state/site-change cycles. We compare donor/acceptor energies from relaxation data to those from asymmetric fits and verify assignments of specific transitions to each observed relaxation feature and access energy values not previously determined. Previous studies have shown that the T-site muonium acceptor level enters the valence band near x = 0.92. We find separate muonium acceptor states with muonium trapped at a Si within the tetrahedral Si_{1-x}Ge_{x} cage region and propose a new charge cycle that involves valence band resonant states.

V1.00080 Modeling of Transition Metal Color Centers in Diamond, NICK GORTHARD, University of Dayton Research Institute, DOUG DUDIS, LUKE BISSELL, Air Force Research Laboratory — Diamond stands out among single-photon sources due to an intrinsically large band gap, efficient electrical excitation, the ability to host bright optical centers, photo-stable emission, room-temperature operation, short excited state lifetimes, and the ability to host hundreds of different color centers. Currently, most of these centers are active in the optical spectrum, but a single-photon source in the IR would represent a significant advancement. In pursuit of this end, the effects of a number of different transition metal atoms upon the diamond lattice have been investigated via cluster calculations using the General Atomic Molecular and Electronic Structure System (GAMESS) code. The importance of cluster size and electron correlation effects is considered, and time-dependent DFT and multi-configurational SCF approaches are compared.

V1.00081 Vacancies and Temperature Effects on the Mechanical Properties of Silicene Nanoribbons, MA. RAYO CHAVEZ-CASTILLO, Instituto de Fisica BUAP, MARIO ALBERTO RODRIGUEZ-MEZA, Depto. de Fisica, ININ, LILIA MEZA-MONTES, Instituto de Fisica BUAP — The study of two-dimensional materials has been increasing. In the past few years a large variety of these kinds of materials has been studied, such as boron nitride, molybdenum disulfide, and silicene. The main potential application of silicene is found in electronic devices, nevertheless, other possible applications can be found. It is necessary to understand the mechanical properties of the material, because it can help us to determine the stability and useful lifetime thereof. We study vacancies and temperature effects on the Young’s Modulus (YM) of silicene nanoribbons (SNRs). To determine the mechanical properties of the nanoribbons, different structural parameters are introduced. We analyze the YM of three square shaped SNRs, whose lengths varies from 3 to 8 nm. Results at room temperature showed that the YM for the ribbon respectively increase with the length in both directions of chirality. On the other hand, for SNRs in the presence of defects (mono- and bi-vacancies) the YM depends on the defect position. It increases as the vacancy approaches the SNRs boundary. We observed that the higher the temperature, the lower the YM with and without vacancies. However, dependence on the length remains the same.

3 We acknowledge the financial support from CONACYT Grant. CB/2009/133251 and VIEP-BUAP.

V1.00082 Optical properties of TiO_{2-x} based Re-RAM switching devices under the effect of oxygen vacancies, MAAMAR BENKRAOUDA, NOUREDDINE AMRANE, UAE University — The tuning of the optical properties of TiO_{2-x} based materials can be achieved by varying the mole fraction. The accurate calculations of linear optical function (refractive index, reflectance, coefficient of absorption, and both imaginary and real dielectric function) were carried out. The dependence of these properties under the effect of the oxygen mole fraction were analyzed. Using controllable mole fraction, various intermediate resistance states are induced. Furthermore, the presence of oxygen vacancies which is linked to the on-state conduction and resistance switching mechanism in the optical properties is studied.

This work was funded by UPAR2013. UAE University

V1.00083 High Efficiency Alternative Current Driven Organic Light Emitting Device, JUNWEI XU, GREGORY SMITH, CHAOCHAO DUN, DAVID CARROLL, Center for Nanotechnology and Molecular Materials, Department of Physics, Wake Forest University, CENTER FOR NANO TECHNOLOGY AND MOLECULAR MATERIALS TEAM — In this work, we introduce the use of field-activated organic light emitter, coupled with a semiconducting gate electrode to create a novel, highly efficient lighting device. A layer of ZnO nanoparticles between the interface of an ITO contact and a PEDOT:PSS injection layer facilitates improved current control over the capacitative characteristics of the device. The advanced capacitive behavior of our devices gives rise to a barrier for carrier injection at low frequencies. Conversely, it promotes the generation of a field-induced polarization current in the active layer at high frequencies. The alternative current driven organic light emitting device obtains the power efficiency over 300 lm/W A at >500 cd/m2, which is the highest efficiency to date among high-lumiance organic light emitting devices, to the best of the authors' knowledge. We interpret these findings as the negative magnetoresistance induces the 'secondary' carriers that would contribute to light.

V1.00084 Technological Concepts for Enhancing Semiconductor Ion Implantation Sources, ADY HERSCHCOVITCH, Brookhaven National Laboratory — Two novel ideas for improving ion sources for the two energy extremes of ion implantation for semiconductor manufacturing are described. Since the invention of the transistor, semiconductor devices have been miniaturized. As semiconductors become smaller shallow implantation is desired and ion energy needed for implantation decreases, resulting space charge (intra-ion repulsion) effects, which reduced beam currents and production rates. To increase production rates, molecular ions are used. Carborane, which is the most stable molecular boron ion leaves unacceptable carbon residue on extraction grids. Special O2 elliptical cross section dissociator that injects O unto the grid can in-situ prevent carbon deposition without loading up power supplies. Pure gaseous processes are desired for enable rapid switch among ion species. For deep implantation and for avoiding the use of molecular phosphorous and arsenic can be generated by introducing phosphi in dissociators via 4PH = P4 + 6H2 in a pure gaseous process (same for arsenic AsH3). In the ion source molecular or high charge state phosphorous and arsenic can be generated. Concepts and devices will be presented.

1 Work supported by Contract No. DE-AC02-98CH1-886 with the US DOE and support from Russian Skolkovo Grant.

V1.00085 Effect of Boron doping on the structural, optical and electrical properties of ZNO nanoparticles produced by the Hydrothermal method, OZGUR OZTURK, Kastamonu University, SEVIM DEMIROZ SENOL, CADIR TERZIOGLU, Abant Izzet Baysal University — Effect of boron doping with B-11 at. % concentration on structural, optical and electrical properties of Zinc oxide nanopowder synthesized by Hydrothermal method has been reported. XRD results reveal that all B doped ZnO nanopolowders have single phase hexagonal structure without any impurity. Positions of main diffracted peaks of ZnO shifted slightly towards small 2θ angle and grain size decreases from 60.39 nm to 34.34 nm with an increase of B doping. SEM analyses indicate that the doping concentration of B affected the surface morphology of ZnO nanoparticles. Optical properties were examined by UV–Vis absorption/diffuse reflectance spectroscopy. The optical band gap of ZnO_{1-x}B_{x} nanoparticles increased from 3.27 to 3.75 eV with increase in B doping. The role of B doping on the transport properties was searched by temperature dependent Hall measurements in range of 180–350 K. The carrier concentration of the samples increased from 0.11x10^{14} to 4.08x10^{14} cm^{-2}, the Hall mobility decreased from 5.61 to 1.22 cm^{2}V^{-1}s^{-1} and electrical resistivity decreased from 10.89 x 10^{4} to 1.25 x 10^{4} ohm-cm with the increase of B doping at room temperature. The electrical resistivity was observed to decrease with both the increase in dopant concentration and the temperature.

2 This research partially supported by Abant Izzet Baysal University Scientific Research Projects Coordination Department under the Grant No. BAP-2013.03.02.609.
V1.00086 Growth and characterization of CH$_3$NH$_3$PbX$_3$ (X=I, Br) single crystals by solution method$^1$. SU JING, SANG LI, Nanjing University of Information Science & Technology, WANG DI, Nanjing University, LIN MIN, Nanjing University of Information Science & Technology — Solar energy conversion using solar cells requires materials that absorb in a broad spectral range, from visible to near infrared, to harvest most of the solar photons, as well as with the capability to convert effectively the incident light into free charges that produce electrical current and voltage. Organic-inorganic perovskite-structured hybrids CH$_3$NH$_3$PbX$_3$ (X = Cl, Br, I or a combination) exhibit good application potentials in the next generation solid-state solar cells. In order to improve the properties of CH$_3$NH$_3$PbX$_3$ based solar cell, the studies on the basic materials are of great necessities. In this work, we present the results of the successful growth of large single crystals of CH$_3$NH$_3$PbI$_3$ and CH$_3$NH$_3$PbBr$_3$ with size up to cm's using hydrochloric acid solution method. The solubilities of CH$_3$NH$_3$PbI$_3$ and CH$_3$NH$_3$PbBr$_3$ in hydrochloric acid were determined by weight method at the temperature range between 300-360K. X-ray diffractometry, scanning electron microscopy were used to study the structure and morphology, and the lattice parameters were estimated using Rietveld refinement method. The study of crystal nucleation, morphology and dimensions show that these are strongly dependent on the supercooling state occurred to the liquid during crystal growth, in which the (100) always exhibits the largest faces on the as-grown crystals. Optical properties of these single crystals were characterized by FT-IR, Raman, photoluminescence and cathode fluorescent spectroscopy.

$^1$National Natural Science Foundation of China (Grant Nos. 51472123) National Natural Science Foundation of China (Grant Nos. 51302268).

V1.00087 Large-scale Synthesis of monolayer MoSe$_2$ via Chemical Vapor Deposition. BYEONGGIL KANG, SKKU Advanced Institute of Nanotechnology(SAINT), Sungkyunkwan University, Suwon, 440-746, Korea, CHANGGU LEE, Department of Mechanical Engineering and SKKU Advanced Institute of Nanotechnology(SAINT), Sungkyunkwan University, Suwon, 440-746, Korea — Molybdenum diselenide (MoSe$_2$) has a direct band gap of 1.55eV for a monolayer utilized photodetector and optoelectronics. Recently, its synthesis methods have been briskly researched as a material for electronic devices from reason why it has similar properties with molybdenum disulfide (MoS$_2$). We present synthesis method for large-scale monolayer MoSe$_2$ through the chemical vapor deposition using Se and MoO$_3$ powder as a precursor. Raman and X-ray photoelectron microscopy confirmed the quality of synthesized MoSe$_2$. Moreover, electrical property was investigated with field effect transistor.

V1.00088 Synthesis of MoS$_2$ flakes by Electrical Arc Discharge of Molybdenum Wire and sulfidization of MoO$_3$ $^1$. VICENTE GONZALES, JOHN SANCHEZ, JESUS VELAZQUEZ-SALAZAR, MIGUEL YACAMAN, University of Texas at Santonio, UTSA DEPARTMENT OF PHYSICS AND ASTRONOMY COLLABORATION — Molybdenum Disulfide (MoS$_2$) is an important inorganic compound in industry due to its robustness, ability to withstand high temperatures, and physical properties. It acts a solid lubricant in oils as well as functioning as an excellent co-catalyst in desulfurization for uses in petroleum refining. In this project, we used electrical arc discharge to first synthesize Molybdenum Trioxide (MoO$_3$), then sulfidized the MoO$_3$ at 800°C to form our MoS$_2$ flakes. We then used a scanning transmission electron microscope (Hitachi 5500) to analyze the structure of our MoS$_2$ flakes and perform a chemical analysis. Electrical arc discharge is an innovative and favorable synthesis method due to the simplicity of the setup, and the large volume of particles produced. We varied parameters such as the voltage and amperage in our electrical arc discharge process to maximize the amount of MoS$_2$ flakes that we could produce. Characterization were done to ensure that the Molybdenum Disulfide was of correct structure (flakes) and to ensure that these flakes were of correct chemical composition. Future applications in industry of these particles directly depend on the ability for us to produce these particles in the correct shape (flakes) and the efficiency by which we can produce them.

$^1$This research was supported by the University of Texas at San Antonio and Dr. Miguel Jose-Yacaman.

V1.00089 Pin diodes based on n-ZnO/i-Al$_2$O$_3$/p-Si. Y.S. WANG, Q.Y. CHEN, W.Y. LIN, C.F. CHANG, W.C. HSIEH, H.C. HUANG, L.W. TU, National Sun Yat-Sen University, P.V. WADEKAR, W.K. CHU, University of Houston, H.H. LIAO, Enli Technology Inc., C.H. LIAO, ROC Military Academy — We focus on the pin-diodes fabricated with n-type ZnO thin films deposited on p-type silicon by RF-sputtering, using very-thin Al$_2$O$_3$ as an insulation layer. By annealing at various temperatures, the domain sizes of the ZnO films would vary accordingly as viewed under scanning electron microscope (SEM). With larger grains, the leakage current was lowered, suggesting that grain boundaries are responsible for the leakage. However, the ZnO films largely remain textured along the c-axis as judged by their clear ZnO (0002) peaks of the XRD theta-2theta scans that are related to the phi-scans of off-axis planes. Furthermore, the XRD data also showed the structural changes of the insulation layer after annealing above certain temperature. For the samples annealed at 750°C and 850°C, the I-V curves showed characteristic pin diodes behaviors. The photoconductivity was measured as a function of intensity of a pulsed laser beam of wavelengths 1064nm, 532nm, 266nm. The photoelectronic IV responses will be discussed in regards to the electronic tunneling structures of the pin junctions and their dependence on the fabrication processes.

V1.00090 Calculation of effective magnetic field of phonon dynamics in the Born Oppenheimer approximation. BANGGUO XIONG, LIFA ZHANG, QIAN NIU, Univ of Texas, Austin — Phonon dynamics with an effective magnetic field can lead to phonon hall effect. We study the effect magnetic field on phonon dynamics due to the coupling to electrons in the Born Oppenheimer approximation. Symmetry properties of the effective magnetic field are discussed in crystals. Two methods to calculate the effective magnetic field are brought up, with model calculations on the honey comb lattice. The application of the methods can be directly applied in first principle calculation.

V1.00091 Rigid Unit Modes; their energy and temperature dependence with aluminium phosphate. ADAM BERLIE$^1$, The Bragg Institute. ANSTO, YUN LIU, Australian National University, DEHONG YU, GORDEN KEARLEY, The Bragg Institute, ANSTO, CHRIS LING, University of Sydney, RAY WITHERS, Australian National University — One of the problems within crystallography is the concept of the average structure where due to dynamical translations or librations the structure is not truly static. This type of behaviour is common within polyhedral based compounds such as APO$_4$ where, in this case, the rigid tetrahedra can move or tilt with respect to each other as a consequence of the instability of the 180° Al-O-P bond. We explore the energy and temperature dependence of these modes using inelastic neutron scattering and heat capacity measurements as well as using computational modelling to assign the observed behaviour to these rigid unit modes.

$^1$Also affiliated to the Australian National University

V1.00092 Phase transition of MoS$_2$ using laser irradiation$^1$. JAE SU KIM, JUNSUK KIM, JINHEE LEE, YOUNGJO JIN, TAESOO KIM, YOUNG HEE LEE, SEONG CHU LIM, Institute for Basic Science, Center for Infragated Nanostucture physics, Department of Energy Science, Sungkyunkwan University, Suwon 440-746 — The multi-layer 2H-MoS$_2$ flakes are transferred to SiO$_2$/Si substrate by mechanical exfoliation method and transformed into 1T-MoS$_2$ by Li intercalation. The phase change by Li doping leads semiconducting 2H-MoS$_2$ to metallic 1T-MoS$_2$ that is confirmed by Raman and PL spectroscopy and I-V measurements. Then, 1T-MoS$_2$ flakes are locally heated to recover to 2H-MoS$_2$ using 532nm-laser beam that can increase the irradiated power up to 10 mW. The characteristics of thermally patterned 2H-MoS$_2$ are investigated by confocal PL and photo-current and I-V measurements. Also, the junction characteristics of 2H- and 1T-MoS$_2$ flakes will be discussed further in this presentation.

$^1$HBS-R011-D1
other two-dimensional transition metal dichalcogenides. Monolayer T-phase TaS
The combination of inherent spin polarization with a semiconducting nature distinguishes the monolayer fundamentally from the bulk compound as well as from strongly localized, which explains the formation of significant magnetic moments. The spin polarization transforms the material into a magnetic semiconductor.

1 Research reported was supported by the King Abdullah University of Science and Technology (KAUST). Computational resources have been provided by KAUST IT.

V1.00094 Spin polarization driven by a charge-density wave in monolayer 1T-TaS
2 QINGYUN ZHANG, LI-YONG GAN, YINGCHUN CHENG, UDO SCHWINGENSCHLOGL, Physical Sciences and Engineering, King Abdullah University of Science and Technology, COMPUTATIONAL PHYSICS AND MATERIALS SCIENCE TEAM — Using first-principles calculations, we investigate the electronic and vibra-
tional properties of monolayer T-phase TaS
2. Our results demonstrate that the formation of a CDW is energetically favorable at low temperature, similar to bulk 1T-TaS
2. Electron-phonon coupling is found to be essential for the lattice reconstruction. In the CDW phase the electronic states near the Fermi level are strongly localized, which explains the formation of significant magnetic moments. The spin polarization transforms the material into a magnetic semiconductor. The combination of inherent spin polarization with a semiconducting nature distinguishes the monolayer fundamentally from the bulk compound as well as from other two-dimensional transition metal dichalcogenides. Monolayer T-phase TaS
2 therefore has the potential to enable two-dimensional spintronics.

V1.00095 Giant valley drifts in uniaxially strained monolayer MoS
2 QINGYUN ZHANG, YINGCHUN CHENG, LI-YONG GAN, UDO SCHWINGENSCHLOGL, Physical Sciences and Engineering, King Abdullah University of Science and Technology, COMPUTATIONAL PHYSICS AND MATERIALS SCIENCE TEAM — Using first-principles calculations, we study the electronic structure of monolayer MoS
2 under uniaxial strain. We show that the energy valleys drift far off the corners of the Brillouin zone (K points), about 12 times the amount observed in graphene. Therefore, it is essential to take this effect into consideration for a correct identification of the band gap. The system remains a direct band gap semiconductor up to 4% uniaxial strain, while the size of the band gap decreases from 1.73 to 1.54 eV. We also demonstrate that the splitting of the valence bands due to inversion symmetry breaking and spin-orbit coupling is not sensitive to strain.

1 Computational resources have been provided by KAUST IT. This work is supported by a KAUST CRG grant.

V1.00096 Electronic structure and bonding in fluorapatites crystals: A
10(PO
6)F
2 (A=Ba, Ca, Pb and Sr)
1. CLAUDIA LOYOLA, Universidad Andres Bello, EDUARDO MENENDEZ-PROUPIN, Universidad de Chile, KRISHNA RAJAN, Iowa State University — In this work we report a computational study of electronic properties of fluorapatites (A
10(PO
6)F
2 with A=Ba, Ca, Pb and Sr) using ab initio calculation. We employed Density Functional Theory using a Plane Wave basis set and pseudopotentials to obtain the band structure, total and partial density of states, electronic charge density and electron localization function. We obtain that Ba-, Ca- and Sr-fluorapatite have a wide band gap in the range of ~5.4 eV, while the Pb-fluorapatites have a band gap of ~3.8 eV and different band structure compared with the rest of fluorapatites. The electron charge density and the electron localization function reveal covalent character of the bond between the oxygen and phosphorus in the tetrahedral substructure for all fluorapatites. We analyze the results and possible causes behind the differences in the electronic structure of these fluorapatites.

3 This work is supported by FONDECYT Insercion a la academia 2014

V1.00097 Excitonic valley polarization and coherence in atomically thin MoS
2 DONG HAK KIM, DAEYOUNG LIM, Department of Applied Physics, KyungHee University — We study the excitonic valley polarization and coherence in few-layer MoS
2 by circular- and linear-polarization-resolved photoluminescence. The valley polarization is largest in monolayer MoS
2 and decreases with the increase in the number of layers or temperature. Contrary to the valley polarization, the linear polarization is negligibly small in monolayer MoS
2 and increases with the increase in the number of layers or temperature. The valley decoherence in monolayer MoS
2 is at least an order of magnitude faster than the valley depolarization or exciton decay at low temperature, implying it has a pure dephasing origin. The valley coherence is steady against the increase in temperature or photoexcitation intensity, excluding phonon or carrier-carrier scattering from the dominant decoherence process. The temperature dependence of the valley polarization can be explained by the center of mass momentum dependent long range electron-hole exchange interaction, whereas that of the linear polarization may be due to relatively temperature-insensitive valley decoherence.

V1.00098 Photoluminescence Saturation and Exciton Decay Dynamics in Transition Metal Dichalcogenide Monolayers DONG HAK KIM, MIN JU SHIN, DAEYOUNG LIM, Department of Applied Physics, KyungHee University — We study the photoluminescence saturation and exciton decay dynamics in monolayer transition transition-metal dichalcogenides (TMDs). Monolayer MoSe
2 shows a PL saturation at a very low excitation intensity, more than two orders of magnitude lower than monolayer MoS
2. Transient reflection spectroscopy shows that nonlinear exciton-exciton annihilation is the dominant exciton decay mechanism in monolayer MoSe
2, in contrast to the exciton decay in monolayer MoS
2. Furthermore, we measure exciton lifetime >125 ps for monolayer MoSe
2 much longer than the several-ps exciton lifetime in MoS
2. We find that that the difference in their exciton lifetime can explain both the dramatically different exciton decay mechanism and PL saturation behavior of MoSe
2 and MoS
2 monolayers.

V1.00099 Carrier recombination in m-plane InN thin film WEI-SHENG CHEN, WEN-JING ZHAO, J.-Y. ZENG, DER-JUN JANG, LI-WEI TU, Department of Physics, Natl Sun Yat Sen Univ — Nonpolar m-plane InN thin films grown on LiAlO
2 substrates by plasma-assisted molecular beam epitaxy have been studied using time-resolved photoluminescence (TRPL) upconversion technique. The carrier densities of 1.97 x 10
19 cm
−3 and mobility of 420 cm
2/Vs were measured by van der Pauw–Hall geometry. The carrier temperature curves at different temperatures, derived from the time-resolved photoluminescence (TRPL) spectra at different time delay, indicate that hot carriers lost most of their excess energy by releasing LO-phonons. The effective LO phonon emission times increase with the lattice temperature, from 53 to 197 fs for 35 and 250 K, respectively. We found that the effective LO emission time of m-plane InN is smaller than that of c-plane InN. The recombination rates were derived from the TRPL measured at the energy closed to the bandgap energy. Similar to c-plane InN, the Shockley-Read-Hall recombination coefficient of m-plane InN shows a 3-fold increase for temperature increasing from 35 to 250 K. The Auger recombination was less effective as compared to that in c-plane InN.
V1.00100 Optical properties of non-polar ZnO using Terahertz time domain spectroscopy, MING-GEN CHUANG, SHU-YU YAO, DER-JUN JANG, QUARK Y. CHEN, Department of Physics, Natl Sun Yat Sen Univ — The m-plane ZnO thin films grown on m-plane sapphire substrates by atomic layer deposition were investigated with the terahertz time domain spectroscopy. The terahertz emission was generated by exciting a LT-GaAs antenna with laser pulses from Ti:sapphire at the wavelength of 800 nm. One of the ZnO samples was thermally annealed with a rapid thermal annealing system with O2 at a temperature of 700 °C. The other ZnO sample was studied without annealing. The refractive indices and extinction coefficients of m-plane ZnO along c- and a-axis were derived and found significant different. For both samples, the extinction coefficient and refractive index decreases monotonically with frequency. While the mobility along a-axis was found about the same after annealing, the mobility along c-axis has been improved significantly due to annealing. The annealing treatment has shown its impact on reducing the carrier concentration of 4.5 × 10^{19} to 3.5 × 10^{18} cm^{-3} for unannealed and annealed ZnO, respectively.

V1.00101 Carrier localization in green emitting InGaN/GaN multiquantum well structure, CHOU-JEN CHENG, Department of Physics, Natl Kaohsiung Normal Univ, ANTARYAMI MOHANTA, DER-JUN JANG, Department of Physics, Natl Sun Yat Sen Univ, MENG-EN LEE, Department of Physics, Natl Kaohsiung Normal Univ — Green emitting InGaN/GaN multiquantum well sample is investigated using photoluminescence (PL) and time-resolved photoluminescence (TRPL) spectroscopy. Carrier localization of energy ∼ 12 meV due to inhomogeneous distribution of In in the InGaN quantum well (QW) layer is observed. The temperature dependence of PL peak energy exhibits S-shape phenomenon and is controversially discussed. We propose that localization is connected to the double-well behavior with increase in temperature. The temperature dependence of radiative life time (τr) shows τr ∼ T^{1/2} dependence with temperature above 200 K which confirms the significant effect of carrier localization at room temperature. Transmission electron microscopy (TEM) study reveals the absence of In-rich regions known for strong carrier localization in the InGaN QW layer which is consistent with the results of PL and TRPL.

V1.00102 Hot carrier cooling in Si-doped InN, JHENG-YU WU, CHIA-SHIA WANG, ANTARYAMI MOHANTA, MING-SUNG WANG, DER-JUN JANG, LI-WEI TU, Department of Physics, Natl Sun Yat Sen Univ — Temperature and excitation power dependent time-integrated photoluminescence of Si doped InN thin films are investigated. Photoluminescence (PL) spectra at low temperatures are described by single emission peak ensued due to free-to-bound? recombination; whereas PL spectra at higher temperatures above 150K are characterized by both band-to-band- and free-to-bound transition. Carrier dynamics of Si doped InN thin films is studied using pump-probe reflection spectroscopy at room temperature. The hot electron cooling process is well described by electron-electron scattering. The dependence of the hot electron cooling rate on total electron density shows sublinear to linear behavior with increase of background electron density. The variation of the carrier recombination lifetime with total electron density implicates the dominance of the defect-related nonradiative recombination channel over other recombination processes.

V1.00103 Comparison between stamping method and one-by-one dry-transfer method for the fabrication of h-BN sandwiched graphene FET in the quantum Hall regime, JEONGMIN PARK, HAEYONG KANG, JOONGGYU KIM, JOEONG-GYUN KIM, YOOHOO YUN, NAHEE PARK, KIEU TRUONG, YORKACK LEE, DONGSUB CHUNG, DONGGYUN KIM, CINAP, IBS, DOES, SKKU, HOYEOL YUN, SANGWOOK LEE, Konkuk University, YOUNGhee LEE, DONGSEOOK SUHN, IBS, DOES, SKKU — We have fabricated a dual-gate graphene field-effect-transistor (FET) for the study of integer Quantum Hall Effect in terms of its edge-state transport. The graphene was encapsulated by hexagonal boron-nitride (h-BN) flakes without any interlayer residues using the ‘stamping-transfer’ method, which is critical for the observation of graphene’s intrinsic transport properties. Using the polypropylene carbonate (PPC) and Polydimethylsiloxane (PDMS), initially top h-BN flake is picked up and graphene flake is picked up by van der Waals’ force between graphene and top h-BN. These two layers are dropped down on the bottom h-BN flake to complete the encapsulated formation. To make the source/drain (S/D) and top-gate electrodes, whole area of graphene is not covered by top h-BN flake. The open areas of graphene, located at both ends, are covered by S/D metal electrodes, which made whole graphene channel region sandwiched by top and bottom hBN. We compared this method with the old one which put the two-dimensional flakes one by one using ‘dry-transfer’ method, and found out a significant difference in the device quality especially at low temperatures and high magnetic fields in the quantum Hall regime.

V1.00104 Exact solutions of fractional Chern insulators: interacting particles in the Hofstadter model at finite size, THOMAS SCARRIDI, STEVEN SIMON, University of Oxford — We show that all the bands of the Hofstadter model on the torus have an exactly flat dispersion and Berry curvature when a special system size is chosen. This result holds for any hopping and Chern number. Our analysis therefore provides a simple rule for choosing a particularly advantageous system size when designing a Hofstadter system whose size is controllable, like a qubit lattice or an optical cavity array. The density operators projected onto the flat bands obey exactly the Girvin-MacDonald-Platzman algebra, like for Landau levels in the continuum or an optical cavity array. The density operators projected onto the flat bands obey exactly the Girvin-MacDonald-Platzman algebra, like for Landau levels in the continuum or an optical cavity array.

V1.00105 Nature of Quasi-electrons and the Continuum of Neutral Bulk Excitations in Laughlin Quantum Hall Fluids, BO YANG, Institute of High Performance Computing, F.D.M. HALDANE, Princeton University — We construct model wavefunctions for a family of single-quasielectron states supported by the ν = 1/3 fractional quantum Hall (FQH) fluid. The charge e∗ = e/3 quasielectron state is identified as a composite of a charge-2e∗ quasiparticle and a −e∗ quasihole, orbiting around their common center of charge with relative angular momentum nh > 0, and corresponds precisely to the “composite fermion” construction based on a filled n = 0 Landau level plus an extra particle in level n > 0. An effective three-body model (one 2e∗ quasiparticle and two −e∗ quasiholes) is introduced to capture the essential physics of the neutral bulk excitations. We also explore different ways of representing many-body wavefunctions in fractional quantum Hall fluids, including the holomorphic wavefunctions, Jack polynomial formalisms and the diagrammatic representations. (Bo Yang and F.D.M. Haldane, PRL 112, 206804).

V1.00106 STRONGLY CORRELATED SYSTEMS INCLUDING QUANTUM FLUIDS AND SOLIDS —

V1.00107 Coexistence and competition of on-site and intersite Coulomb interactions in Mott-molecular-dimers, ALBERTO ARRUDA, RAFFAEL JULIANO, THIAGO WERLANG, LUIS CRACO, Instituto de Física - Universidade Federal de Mato Grosso — Recent findings of Mott-Hubbard physics in ultracold atoms trapped in periodic potentials have reinvigorated the search for quantum simulators of fermionic and bosonic Hubbard-like models. With this in mind, we performed a systematic study of a two-site realization of the Hubbard model, i.e. in a regime where this model can exactly treated. Particularly, we reveal the interplay between on-site (U) and intersite (V) Coulomb interactions in the extended two-site Hubbard model. Due to its atomic-like form quantum correlations intrinsic to Mott-molecular-dimers are exactly computed. Our results for physical quantities such as double occupancy and specific heat are consistent with those obtained for the one-band Hubbard model, suggesting that a two-site Hubbard model is able to capture the essential thermodynamic properties of strongly interacting electron systems. It is shown that intersite Coulomb interactions promotes the formation of doublons, which compete with the spin-singlet state induced by the on-site Coulomb repulsion. Our results are expected to be relevant for understanding electronic and thermodynamical properties of interacting electrons in strongly coupled magnetic atoms.
V1.00108 ABSTRACT MOVED TO G22.00015 –

V1.001109 Carrier dynamics in EuTiO$_3$ films probed by femtosecond pump-probe spectroscopy$^1$

ZHONGGUO LI, Harbin Institute of Technology, RUN ZHAO, WEIWEI LI, Soochow University, HAIYAN WANG, Texas A&M University, HAO YANG, Soochow University, XUERU ZHANG, YUXIAO WANG, TAI-HUEI WEI, YING-LIN SONG, Harbin Institute of Technology — Recently, perovskite oxide EuTiO$_3$ has attracted considerable attention due to its intriguing multiferroic properties. To gain a deeper understanding of its fascinating properties, it is essential to characterize the competing interactions between charge, lattice, spin, and orbital parameters. Here we present optical studies of the ultrafast carrier dynamics in EuTiO$_3$ films grown on SrTiO$_3$ substrates by probing photo-induced transient absorption (TA) in the weak excitation limit. All the signals were measured at room temperature. The transient curve of EuTiO$_3$ exhibits a fast rise after photo excitation (approximately 2 ps) and a long decay component with time constant of several nanoseconds, which are attributed to carrier-phonon coupling and carrier recombination respectively. The absorption change of EuTiO$_3$ near zero temporal delay is found to be quite different from the SrTiO$_3$ substrates, implying carrier-phonon interactions differ distinctively between these two materials. Our results could be helpful to understand the microscopic interactions in perovskite oxide.

$^1$The authors acknowledge the support of the National Natural Science Foundation of China.

V1.001110 Investigation of 2-dimensional electron liquid at the interface of La(1-x)Al(1+x)O$_3$/SrTiO$_3$ $^1$

MING SHIU TSAI, WEI FAN HSIU, HAO YU CHEN, WEI LI LEE, Academia Sinica, Taiwan, ACADEMIA SINICA. TAIWAN TEAM — The emergence of two dimensional electron liquid (2DEL) at the interface between two insulating oxides of lanthanum aluminate (LaAlO$_3$) and strontium titanate (SrTiO$_3$) shows unusual superconductivity and magnetism compared to conventional semiconductor-based 2DEG systems. One important issue resides on the influence of the stoichiometry to the 2DEL. Here, we report the structural analysis and magneto-transport results on a series of La(1-x)Al(1+x)O$_3$/SrTiO$_3$ with different x grown by oxide molecular beam epitaxy (OMBE) with in-situ growth monitoring using reflection high electron energy diffraction (RHEED). Detailed low temperature magneto-transport data and its correlation to the stoichiometry and film strain will be presented and discussed.

V1.001111 Double Charge Ordering States and Spin Ordering State Observed in a RAF$_2$O$_4$ System$^1$

1. FEI SUN, RUI WANG, Institute of Physics, Chinese Academy of Sciences, CYNTHIA AKU-LEH, IScences, Ann Arbor, Michigan, USA, HUAIXIN YANG, Institute of Physics, Chinese Academy of Sciences, RUI HE, Department of Physics, University of Northern Iowa, Cedar Falls, USA, JIMIN ZHAO, Institute of Physics, Chinese Academy of Sciences — Charge, spin, and lattice degrees of orderings are of great interest in the layered quantum material RFe$_2$O$_4$ (R = Y, Er, Yb, Tm, and Lu) system. Recently many unique properties have been found using various experimental methods. However so far the nature of the two-dimensional (2D) charge ordering (CO) state is not clear and no observation of its fine structure in energy has been reported. Here we report unambiguous observation of double 2D CO states at relatively high temperature in a polycrystalline Er$_{1.4}$Y$_{0.6}$Fe$_2$O$_4$ using Raman scattering. The energy gaps between the 3D and the double 2D states are 170 meV (41.2 THz) and 193 meV (46.6 THz), respectively. We also observed a spin ordering (SO) state at below 210 K with characteristic energy of 45 meV (10.7 THz). Our investigation experimentally identified new fine structures of quantum orders in the system, which also extends the capability of optical methods in investigating other layered quantum materials.

$^1$National Basic Research Program of China (2012CB821402), National Natural Science Foundation of China (11274372)

V1.001112 Ultrafast dynamics of titanate octahedra tilting modes in a THz laser pulse

MINGQIANG GU, JAMES M. RONDINELLI, Northwestern University — Using first-principles calculation, the electronic band structure and electric dipole moment for orthorhombic titanate are examined. To explore the energy dissipation after pulse excitation, the light-lattice coupling is treated with the mode oscillator model. By solving the equation of motion, we investigate the dynamics of the tilting modes. The evolution of the optical transition matrix elements as functions of different octahedra tilting modes and mode amplitudes are also evaluated, which provides theoretical base for the future experiments.

V1.001113 Correlating valence state, site preference and co-substitution to the magnetoelastic properties of cobalt ferrite$^1$

1. CAJETAN NLEBEDIM$^2$, Ames Laboratory, U.S. Department of Energy, DAVID JILES$^3$, Department of Electrical and Computer Engineering, Iowa State University — Understanding how to influence the physics of magnetism, especially the relationship between magnetic susceptibility and stress, can be very useful in designing non-contact stress and torque sensors using magnetoelastic materials. This is particularly important considering that materials rarely occur in states desirable for direct applications. In this work we show that the magnetoelastic properties of cobalt ferrite are strongly dependent on the valence states and site preferences of substituted cations. It was found that co-substitution of magnetic and non-magnetic cations, is key to achieving simultaneous improvement in magnetostrection amplitude and strain sensitivity to applied magnetic field. Nevertheless, Curie temperature decreased, irrespective of the valence state, site preference or co-substitution. This presentation will show why tetravalent Ge resulted in superior magnetostrictive properties compared to other tetravalent, trivalent and divalent cations substituted into the crystal lattice of cobalt ferrite.

$^1$This work was supported by the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. The research was performed at Ames Laboratory, operated for the USDOE by Iowa State University (contract #DE-AC02-07CH11358).

$^2$Also affiliated to the Department of Electrical and Computer Engineering, Iowa State University

$^3$Also affiliated to Ames Laboratory, U.S. Department of Energy

V1.001114 Quantum Monte Carlo calculations of structural and electronic properties in the correlated oxide NiO$^1$

1. CHANDRIMA MITRA, JARON KROGEL, JUAN A. SANTANA PALACIO, FERNANDO A. REBOREDO, Oak Ridge National Laboratory — Transition metal oxides pose difficulties for condensed matter theories due to the presence of strong electronic correlations. The complex interplay among correlation and exchange in d subshells, crystal field effects, p-d hybridization and charge transfer gives rise to a rich variety of structural and electronic phases. NiO is one such challenging d system, where conventional band theory fails. Compared to the experimental value, the cohesive energy of bulk NiO computed within DFT-LDA differs by almost a factor of 18 %. Band gap computed within standard local or semi-local functionals are off by a factor of 80 %. A quasi-particle correction like the G$^W$ approach cannot correct the band gap and is still far too low. In this work we adopt the Diffusion Monte Carlo (DMC) approach to study the structural and electronic properties of NiO. Trial wave-functions were self consistently generated in a Slater-Jastrow form. To test pseudopotentials used, DMC calculations were done on atomic Ni and O and their computed ionization potentials showed excellent agreement with experiments (within 0.04%). The equilibrium bond length and binding energy of the NiO dimer were also computed that were 0.001% and 0.03%, respectively, from experimental values. DMC calculations of equation of state and band gap of bulk NiO will be presented.

$^1$We gratefully acknowledge support from U.S Department of Energy, Basic Energy Sciences, Materials Science and Engineering Division.
Investigation of the Band Gap in Co$_3$O$_4$. MARK SHOLTE, CHUNGWEI LIN, KRISTY KORMONDY, University of Texas System, TIMOTHY NUNELEY, New Mexico State University, AGRAM POSADAS, University of Texas System, STEFAN ZOLLNER, New Mexico State University, ALEXANDER DEMKOV, University of Texas System — Co$_3$O$_4$ is a strongly correlated oxide with a spinel structure and G-type antiferromagnetic order at temperatures below 40 K. It is a widely studied material owing to its applications in gas sensing, spintronics, batteries, and catalysis. The strong correlation and magnetism make it a difficult material to model from first principles. Density functional theory calculations require the use of a Hubbard U to correctly model its magnetic behavior. The band gap is sensitive to the choice of U allowing one to tailor the gap to a wide range of values. This often provides a phenomenological approach to determining U, but in the case of Co$_3$O$_4$ there is no experimental consensus on the actual value of the band gap. We utilize an alternate approach by matching the theoretical valence band structure to the actual valence band data obtained via x-ray photoemission spectroscopy. This generated set of U values is used to compute an absorption spectrum, which is in good agreement with ellipsometry results.

Electronic Structures of the Charge Density Wave System RTe$_2$ (R=Ce, Pr) investigated by ARPES. JEONGSOO KANG, EUNSOOK LEE, D.H. KIM, The Catholic University of Korea, JONATHAN DENLINGER, Lawrence Berkeley National Laboratory, B.H. MIN, Y.S. KWON, DGIST, JUNWON KIM, KYOO KIM, B.I. MIN, Pohang University of Science and Technology — The rare-earth (R)-based RTe$_2$ compounds are known as the charge-density-wave (CDW) systems. In this work, we have investigated the electronic structures of RTe$_2$ (R=Ce, Pr) by employing angle-resolved photoemission spectroscopy (ARPES) experiment and the first-principles band structure calculations. The overall shapes and sizes of the measured Fermi surfaces (FSs) of RTe$_2$ are found to be similar to those of the calculated FSs for the undistorted structures. The metallic states crossing the Fermi level (E_F) are observed in ARPES even in the CDW state, indicating that the metallic states remain under the CDW transition with the remnant ungapped FSs. R 4f/ PES spectra exhibit that the 4f hybridization peak (4f$^n$$e_{5/2}$) in R=Pr is located deeper than in R=Ce, resulting in the much weaker 4f spectral intensity near E_F in R=Pr. The shadow bands and the corresponding very weak FSs are found to arise from the band folding due to the interaction of Te(1) layers with R-Te(2) layers and the CDW-induced FS reconstruction. The E_F-crossing states are stronger with the linear vertical polarization than with the linear horizontal polarization. The photon-energy maps in ARPES demonstrate the two-dimensional character of the near-E_F states.

Circular dichroism of chiral photon crystal liquid layers with enclosed defect inside. ASHOT GEVORYAN, Yerevan State University, Armenia, ARMEN KOCHARIAN, California State University, Los Angeles, GAGIK VARDANYAN, NNN Inc., Granada Hills, CA — The photonic crystals of artificial and self-organizing structures with spatial periodic changes in dielectric and magnetic properties have attracted considerable interest recently due to unusual physical properties and wide practical applications. The chiral periodic structure in the scale of optical wavelength gives rise to strong and characteristic circular dichroism responses at visible wavelengths. Here we investigate photonic density, circular dichroism and peculiarities of absorption and emission spectra at various eigen polarizations in multilayered one-dimensional chiral soft matter with two layers of CLCs and an isotropic defect layer inside. The circular dichroism is defined by differences in light energy absorption A(l, l') in the system (l, l') are the reflection and transmission coefficients, respectively) and A(l, l') are the light absorptions, if the incident light has left and right circular polarizations, respectively. This problem can be solved by the modified Ambartsumian's layer addition method. The influence of absorption and gain on the circular dichroism, absorption and emission spectra is established in cholesteric liquid crystal (CLC) cell with an isotropic defect layer inside.

Fermion-sign-free Majorana-quantum-Monte-Carlo studies of quantum critical phenomena of Dirac fermions in two dimensions. ZIXIANG LI, YIFAN JIANG, HONG YAO, Institute for Advanced Study, Tsinghua University, Beijing, 100084, China — Quantum critical phenomena may be qualitatively different when massless Dirac fermions are present at criticality. Using our recently-discovered fermion-sign-free Majorana quantum Monte Carlo (MQMC) method, we investigate the quantum critical phenomena of spinless Dirac fermions on the honeycomb lattice having N_s = 2L^2 sites with largest L = 24, at their charge-density-wave (CDW) phase transitions. By finite-size scaling, we accurately obtain critical exponents of this so-called Gross-Neveu chiral-ising universality class of two (two-component) Dirac fermions in 2+1D: $\eta = 0.45(2)$, $\nu = 0.77(3)$, and $\beta = 0.60(3)$, which are qualitatively different from the mean-field results but are reasonably close to the ones obtained from renormalization group calculations.

Beyond structural bottleneck: the nature of nonthermal optically induced ultrafast phase switching in V$_2$O$_3$. ZHENHENG TAO, JILA, Univ of Colorado - Boulder, TZONG-RU T. HAN, FARAN ZHOU, Department of Physics and Astronomy, Michigan State University, DAVID TORGES, TONY WANG, NELSON SEPULEVIDA, Department of Material Science Engineering, Michigan State University, CHONG-YU RUAN TEAM, NELSON SEPULEVIDA TEAM — Ultrafast manipulation of the electronic states of strongly correlated electron crystal near room temperature, such as V$_2$O$_3$, encompasses enormous opportunities in high-speed electronics and photonics. However, its strong coupling to the first-order structural phase transition presents a bottleneck effect, which leads to cracking and various instabilities. Here, we show that repetitive ps or even sub-ps phase switching can be initiated by using mid-infrared photons where the rapid transformation is driven by instantaneous shift of chemical potential, rather than lattice or electronic heating. Using fs electron crystallography, we establish the cooperative doping-induced multi-step atomic pathway, which leads to a metal-insulator transition at a fractional energy dose.

First-principles study of Sr$_2$Ir$_{1-x}$Rh$_x$O$_4$: charge transfer, spin-orbit coupling change, and the metal-insulator transition. JAE-HOON SIM, Department of Physics, KAIST, Daejeon 305-701, Korea, HEUNG-SIK KIM, Department of Physics, University of Toronto, Toronto, Ontario MSS 1AT, Canada, MYUNG JOON HAN, Department of Physics, KAIST, Daejeon 305-701, Korea — Using first-principles density functional theory (DFT) calculations, we investigated the electronic structure of Rh-doped iridate Sr$_2$Ir$_{1-x}$Rh$_x$O$_4$ for which the doping (x) dependent metal-insulator transition (MIT) has been reported experimentally and the controversial discussion developed regarding the origin of this transition. Our DFT+U calculation shows that the value of $\langle L,S \rangle$ remains largely intact over the entire doping range considered here for $\langle x = 0.0, 0.125, 0.25, 0.50, 0.75, \text{ and } 1.0 \rangle$ in good agreement with the branching ratio measured by x-ray absorption spectroscopy. Also contrary to a previous picture to explain MIT based on the charge transfer between the transition-metal sites, our calculation clearly shows that those sites remain basically isoelectronic while the impurity bands of predominantly rhodium character are introduced near the Fermi level. As the doping increases, this impurity band overlaps with lower Hubbard band of iridium, leading to metal-insulator transition. The results will be discussed with comparison to the case of Ru doping.

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2 Computational resources were supported by The National Institute of Supercomputing and Networking/Korea Institute of Science and Technology Information with supercomputing resources including technical support (Grant No. KSC-2013-C2-23).
V1.00121 Evidence of a quantum critical point in Ce$_{1-x}$Yb$_x$CoIn$_5$ alloys at high Yb doping$^1$. Y.P. SINGH, D.J. HANEY, X.Y. HUANG, Kent State University, B.D. WHITE, M.B. MAPLE, University of California, San Diego, M. DZERO, C.C. ALMASAN, Kent State University — We performed this study on single crystals of Ce$_{1-x}$Yb$_x$CoIn$_5$ alloys with the motivation to further explore some of the previously reported unusual behaviors such as robust coherence and superconductivity, non-Fermi liquid (NFL) behavior, and the possibility of quantum criticality in higher Yb doping. Our specific heat and electronic magneto-transport measurements on the alloy with $x = 0.75$ nominal doping down to temperatures ($T$) as low as 0.5 K and magnetic fields ($H$) as high as 14 T. Our analysis of both specific heat and resistivity data unveils the presence of a crossover from NFL behavior at high temperatures to Fermi-liquid (FL) behavior at lower temperatures. Our analysis also indicates that the origin of the NFL behavior is a result of quantum fluctuations of unknown origin. The H-T phase diagram extracted from resistivity and specific heat shows that the crossover from NFL to FL behavior at zero temperature occurs at $H = 0$. This implies that the alloy with $x = 0.75$ Yb concentration is quantum critical, i.e., $\chi_c = 0.75$. This result of zero field quantum critical point at $x = 0.75$ is also confirmed from our analysis of magneto-resistance data.

$^1$This work was supported by the National Science Foundation (grant NSF DMR-1006606) and Ohio Board of Regents (grant OBR-RIP-220573) at KSU, and by the U.S. Department of Energy (grant DE-FG02-04ER46105) at UCSD.

V1.00122 Two-channel Kondo physics from arsenic bond oscillations in zirconium arsenide selenide, STEFAN KIRCHNER, Center for Correlated Matter, Hangzhou, TOMASZ CICHOREK, L. BOCHENEK, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, MARCUS SCHMIDT, Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany, RAINER NIEWA, Institute of Inorganic Chemistry, University of Stuttgart, Germany, A. CZULUCKI, G. AUFLERMAN, FRANK STEGLICH, RUEDIGER KNIEP, Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — The two-channel Kondo effect is a fascinating but extremely fragile many-body state that has been theoretically discussed extensively. We address metallic compounds of a specific (PdFCI) structure for which a $-AT^{1/2}$ term to $p(T)$ is frequently observed, in line with the two-channel Kondo effect. The origin of this anomaly has remained enigmatic since here, solely the interaction between electrons may account for this behavior, and the two-channel Kondo state is not expected to occur. By combining chemical and structural investigations with various physical property measurements we show that the magnetic field-independent $-AT^{1/2}$ term to the low-T resistivity observed over two decades in ZrAs$_2$Se$_2$ with $1.90 \leq x + y \leq 1.99$ originates from vacancies in the layer exclusively built up by As. Furthermore, we can trace back the two-channel Kondo effect in this material to a dynamic Jahn-Teller effect operating at these vacancies. All physical properties of the investigated compounds support this conclusion. Our findings will be relevant also for other metallic systems with pnictogen-pnictogen bondings, e.g., cage-forming compounds like the skutterudites.

V1.00123 When do interactions with Goldstone bosons lead to non-Fermi liquids, HARUKI WATANABE, ASHVIN VISHWANATH, UC Berkeley — There are few general physical principles that protect the low-energy excitations of a quantum phase. Of these, Goldstone’s theorem and Landau-Fermi liquid theory are the most relevant to solids. In this talk, I will present a general analysis of when non-Fermi liquid behavior can arise in electronic systems due to coupling to Goldstone modes. We unify previously known cases using a single criterion and predict a new candidate involving phonons under a magnetic field.

V1.00124 Evaluation of the magnetic field induced glassy behavior and oscillating magneto-caloric effect in Zn$_{0.05}$Ni$_{0.95}$Cr$_2$O$_3$ spinel oxide, KAKARLA DEVI CHANDRASEKHAR, Department of Physics, National Sun Yat Sen University, Taiwan, JYOTHINAGARAM KRISHNA MURTHY, ADYAM VENIMADHAV, Cryogenic Engineering Centre, Indian Institute of Technology Kharagpur, India, HUNG-DUEN YANG, Department of Physics, National Sun Yat Sen University, Taiwan, PROF. H. D. YANG TEAM, PROF. A. VENIMADHAV COLLABORATION — Polycrystalline Zn (5%) doped NiCr$_2$O$_3$ sample was prepared by standard solid state reaction method. Room temperature structural refinement through X-ray diffraction confirm the cubic crystal structure with Fd-3m space group. Temperature dependent dc and AC magnetic measurements revealed multiple magnetic transitions. Doping small amount of non Jahn-Teller (J-T) ion (Zn$^{2+}$) in place of J-T site (Ni$^{2+}$) shows pronounced influence on the magnetosstructural transitions. We have found a frequency independent magnetic transitions in the AC susceptibility measurement indicate the absence of glassy magnetic behavior under zero applied dc bias field. However, an unusual new glassy magnetic transition was discerned under the small dc magnetic field (3 kOe) in the AC susceptibility measurement. We have demonstrated oscillating magneto-caloric effect through isothermal magnetization measurements at low temperature. The observed unusual magnetic properties can be ascribed to the strong magnetic coupling and competing interaction between the spin-lattice-orbital interactions.

V1.00125 INSULATORS AND DIELECTRICS —

V1.00126 Crystal structure and physical properties of Cr oxide with K$_2$NiF$_3$-type structure, TING-HUI KAO$^1$, National Sun-Yat Sen University, Kaohsiung 804, Taiwan, HIROYA SAKURAI, TARAS KOLODIAZHNYI, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan, YUTARO SUZUKI, MOMOKO OKABE, TORU ASAKA, KAKARLA DEVI CHANDRASEKHAR, Department of Physics, National Sun Yat Sen University, Kaohsiung 804, Taiwan, National SUN-YET SEN UNIVERSITY TEAM, NATIONAL INSTITUTE FOR MATERIALS SCIENCE TEAM, NAGOYA INSTITUTE OF TECHNOLOGY COLLABORATION, KOBE UNIVERSITY COLLABORATION — Ruddlesden-Popper (RP) structure materials have been attracted much attention due to their interesting physical properties including high-Tc superconductivity, charge stripe, itinerant ferromagnetism and so on. In this work we are presenting physical properties of some of the K$_2$NiF$_3$-type structure compounds. YSrCrO$_4$ is first synthesized and found to be a hetto-type K$_2$NiF$_3$ structure. The space group of YSrCrO$_4$ is determined to be orthorhombic Pccn by the electron diffraction and the powder X-ray diffraction. YSrCrO$_4$ shows two-dimensional (2D) spin correlations and a canted antiferromagnetic (AF) ordering. Evidence of AF ordering of the Cr oxides is obtained microscopically from ESR. The dielectric measurements suggest existence of in-gap states, while no magneto-dielectric coupling was observed in the above compounds.

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V1.00127 Creep-free ac hysteretic dynamics in epitaxial ferroelectric BiFeO$_3$ films$^1$. YEONGJAE SHIN, BYUNG CHUL JEON, SANG MO YANG, CCES-IBS, Dept of Physics & Astronomy, Seoul N. Univ., Seoul, Republic of Korea, INROK HWANG, EMRC, KIST, Seoul, Republic of Korea, MYUNG RAE CHO, Dept of Physics & Astronomy, Seoul N. Univ., Seoul, Republic of Korea, DANIEL SANDO, SEUNG RAN LEE, CCES-IBS, Dept of Physics & Astronomy, Seoul N. Univ., Seoul, Republic of Korea, JONG-GUL YOON, Dept. of Physics, Univ. of Suwon, Hawseong, Gyeonggi-do, Republic of Korea, TAE WON NOH, CCES-IBS, Dept of Physics & Astronomy, Seoul N. Univ., Seoul, Republic of Korea — Dynamics of domain wall (DW) in ferroelectric (FE) films principally governs their switching properties under applied electric field ($E$). At finite temperature ($T$), the DW motion and their FE switching characteristics can be understood only by introducing the creep motion. Despite this importance, there have been little studies on creep motion of FE films under ac-driven force. In this work, we investigate ac-driven hysteretic dynamics of FE domains in epitaxial BiFeO$_3$ (BFO) films through polarization-electric field hysteresis loops with varying frequency and other switching characters. All BFO films were grown at the optimized growth condition, by employing different bottom electrodes of La$_{0.67}$Sr$_{0.33}$MnO$_3$ (LSMO) and SrRuO$_3$ (SRO); only BFO/SRO shows nearly creep-free hysteretic dynamics. We argue that inhomogeneous internal $E$ plays a significant role in such distinctive FE dynamics of BFO domains, which are affected by surface morphologies of bottom electrodes. Our results highlight that growth-mode-induced interfacial structure between an FE film and a bottom electrode result in engineering domain dynamics of FE switching characteristics.

$^1$This work was supported by IBS-R009-D1.

V1.00128 Application of the Wang-Landau Algorithm applied to Ferroelectrics. SAAD BINOMRAN, King Saud Univ, IGOR KORNEV, Laboratoire SPMS, UMR 8580 du CNRS, Ecole Centrale Paris, 92295 Chatenay-Malabry, France, LAURENT BELLAICHE, Institute for Nanoscience and Engineering and Physics Department, University of Arkansas, Fayetteville, Arkansas 72701, USA — The conventional description of phase transitions in ferroelectrics is based on canonical thermodynamic functions and always assumes the thermodynamic limit of an infinite system. However, ferroelectrics at nanoscale recently became of high interest due to their potential applications in miniaturized devices. It is this timely and more appropriate to use the microcanonical ensemble when mimicking ferroelectric systems. Here, a first-principles-derived scheme, combined with an efficient Monte Carlo microcanonical technique, is used to gain new insight into the paraelectric to ferroelectric phase transition and the effect of the electric field on properties of BaTiO$_3$ systems. In this presentation, we will show the temperature variation of the specific heat for different lattice sizes in BaTiO$_3$ systems. The nature of the phase transition and the behaviour of the specific heat versus the lattice size will be documented. In addition, the effect of the electric field on the character of the phase transitions in BaTiO$_3$ systems will be investigated by showing the free energy ($F$) versus the internal energy ($U$) curves. Electrocaloric effects can also be easily computed and will be discussed.

V1.00129 Evolution of multiple dielectric responses and relaxor-like behaviors in pure and nitrogen-ion-implanted (Ba, Sr)TiO$_3$ thin films. JING YANG, YANHONG GAO, WEI BAI, YUANYUAN ZHANG, East China Normal University, HONG SHEN, JINGLAN SUN, XIANGJIAN MENG, Shanghai Institute of Technical Physics, CHUNGANG DUAN, XIAODONG TANG, JUNHAO CHU, East China Normal University, MENG XIANGJIAN TEAM, CHU JUNHAO TEAM — Multiple dielectric responses are comparatively investigated in the pure and nitrogen-ion-implanted (Ba, Sr)TiO$_3$ (BST) films. Larger diffusive degree of phase transition and more relaxor-like features than those of pure BST films are observed in implanted ones, where the long-range-dipolar-correlated-orders were further segregated into local polar orders after the implantation.

V1.00130 Effect of ferroelectric layer on the magnetic properties of ferromagnetic layer. SRINIVASA RAO SINGAMANENI, North Carolina State University, JOHN T. PRATER, Army Research Office, JAY NARAYAN, North Carolina State University — In this presentation, we show the integration of classical two-phase multiferroic heterostructures composed of room-temperature ferroelectric BaTiO$_3$ (BTO) and ferromagnetic La$_{0.67}$Sr$_{0.33}$MnO$_3$ (LSMO) epitaxial thin films grown on technologically important substrate Si (100) [1-3]. Bilayers of BTO/LSMO thin films display ferromagnetic Curie transition temperatures of ~350 K, close to the bulk value, that are independent of BTO films thickness in the range of 25-100 nm. Discontinuous magnetization jumps associated with BTO structural transitions were suppressed in $M(T)$ curves, probably due to substrate clamping effect. Interestingly, at cryogenic temperatures, the BTO/LSMO structure with BTO layer thickness of 100nm shows almost 2-times higher magnetic coercive field, 3-times reduction in saturation magnetization and improved squareness compared to the sample without BTO. We attribute that to the strong in-plane spin pinning of the ferroelectric layer induced by BTO layer at BTO/LSMO interface. This work demonstrates that it is possible to manipulate the magnetic properties of ferromagnetic layer by varying the thickness of ferroelectric layer, without applying external electric field.


V1.00131 On Structural States of Multiferroic InMnO$_3$. TREVOR TYSON, TIAN YU, New Jersey Institute of Technology, JIANNING BAI, MILINDA ABEEKOON, Brookhaven National Laboratory, ROGER LALANCELLETTE, Rutgers University — InMnO$_3$ (with small site ion) was recently found to be ferroelectric and to crystallize with space group P63cm under certain preparation conditions (Appl. Phys. Lett. 102, 172901 (2013)). We have conducted detailed structural studies to explore the phase diagram and to identify the structural forms of InMnO$_3$ under varying preparation conditions. Detailed diffraction measurement results will be presented. This work is supported by DOE Grant DE-FG02-07ER46402.

V1.00132 Anderson Chern insulators. JAMES JUN HE, TONG ZHOU, YAO LU. The Hong Kong Univ of Science and Technology, Z.C. GU, Perimeter Institute, Canada, K.T. LAW. The Hong Kong Univ of Science and Technology — Previously, it was shown that quantum spin Hall insulators (QSHI) with helical edge states can be turned into a trivial insulator with Chern number $N = 0$ by applying magnetic fields. Further increase of the magnetic fields can result in a quantum anomalous Hall insulator (QAHI) which supports chiral edge state with $N = 1$. In this work, we show that for intermediate magnetization strengths, before the QSHI is turned into a QAHI, a topologically non-trivial phase which supports a single branch of chiral edge states can be obtained by increasing non-magnetic disorder. We call this phase the Anderson Chern insulator phase. In contrast to QAHI in which the chiral edge states are protected by the bulk gap, the gapless chiral edge states in Anderson Chern insulators survive even though the bulk gap is closed by disorder. Moreover, an Anderson Chern insulator exhibits quantized conductance of $e^2/h$ instead of $2e^2/h$ as for topological Anderson insulators. Therefore, we propose that this Anderson Chern insulator phase is a new phase of topological matter.

V1.00133 Topological properties of linear circuit lattices, VICTOR V. ALBERT, LEONID I. GLAZMAN, LIANG JIANG, Yale University — Motivated by the topologically insulating (TI) circuit of capacitors and inductors proposed and tested in [1], we present a related circuit with less elements per site [2]. The normal mode frequency matrix of our circuit is unitarily equivalent to the tight-binding matrix of a quantum spin Hall insulator. Spinful fermionic time-reversal symmetry manifests itself in the TI circuit context as a result of a discrete symmetry of the circuit; elastic backscattering between edge normal modes does not occur whenever a circuit perturbation is invariant under such a symmetry. We also generalize the idea and provide a platform to simulate tunable and locally accessible lattices with arbitrary spin-orbit hopping. A simulation of a non-Abelian Aharonov-Bohm effect using such linear circuit designs is discussed.


V1.00134 ABSTRACT MOVED TO S22.0008

V1.00135 ABSTRACT WITHDRAWN

V1.00136 Growth and Characterization of Large Scale (Sb\textsubscript{1−x}Bi\textsubscript{x})\textsubscript{2}Te\textsubscript{3} Thin Films on Mica\textsuperscript{1}, YAN NI, ZHEN ZHANG, DAVID JILES, Department of Electrical and Computer Engineering, Iowa State University — Topological insulators (TIs) attract attentions for both fundamental science and potential applications because of their bulk band inversion arising from the strong spin orbit coupling. However, it is necessary to tune the Fermi level and Dirac cone in 3D TI (Sb\textsubscript{1−x}Bi\textsubscript{x})\textsubscript{2}Te\textsubscript{3} to make an ideal system for TI applications. In this work, we report high quality (Sb\textsubscript{1−x}Bi\textsubscript{x})\textsubscript{2}Te\textsubscript{3} thin films grown on mica substrate by molecular beam epitaxy. The surface roughness of the thin film can reach as low as 0.7 nm in a large area by van der Waals epitaxy. (Sb\textsubscript{1−x}Bi\textsubscript{x})\textsubscript{2}Te\textsubscript{3} thin film with x = 0.04 shows a local maxima in the room temperature sheet resistance, which indicates a minimization of the carrier density due to band structure engineering. Moreover, for higher Bi concentration, due to an increase of the surface roughness and corresponding reduction of electron mobility, the sheet resistance increases. Our results on the feasibility of depositing (Sb\textsubscript{1−x}Bi\textsubscript{x})\textsubscript{2}Te\textsubscript{3} in wide Bi range on mica substrate will be helpful for the application of TI at room temperature and flexible electronics.

\textsuperscript{1}Authors would like to thank the financial support from the U.S. National Science Foundation under the Award No. 1201883.

V1.00137 Evidence of a Positron bound state on the surface of Bi\textsubscript{2}Te\textsubscript{3}Se\textsubscript{2}, K. SHASTRY, Z.H. LIM, P.V. JOGLEKAR, VARGHESE ANTO CHIRAYATH, University of Texas at Arlington, B.A. BADIH, D. HEIMAN, B. BARBIELLINI, Northeastern University, A.H. WEISS, University of Texas at Arlington — We describe experiments aimed at probing the sticking of positrons to the surfaces of topological insulators performed at University of Texas at Arlington using the Positron Annihilation induced Auger electron Spectrometer. A magnetically guided beam was used to deposit positrons at the surface of Bi\textsubscript{2}Te\textsubscript{3}Se\textsubscript{2} sample at energy of ∼ 2 eV. Peaks observed in the energy spectra and intensities of electrons emitted as a result of positron annihilation showed peaks at energies corresponding to Auger peaks in Bi and Te providing clear evidence of Auger emission associated with the annihilation of positrons in a surface bound state. Theoretical estimates of the binding energy of this state are compared with estimates obtained by measuring the incident beam energy threshold for secondary electron emission and the temperature dependence positronium emission. The experiments provide strong evidence for the existence of a positron bound state at the surface of Bi\textsubscript{2}Te\textsubscript{3}Se\textsubscript{2} and indicate the practicality of using positron annihilation to selectively probe the critically important top most layer of topological insulator system.

\textsuperscript{2}Welch grant 1100 NSF DMR 0907679.

V1.00138 Collective modes at a surface of a topological insulator\textsuperscript{1}, JHIH-SHENG WU, M.M. FOGLER, D.N. BASOV, UCSD — We investigate hybrid plasmon-phonon modes of a polar topological insulator that originate from interaction among the quasiparticles of surface and bulk states, and also optical phonons. As an example, we study electron-doped Bi\textsubscript{2}Se\textsubscript{3}. We analyze the dispersion of the collective modes of this compound for (i) a bulk sample with a depletion layer created by acceptor adsorbates on the surface and (ii) a thin film. In the first case, we show that a depletion layer gives rise to two energy-momentum regions, where the surface states dominate the collective modes over the bulk carriers. In a thin film, the phonons are more prominent than the bulk carriers. The anisotropy of the phonon response makes the thin film behaves as a waveguide. We discuss how these various collective modes can be detected by scanning near-field optical microscopy.

\textsuperscript{1}Supported by ONR and UCOP.

V1.00139 Magnetic properties of graphite nanostructures in carbon microspheres\textsuperscript{1}, EDUARE SHAROYAN, ARAM MANUKYAN, ARMEN MIRZAKHANYAN, ARMEEN KOCHARIAN, OSCAR BERNAL, California State University, Los Angeles — Carbon microspheres with interesting magnetic properties are prepared by solid-phase pyrolysis using as a precursor the metal-free phthalocyanine H\textsubscript{2}PC\textsubscript{5}. At any other temperature, a mixture of oxides consisting of V2O5 and VO2 was observed in the films. Annealing \begin{equation*} t=60\text{min} \end{equation*} carbon microspheres have average \begin{equation*} d=5-300 \end{equation*} diameter, and \begin{equation*} N=3-10 \end{equation*} in wide Bi range on mica substrate will be helpful for the application of TI at room temperature and flexible electronics.

\textsuperscript{1}The research was supported by State Committee Science MES RA, project # SCS 13-1C090 and National Science Foundation grant: NSF-DMR 1105380.

V1.00140 Reduction of Vanadium Oxide (VOx) under High Vacuum Conditions as Investigated by X-Ray Photoelectron Spectroscopy\textsuperscript{1}, A. CHOURASIA, Texas A&M University—Commerce — Vanadium oxide thin films were formed by depositing thin films of vanadium on quartz substrates and oxidizing them in an atmosphere of oxygen. The oxidation was done by the e-beam technique. The oxide films were annealed at different temperatures for different times under high vacuum conditions. The technique of x-ray photoelectron spectroscopy has been employed to study the changes in the oxidation states of vanadium and oxygen in such films. The spectral features in the vanadium 2p, oxygen 1s, and the x-ray excited Auger regions were investigated. The Auger parameter has been utilized to study the changes. The complete oxidation of elemental vanadium to VO2 was observed to occur at 700°C. At any other temperature, a mixture of oxides consisting of VO2 and VO2 was observed in the films. Annealing of the films resulted in the gradual loss of oxygen following by reduction in the oxidation state from +5 to 0. The reduction was observed to depend upon the annealing temperature and the annealing time.

\textsuperscript{1}Organized Research, TAMU-Commerce
V1.00141 Investigation of InBi intermetallic compounds as possible topological insulators, Y.T. LIN, Q.Y. CHEN, W.C. HSEIH, C.F. CHANG, F.C. CHUANG, National Sun Yat-Sen University, H.H. LIAO, Enli Technology Inc., Kaohsiung, Taiwan — InBi intermetallic compounds were found to be potentially 2-dimensional topological insulators from first-principle calculations. In our experiment, InBi, In$_2$Bi$_3$ and In$_3$Bi$_5$ were fabricated either in bulk or thin film, by depositing In and Bi into 2 layers by e-beam evaporation of proper thickness ratios for each stoichiometry. The bi-layers were rapid thermal annealed to accomplish the reaction or intermixing well above their temperatures of phase transition. EDS and secondary electron imaging were used to determine the obtained stoichiometry. CVD using a 3-zone furnace was as tested with various combinations of zone temperatures, types and flow rates of carrying gases to investigate the feasibility of epitaxial growth. Samples were characterized by XRD to obtain the crystalline phase, magneto-transport measurements to determine the carrier concentration and mobility using a PPMS to correlate the measured results. We will ponder on the implication of our findings in regards to the possibilities of being a candidate for topological insulator as predicted by the calculations.

V1.00142 Optical and Electronic Properties of Diisopropylammonium Bromide molecular ferroelectric crystal (DIPAB), AHMAD ALSAAD, Jordan university of Science and Technology, NABIL AL-AQTASH, RENAT SABIRIANOV, University of Nebraska at Omaha — Diisopropylammonium Bromide molecular ferroelectric crystal (DIPAB) could be considered as a potential alternative for perovskite ferroelectric materials. We report the results of ab-initio calculations of electronic band structure and density of states to underline and explain the optical properties of P$^2$$_1$/c ferroelectric phase of DIPAB. In particular, we present the results on complex dielectric function, absorption, reflectivity, energy-loss spectra, and complex refractive index, as functions of the frequency of the incident electromagnetic wave. We found that the optical band gap of the polar ferroelectric phase of DIPAB is $\approx 5$ eV consistent with the steepest rise in the absorption spectra. Furthermore, we found that the ferroelectric phase of DIPAB exhibits two fundamental oscillator bands at 5.91 and 6.4 eV, which correspond to the optical transitions from the valence band of bromine to the conduction band of nitrogen and carbon. Analysis of optical spectra in the 0-4.8 eV photon energy range reveals that this phase is characterized by high transparency, no absorption and a small reflectivity in this range. We found that the sharp maxima in the energy-loss occur at 14.35 and 15.82 eV in polar phase. The peak value of volume loss, 15.82 eV in polar phase, coincides with the zero values of the real part of the corresponding dielectric functions.

V1.00143 Electromagnetic Wave Transmission Through a Nano-Hole, NORMAN HORING, DESIRE MIESSEIN, Stevens Institute of Technology, GODFREY GUMBS, Hunter College, CUNY, HUNTER COLLEGE-CUNY COLLABORATION. STEVENS INSTITUTE OF TECHNOLOGY COLLABORATION — An integral equation formalism is presented to describe electromagnetic wave transmission through a subwavelength nano-hole in a thin plasmonic sheet. The dyadic Green’s function for the associated Helmholtz problem is employed. Taking the subwavelength radius of the nano-hole to be the smallest length of the system, we have obtained an exact solution of the integral equation for the dyadic Green’s function analytically. This dyadic Green’s function is then used in the numerical calculations of EM wave transmission through the nano-hole for normal incidence of the incoming wave train. The EM transmission involves two distinct contributions, one emanating from the nano-hole and the other is directly transmitted through the thin plasmonic layer itself. The transmitted radiation exhibits interference fringes in the vicinity of the nano-hole, and they tend to flatten as a function of increasing lateral separation from the hole.

V1.00144 PT-symmetric Floquet Lattices, NICHOLAS BENDER, MAHBOOBEH CHITSAZI, HUANAN LI, FRED ELLIS, TSAMPIKOS KOTTOSS, Wesleyan University — We investigate spectral and dynamical properties of periodically driven PT-symmetric dimer systems and show that in the Floquet space they are described by Parity-Time symmetric lattices. The topology of the Floquet lattice depends on the complexity of the driving. For the simplest driving scheme associated with a sinusoidal coupling, we show that as the gain/loss parameter increases, the Floquet spectrum and the corresponding eigenvectors undergo a transition from an exact to a broken PT-symmetric phase via an Exceptional Point singularity. The phase transition is also reflected in the associated Floquet dynamics. This paves the way to experimentally investigate extended lattice dynamics in PT-systems. Arealization in the RF domain is reported and compared with the theoretical analysis.

V1.00145 Effects of stoichiometry and crystalline morphology on transport in topological insulator nanowires$^1$, INA KORZHOVSKA, HAIMING DENG, LUKAS ZHAO, The City College of New York, MARCIN KONCZYKOWSKI, TRAVIS WADE, Ecole Polytechnique, France, LIA KRUSIN-ELBAUM, The City College of New York — In nanostructured topological insulators with increased surface-to-volume ratio the contribution of charge transport through topological surfaces relative to the bulk will be enhanced. Here we report on electrochemical synthesis and characterization of Bi$_2$Te$_3$ and Sb$_2$Te$_3$ nanowires in which the effect of materials’ stoichiometry as well as nanowire size was investigated. Nanowires were grown in porous anodic aluminum oxide membranes with pore diameters varying from 18 to 150 nm. Stoichiometry and the wire morphology were tuned by electrochemical cell voltages in the 30 - 150 mV range. Topological signatures and surface conductance are affected by both crystallinity and chemical composition. We found that in the narrow range of the electrochemical potential (130 mV-150 mV) when stoichiometry changes were very small the nanowire conductance could still be hugely different. The results of high-field magnetotransport and I-V characteristic measurements on nanowires with crystallinity and morphology controlled by a suitable annealing protocol and imaged using transmission (TEM) and scanning (SEM) electron microscopies will be presented.

$^1$Supported by NSF-DMR-1312483, and DOD-W911NF-13-1-0159

V1.00146 Laser induced oxidation and optical properties of bismuth telluride nanofilaments, ZHIPENG YE, Univ of Northern Iowa, SUKRIT SUCHARITAKUL, Case Western Reserve Univ, COURTNEY KEISER, TIM E. KIDD, Univ of Northern Iowa, XUAN P. A. GAO, Case Western Reserve Univ, RUI HE, Univ of Northern Iowa — Bi-Te nanofilaments (NPs) grown by low pressure vapor transport method were studied by Raman spectroscopy, atomic force microscopy (AFM), energy-dispersive X-ray spectroscopy (EDS), and Auger electron spectroscopy (AES). We find that the surface of relatively thick (more than tens of nanometers) Bi$_2$Te$_3$ NPs is oxidized in the air and forms a bump under heating with moderate laser power, as revealed by the emergence of Raman lines characteristic of Bi$_2$O$_3$ and TeO$_2$ and characterization by AFM and EDS. Further increase of laser power burns holes on the surface of the NPs. Thin (thicknesses less than 20 nm) NPs with stoichiometry different from Bi$_2$Te$_3$ were also studied. Raman lines from non-stoichiometric NPs are different from those of stoichiometric ones. Thin NPs with the same thickness but different stoichiometries show different color contrast compared to the substrate in the optical image. This indicates that the optical absorption coefficient in thin Bi-Te NPs strongly depends on their stoichiometry. Controlling the stoichiometry in the Bi-Te NPs growth is thus very important for their thermoelectric, electronic, and optical device applications.

$^3$Supported by American Chemical Society Petroleum Research Fund (Grant 53401-UNI10), NSF (No. DMR-1206530, No. DMR-1410496, DMR-1151534), UNI Faculty Summer Fellowship and a UNI capacity building grant.
V1.00147 Investigation of Interactions between the Doped Rare Earth Ions and Encaged Radicals in C12A7:RE3+ — Using Optical and EPR Spectroscopy, CARTER LAYFIELD, LI MA, XIAO-JUN WANG, Georgia Southern Univ — Doped calcium aluminates (C12A7) (C12A7:Eu3+ and C12A7:Mn2+) have been prepared using solid state reaction methods. The Eu3+ and Mn2+ dopants can both occupy the Ca2+ positions in C12A7. The unique cage-like structure of C12A7 allows different anions, such as oxygen, hydrogen to be trapped in cage by modifying the sample preparation or treatment conditions. The effects of these encaged anions/radicals on the local symmetries of Ca2+ have been studied using photoluminescence from C12A7 doped with Eu3+, which is a sensitive environmental probe. The effects can also be independently observed from the hyperfine structure of electron paramagnetic resonance spectra in C12A7 doped with Mn2+. Our results showed: 1) the presence of 5D0 to 7F0 transition implies that Eu3+ sits at a non-centrosymmetric site in all caged radical centers; 2) this singlet transition is doubled when superoxides are encaged in C12A7, indicating that the sites of calcium (or Eu2+) ions are not identical due to the distortion of the encaged anions; 3) a blue shift of the transition occurred due to nephelauxetic effects in asymmetry sites. We have also observed double sets of EPR signals of sextet hyperfine splitting for Mn2+ in C12A7-O but single sets in C12A7-H. We conclude that the local symmetry around Ca2+ positions are distorted more when superoxide is encaged in C12A7. Finally, RE3+ doped C12A7 samples have been systematically prepared and the interactions between the encaged ions and RE3+ emission centers studied using EPR spectroscopy.

V1.00148 Enhanced spin orbit interaction of graphene by Ir cluster decoration, PEI-QUN WANG, YUJUN QIN, ZHAOQIU LI, SIQI WANG, BAIGENG WANG, Nanjing University, COLLABORATIVE INNOVATION CENTER OF ADVANCED MICROSTRUCTURES TEAM — Enhancing the strength of the intrinsic spin orbit (SO) coupling in graphene is a critical issue in achieving the quantum spin Hall effect predicted by Haldane et al. Here we report the measurements of the weak localizations in graphene, which has been decorated by Ir clusters. The SO scattering rate ($\tau_{SO}$) is extracted by fitting the curves using the formula of E. MacCan. It is found that $\tau_{SO}$ is monotonically dependent on the electronic relaxation time. Further analysis points that it obeys an Elliot-Yafet relaxation, which can be attributed to the dominance of Kane-Mele $\tau_{SO}$ interaction. The SO interaction strength can be extracted by fitting the $\tau_{SO}$ data dependent on the gate voltage. After considering the temperature effect, an SO strength value of $5 \sim 7$ meV is achieved, which has been greatly enhanced as compared to that of pristine graphene.

V1.00149 Zero modes in superconducting nanowires with Desselhaus spin-orbit coupling, HSICHIANG KAO, National Taiwan Normal University — Using chiral decomposition, we are able to find analytically the zero modes in the Kitaev ladder model and superconducting nanowires with Desselhaus spin-orbit coupling. Analytic conditions for the existence of zero modes are obtained. As a result, we are able to predict the number of zero modes in these systems. Moreover, we find that when suitable resonance condition is satisfied exact zero modes exist even in finite systems contrary to the common belief.

V1.00150 Chiral Majorana edge modes in d-wave superconductor/antiferromagnet heterostructures, PIN GAO, TAI KAI NG, VIC KAM TUN-E LAW, Hong Kong Univ of Sci & Tech — In this work, we study the heterostructure of a d-wave superconductor coupled to an antiferromagnet. We show that Majorana fermion edge states can be created in the system even in the absence of spin-orbit coupling, given that a supercurrent is induced in the superconductor. The Majorana edge states exist even the bulk is gapless and they propagates perpendicular to the direction of the supercurrent. The Majorana modes can be detected through tunneling and heat transport measurements.

V1.00151 Chiral magnetic effect in two-band lattice model of Weyl semimetal, MIN-FONG YANG, Tunghai University, MING-CHE CHANG, National Taiwan Normal University — Employing a two-band model of Weyl semimetal, a definite result on the existence of the chiral magnetic effect (CME) is established within the linear-response theory. The crucial role played by the limiting procedure in deriving correct transport properties is clarified. Besides, in contrast to the prediction based on linearized effective models, the value of the CME coefficient in the uniform limit shows nontrivial dependence on various model parameters. Even when these parameters are away from the region of the linearized models, such that the concept of chirality may not be appropriate, this effect still exists. This implies that the Berry curvature, rather than the chiral anomaly, provides a better understanding of this effect.

V1.00152 Magnetic ordering at the topological insulator-magnetic insulator interface, KARAN BANERJEE, JEAN BESBAS, Nati Univ of Singapore, PENG REN, Nanyang Technological University, LAN WANG, RMIT University, HYUNSOO YANG, Natl U of Singapore — The spin momentum locking property of topological insulators is key to their practical utility. However, due to large bulk contribution and defects, it has been difficult to harness it. One of the possible solutions is to use heterostructures of topological insulators and magnetic insulators which can make the spin momentum locking robust at the interface. Here we report on the angular dependence of magnetoresistance on heterostructures of the topological insulator BiSbTeSe$_2$ and the magnetic insulator YIG. We find that a four-fold symmetry arises in the in-plane angular dependence spectrum above a critical external field indicating the presence of magnetic ordering at the interface. We demonstrate that the interfacial magnetic ordering arises from a spin polarized interface state which is distinct from the topological surface state.

V1.00153 Superlattice valley engineering for designer topological insulators, XIAO LI, The University of Texas at Austin, FAN ZHANG, The University of Texas at Dallas, QIAN NIU, The University of Texas at Austin, JI FENG, Peking University — A topological insulator is a novel state of quantum matter, characterized by symmetry-protected Dirac interfacial states within its bulk gap. Tremendous effort has been invested into the search for topological insulators. To date, the discovery of topological insulators has been largely limited to natural crystalline solids. Therefore, it is highly desirable to tailor-make various topological states of matter by design. Starting with but a few accessible materials or elements. Here, we establish that valley-dependent dimerization of Dirac surface states can be exploited to induce topological quantum phase transitions, in a binary superlattice bearing symmetry-unrelated interfacial Dirac states. This mechanism leads to a rich phase diagram and allows for rational design of strong topological insulators, weak topological insulators, and topological crystalline insulators. Our ab initio simulations further demonstrate this mechanism in [111] and [110] superlattices of calcium and tin tellurides. While our results reveal a remarkable phase diagram for the binary superlattice, the mechanism is a general route to design various topological states.

V1.00154 Orbital and spin magnetization induced by electric current in crystals with helical structure, TAIKI YODA, TAKEHITO YOKOYAMA, SHUICHI MURAKAMI, Tokyo Institute of Technology — Crystals with helical lattice structure lack inversion and mirror symmetries. In such systems with low symmetry, we expect various physical phenomena which never occur in systems having high symmetry. In particular, because a helix is similar to a solenoid, we expect that an electric current will induce orbital and spin magnetization. To confirm this scenario, we introduce a simple tight-binding model with helical lattice structure. Using this model, we calculate the orbital and spin magnetization induced by electric field along the helical axis. The resulting orbital magnetization in response to the electric field is along the helical axis. The direction of the induced orbital magnetization is opposite for the right-handed helix and the left-handed one. Furthermore, when the spin-orbit coupling is included, the spin magnetization is also induced along the helical axis as well. This spin magnetization comes from a radial spin texture on the Fermi surface, which is totally different from the Rashba system having tangential spin texture. We also show that by changing the model parameters the model shows characteristic phase transitions into a Weyl semimetal and a weak topological insulator.
V1.00155 Linked Temperature Evolution of the bulk gap and helical topological surface states in SmB$_6$1, J.D. DENLINGER, Lawrence Berkeley National Lab, J.W. ALLEN, KAI SUN, U. of Michigan, JEONGSOO KANG, Catholic U. of Korea, J.W. KIM, C.J. KANG, J.H. SHIM, B.I. MIN, POSTECH, D.-J KIM, Z. FISK, UC Irvine — The paradigm mixedvalent insulator SmB$_6$ with a temperature dependent bulk gap has recently become the first paradigm example of a strongly correlated topological insulator with f-d band inversion and with experimental evidences for in-gap surface states and surface transport. In this work temperature- and polarization-dependent angle-resolved photoemission on cleaved SmB$_6$ quantifies the T-evolution of (i) the Sm 4f state coherency, (ii) the X-point f-conduction band energy and many-body gap destabilization, and (iii) the intimately connected state of topologically protected in-gap states. DFT and DFT-DMDFT calculations confirm early theory [1] that hybridization between boron 2p and Sm 4f states provides crucial assistance in the full opening of the many-body f-d gap. Also a dimensional crossover above 100K from 3D bulk d-band states crossing $E_F$ at high T to low T 2D in-gap surface states is shown to coincide with the development of a circular dichroism signature of in-gap state helicity.

[1] Supported by U.S. DOE at the Advanced Light Source (DE-AC02-05CH11231).

V1.00156 Low temperature magnetoresistance studies in MBE grown topological insulator thin films1, RIK DEY, ANUPAM ROY, TAMNOY PRAMANIK, SAMARESH GUCHHAIT, SUSHANT SONDE, AMRITESH RAI, SARMITA MAJUMDER, BAHINIMAN GHOSH, LEONARD REGISTER, SANJAY BANERJEE, Microelectronics Research Center, Univ of Texas at Austin — We studied low temperature magnetoresistance in molecular beam epitaxy grown topological insulator Bi$_2$Se$_3$ and Bi$_2$Te$_3$ thin films. The surface and structural characterization of the grown films showed smooth epitaxial growth on Si(111). The magnetoresistance has been measured at low temperatures (2 - 20 K) with magnetic fields upto 9 T. The full range perpendicular field magnetoresistance has been explained with the original Hikami-Larkin-Nagaoka theory. Altshuler-Aronov theory of localization has been used to understand the full range parallel field magnetoresistance. Various scattering times have been estimated by fitting the magnetoresistance data with the theory. It is shown that the Zeeman effect is not needed to explain the magnetoresistance and has not been considered in the theory either. The angle dependent anisotropic magnetoresistance has also been observed and explained using the above theories.

V1.00157 Dirac Semimetal Films as Spin Conductors on Topological Substrates1, XIAOXIONG WANG, Nanjing University of Science and Technology, GUANG BIAN, University of Illinois at Urbana-Champaign, PENG WANG, Shandong University of Science and Technology, T.-C. CHANG, University of Illinois at Urbana-Champaign — Spin-momentum locked states, notably those found on the surfaces of topological insulators, are promising for low-power electronic devices based on spin transport. Here we report a much more versatile case involving a Dirac semimetal film on a topological insulator substrate. Such a film can carry highly spin-polarized conduction channels by electronic coupling to the substrate. The spin channel width, defined by the film thickness, is at the designer’s disposal, thus permitting optimization of the system parameters. The concept and underlying physics of such quasi-bulk spin channels are confirmed by calculations of a model system involving Bi$_2$Se$_3$ as the substrate and its low-Z substitute as the overlayer film. The results demonstrate Dirac semimetals as an important class of material for spintronic applications.

V1.00158 Detection of entanglement by helical Luttinger liquids, KOJI SATO, Tohoku Univ, YAROSLAV TSERKOVNYAK, University of California, Los Angeles — A Cooper-pair or electron-hole splitter is a device capable of spatially separating entangled fermionic quasiparticles into mesoscopic solid-state systems such as quantum dots or quantum wires. We theoretically study such a splitter based on a pair of helical Luttinger liquids, which arise naturally at the edges of a quantum spin Hall insulator. Equipping each helical liquid with a beam splitter, current-current cross correlations can be used to construct a Bell inequality whose violation would indicate nonlocal orbital entanglement of the injected electrons and/or holes. Due to the Luttinger-liquid correlations, however, the entanglement is suppressed depending on ambient temperature and voltage bias.

V1.00159 SUPERCONDUCTIVITY –

V1.00160 Hole doping study in antiferromagnetic BaFe$_2$Se$_3$ and BaMn$_2$As$_2$1, JIN-KE BAO, GUANG-HAN CAO, Zhejiang Univ — Motivated by the close relationship between antiferromagnetism and superconductivity, we studied hole doping in two antiferromagnetic compounds BaFe$_2$Se$_3$ and BaMn$_2$As$_2$. BaFe$_2$Se$_3$ has a block antiferromagnetic transition around 250 K with a magnetic moment 2.8 $\mu_B$/Fe and BaMn$_2$As$_2$ exhibits a C-type antiferromagnetism with a large Néel temperature $T_N = 625$ K and a large order moment 3.9 $\mu_B$/Mn. We did the explicit investigations on the Ba$_{0.8}$K$_{0.2}$Fe$_2$Se$_3$ compound which had anisotropic Heisenberg-like spin glass and variable range hopping conductivity [J. K. Bao et al., J. Phys.: Condens. Matter 26, 026002 (2014)]. As for the semiconducting BaMn$_2$As$_2$, potassium doping introduces holes into this system and makes it a metal. Moreover, weak ferromagnetic transition appears for the heavily potassium doping [J. K. Bao et al., Phys. Rev. B 85, 144523 (2012)]. However, the origin of weak ferromagnetism in the heavily doped Ba$_{1-x}$K$_x$Mn$_2$As$_2$ is still an open question.

V1.00161 ABSTRACT WITHDRAWN

V1.00162 Doping effects of transition metals on superconducting properties of (Ca,RE)FeAs$_2$, HIROYUKI YAKITA, HIRAKU OGINO, TOMOYUKI OKADA, AKIYASU YAMAMOTO, KOJI KISHIO, JUN-ICHI SHIMOYAMA, Univ of Tokyo, AKIRA IYO, HIROSHI EISAKI, AIST, ALBERTO SÁLA, Univ of Tokyo, AIST, Univ of Genova — At the previous March Meeting, we reported new iron based superconductors (Ca,RE)FeAs$_2$ (Ca112) (RE = La-Nd, Sm-Gd)1,2. Superconducting transition was observed in all samples except for Ce-doped sample, and $T_c$ of La-doped sample exceeded 30 K. In this study, we have synthesized transition metals (TM = Mn, Co, Ni) co-doped Ca112 samples. Mn co-doping suppressed superconductivity. On the contrary, enhancement of $T_c$ with sharp superconducting transitions was observed in most of the Co or Ni co-doped samples. $T_c$ of Co co-doped samples decreased with a decrease in ionic radii of $RE^{3+}$ from 38 K for $RE$ = La to 29 K for $RE$ = Gd, though Eu doped sample showed exceptionally low $T_c$. $J_e$ value of La and Co co-doped sample estimated from magnetization measurement is approximately 2.0 x 10$^4$ Acm$^{-2}$ at 2 K suggesting bulk superconductivity. [1] H. Yakita et al., J. Am. Chem. Soc. 136 (2014) 846 [2] H. Yakita et al. APS March Meeting 2014 C1 00090

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V1.00164 Work supported by National Basic Research Program of China (No. 2011CB00137) and National Science Foundation of China (No. 11101003).
V1.00163 Magnetic, Transport Properties, Lower Critical Field, Penetration Depth, Anisotropy and Gap Evidences of Ca_{10} (Pt_{n}As_{x}) (Fe_{2−n}Pt_{n}As_{2})_{5} (n = 3 And 4) Superconductors, KALYAN SAMSAL, YUYI XUE, PAUL C.W. CHU, Texas Center for Superconductivity, Department of Physics, University of Houston — Platinum iron arsenides Ca_{10}(Fe_{2−n}Pt_{n}As)_{5} (n = 3 & 4) are first Fe based superconductors with metallic spacer layers. Crystal structure have stacks of Ca (Pt_{n}As_{x}) Ca (Fe_{2−n}Pt_{n}As) consists of superconducting Fe_{2−n}As layers alternating with Pt_{n}As layers, forming a triclinic P1, 1038phase with n = 3 and tetragonal P4/n, 1048phase with n = 4. Two different negatively charged layers [(FeAs)_{1−x}^{1+}−] and (Pt_{1−x}As)_{m+} compete for electrons provided by Ca^{2+}. In parent compound Ca_{10}(FeAs)_{5}(PtAs), no excess charge dopes FeAs-layer, and superconductivity is induced by Pt-substitution. Additional Pt in Pt_{n}As layers shift charge balance between layers and T_{c} raises to 38 K, but decreases again if additionally Pt is substituted for Fe. Charge doping is supported by T_{c} ≈ 30 K in electron-doped La-1038, x ≈ 0.2 (Ca_{1−x}La_{x})_{5}(Pt_{2}As)_{5} without significant Pt-substitution. Magnetic properties were explored. Magnetization measurements reveal fish-tail hysteresis loop and relatively high critical current density at low T. Lower critical field, H_{c2} derived from vortex penetration into single crystals. Ginsburg-Lauder parameters extracted from reversible magnetizations data. Upper critical field determined by resistive transition shows large anisotropy. With La doping, the structural/magnetic phase transitions are suppressed. T-dependency of the H_{c2} is compared with BCS-gap models and anisotropy of H_{c1} will be discussed.

V1.00164 Nematic phase in strain free detwined BaFe2-xNixAs2, HAORAN MAN, Rice Univ, XINGYE LU, None, JUSTIN CHEN, EMILIA MOROSAN, PENGCHENG DAI, Rice Univ, PENGCHENG DAI'S GROUP TEAM — Here I present the transport and neutron scattering results in BaFe2−xNixAs2. The crystal is detwined using pressure and then the pressure is released at base temperature before the experiment. In the detwined sample, the anisotropy persist at a temperature higher than the both structural and magnetic transition, but the temperature range is much lower than the anisotropy induced by pressure.

V1.00165 Disorder induced correlation gap suppresses superconductivity in the 5d metallic perovskite Ba_{1−x}La_{x}PbO_{3}, CAROLINA ADAMO, Stanford University, DANIEL SHAI, BREDAFA FAETH, Cornell University, PHILIP WU, Stanford University, KYLE SHEN, DARRELL SCHLOM, Cornell University, MALCOLM BEASLEY, Stanford University — We report the synthesis and characterization of the electronic structure of thin films of the perovskite Ba_{1−x}La_{x}PbO_{3} grown by oxide molecular-beam epitaxy. Using angle-resolved photoemission spectroscopy our measurements reveal a Fermi surface consistent with density functional calculations at low doping, but indicate the formation of an energy gap at higher doping values (x ∼ 0.2), consistent with electrical transport measurements. By comparison with temperature-dependent point contact tunneling spectroscopy measurements, we show this behavior is consistent with a disorder-driven correlation gap. Moreover the photoemission data reveal a density of states that is not linear at high binding energies, suggesting discrepancy with previous tunneling density of states measurements of superconducting oxides.

V1.00166 Superconductivity and Eu Valence Instability in Undoped Eu3Bi2S4F4, HUI-FEI ZHAI, PAN ZHANG, GUANG-HAN CAO, Department of Physics, Zhejiang University, Hangzhou 310027, P. R. China — We recently synthesized a novel bismuth sulfurofluoride, EuBiSF_{2}.[1] A CDW-like transition occurs at 280 K, below which SC emerges at 0.3 K. The Eu ions show an anomalously mixed valence about +2.2. With structural design, we successfully synthesized a new europium bismuth sulfofluoride, EuBi_{2}F_{5}.[2] Two crystallographic twins, EuBi_{2}F_{5}−type EuBiSF_{2}[1] and EuBi_{2}F_{5}−type EuBiS_{2}[2], stack alternately along the crystallographic c axis. There are two crystallographically distinct Eu sites, Eu(1) and Eu(2) at the Wyckoff positions 4e and 2a, respectively. Our bond valence sum calculation, based on the refined structural data, indicates that Eu(1) is essentially divalent, while Eu(2) has an average valence of +2.64(5). This anomalous Eu valence state is preserved at low temperatures and magnetic properties, but indicated by Mössbauer and magnetization measurements. The Eu^{3+} components donate electrons into the conduction bands that are mainly composed of Bi 6px and 6py states. Consequently, the material itself shows metallic conduction and superconducts at 1.5 K without extrinsic chemical doping. [1] Hui-Fei Zhai et al., Phys. Rev. B90, 064518 (2014). [2] Hui-Fei Zhai et al., J. Am. Chem. Soc. 2014, 136, 15386−15393.

V1.00167 Polycrystalline Silicon Thin Films at Low Temperature using SiF_{4} / SiH_{4} mixture, MONIRUZZAMAN SYED, Lemoine Owen College, TAKAO INOKUMA, YOSHIHIRO KURATA, SEIIICHI HASEGAWA, Kanazawa University — Polycrystalline silicon films with a strong (110) texture were prepared at 400°C by a plasma-enhanced chemical vapor deposition using different SiF_{4} flow rates ([SiF_{4}] = 0−0.5 sccm) under a fixed SiH_{4} flow rate ( [SiH_{4}] = 1 or 0.15 sccm). The effects of the addition of SiF_{4} to SiH_{4} on the structural properties of the films were studied by Raman scattering, X-ray diffraction (XRD), Atomic force microscopy and stress measurements. For [SiH_{4}] = 1 sccm, the crystallinity and the (110) XRD grain size monotonically increased with increasing [SiF_{4}] and their respective maxima reach 90% and 900 Å. However, for [SiH_{4}] = 0.15 sccm, both the crystallinity and the grain size decreased with [SiF_{4}]. Mechanisms causing the change in crystallinity are discussed, and it was suggested that an improvement in the crystallinity, due to the addition of SiF_{4}, is likely to be caused by the effect of a change in the surface morphology of the substrates along with the formation of SiF_{4} by reaction of SiF_{4} and the substrate.

V1.00168 Electronic conduction in Sr_{2}RuO_{4} and Sr_{2}RhO_{4} thin films, YOSHIHARU KROCKENBERGER, HIROSHI IRIE, JOSH KUO, HIDEKI YAMAMOTO, NTT Basic Research Labs — Transition metal oxides belonging to the Ruddlesden-Popper series, e.g., T^{2+}La_{2−n}Cu_{n}O_{3}, Sr_{2}RuO_{4}, and Sr_{2}RhO_{4}, share several geometrical- and associated electronic features. In all cases, squares of transition metal oxide layers are separated by insulating layers, hence, the observed electronic conduction is anisotropic. So far, much attention has been attributed to the metallic conduction in cuprates and ruthenates and metallic conduction in rhodates has been sparsely acknowledged. This is partly due to the absence of superconductivity in the RhO_{2} planes. We show that the metallic conduction in RhO_{2} planes is subject to d[Rh-O] distance which can be tuned by epitaxial strain.

V1.00169 Investigation of the changes in the density of states in the Copper-Titanium system, A. CHOURASIA, Texas A&M University-Commerce — The density of states and structure parameters in the copper-titanium system have been investigated by DFT. Various compounds of the copper and titanium (such as CuTi, CuTi_{2}, CuTi_{3}, Cu_{3}Ti) have been studied. The DFT calculations were performed using the GGA exchange-correlation potential. For each compound the atoms were relaxed by minimizing the forces and allowing changes in the unit cell. Geometrical structure and variations in the density of states in the vicinity of the Fermi level have correlated with the near neighbors of copper/titanium.

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1Supported by NSF of China (grant no. 11190023 and 90922002), the National Basic Research Program of China (grant no. 2010CB923003 and 2011CBA00103), and the Fundamental Research Funds for the Central Universities of China (grant no. 2013FZA3003).

Organized Research, TAMU-Commerce

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V1.00170 A Model Approach to Flux-Pinning Properties of YBCO Vortex States via Non-Superconducting Impurities, RONALD GAMBLE, KLINTON DAVIS, ABEBE KEEBEDE, North Carolina A&T State Univ — Thin film YBCO samples with added non-superconducting nanodot defects of CeO2 and BaSnO3 are the focus of recent high-temperature superconductor studies. Examining the structure shows that quantized magnetic fluxortices from within the sample arrange themselves in a self-assembled lattice. The nanodots, with non-superconducting properties, serve to present structural properties to restrict motion of these vortices under a pinning-force card to enhance the critical current density. A formulation of a new model for the system by a variation in the electron pair velocity via the virtual work from the nanodot defects in accordance to the Abrikosov-Gor'kov theory is presented. With the zero net force on the vortex, the vortex-core radius and pinning force constant don't set in for the optimal deposition parameters of number density, growth geometry and mass density of these nanodot structures. With a calculation of pair velocities from a similar work, a comparison is made between experimental and theoretical velocity calculations using growth geometry and chemical potential. This will yield insight into how the current density for a doped high-temperature superconductor will be modified and tuned based on the density of the nanodots themselves.

V1.00171 Superconductivity enhanced by Se-doping in Eu2Bi2S4F4, PAN ZHANG, HUI-FEI ZHAI, GUANGHAN CAO, ZHUAN XU, Department of Physics, Zhejiang University — We investigated the negative chemical pressure effect of Eu2Bi2S4F4 by partially substituting S with Se. The "parent" compound Eu2Bi2S4F4 is a new member of the BiS2-based superconductors. [H.-F. Zhai et al., J. Am. Chem. Soc. 136, 15386–15393, (2014)] It shows anomalous Eu valence and superconductivity of $T_c = 1.5$ K without chemical doping. With S/Se-doping, we found that a CDW-like anomaly is gradually suppressed to lower temperatures, and meanwhile the superconductivity ($SC$) is enhanced. For Eu2Bi2Se2F4, $T_c$ reaches 3.4 K. Magnetization measurements reveal an average Eu valence of $\sim 2.06$, which means that Se doping does not introduce extra electrons but instead, lowers down to a low electron doping level of $x \sim 0.1$. Therefore, the present system manifested itself as a rare example of existence of SC at very low doping levels.

V1.00172 Characterization of Titanium Nitride thin films Sputtered at Room Temperature, WEIQI HUANG, STEPHEN ARNASON, MATTHEW BELL, University of Massachusetts Boston — Thin film titanium nitride (TiN) has become widely used in photon detection with microwave kinetic inductance detectors and recently as resonant structures in superconducting quantum information circuits. The attractive properties of the material are its widely tunable critical temperature, large surface inductance, and low losses at microwave frequencies when incorporated into resonant circuits. We report on thin films of TiN sputter-deposited on intrinsic silicon substrates at room temperature for various nitrogen flow rates and deposition pressures. Characterization of the inductance and microwave losses in lumped-element resonators fabricated from these films will also be discussed.

V1.00173 Anisotropy of superconducting properties of flexible magnesium-diboride-coated carbon nanotube yarns, JULIA BYKOVA, MÁRCIO DIAS LIMA, AUSTIN HOWARD, NanoTech Institute, The University of Texas at Dallas, M. TARANOV, K. KONYUKHOV, Moscow Institute of Steel and Alloys, MYRON SALAMON, MPA-CMMS, Los Alamos National Laboratory, RAY BAUGHMAN, ANVAR ZAKHIDOV, NanoTech Institute, The University of Texas at Dallas — Flexible ultralight magnesium-diboride-coated carbon nanotube (MgB$_2$-CNT) yarns have critical temperatures up to 37 K, high critical fields and currents comparable with conventional superconducting wires. Superconducting yarns containing MgB$_2$-CNT nanofibers were prepared by conformal coating of CNT sheets with boron in photothermal chemical vapor deposition, and annealing in magnesium vapors. Magnetic transport measurements in a magnetic field, whose direction is varied relative to the sample orientation, showed anisotropy in superconducting properties. The critical field anisotropy ratio $H_{c2}/H_{c1}$ reaches 1.2-1.4 over a wide temperature range below $T_c$, comparable to but slightly lower than the factor 1.4-2 of epitaxial MgB$_2$ thin films. An X-ray diffraction study confirmed the crystalline anisotropy of composite wires and showed, that the MgB$_2$ grains prefer to grow with the a-plane parallel to the carbon nanotube walls and the yarn axis.

V1.00174 Plasma and thermal assisted selenization for the preparation of chalcopyrite light-absorbing layers, ZEHRA CVHER, ZHI HUANG, YUHANG REN, Hunter College, City University of New York, HUNTER COLLEGE, CITY UNIVERSITY OF NEW YORK TEAM — Chalcopyrite compound has attracted much attention recently because of their application in high efficient photovoltaic devices. In order to obtain a decent chalcopyrite photovoltaic device, it is very critical to optimize the metallic precursor layers and choose a suitable selenization technique. We demonstrate plasma and thermal assisted selenization methods for preparing Cu(In,Ga)Se$_2$ (CIGS) semiconductor films using elemental selenium vapor. The selenization process includes the modification of the ionization state of Se species by radio frequency plasma and/or thermal heating and homogenous control of interactions with CuInGaSe$_2$ metallic precursors. We obtained CIGS absorber layers with improved homogeneity and crystallinity. The result is explained by the enhancement of reaction kinetics between the reduced Se phase and metallic precursor layers.

V1.00175 A15 compounds, HTSC and strong coupling superconductors, SNEHADRI OTA, Institute of Physics, Bhubaneswar 751005, Orissa, India — We suggest that it is possible to understand the origin of high $T_C$ in the framework of strong coupling theory of superconductors. An exploratory investigation of materials with promising structural or electronic motifs is presented. The electron-phonon coupling constant $\lambda$ has been found to be inversely proportional to the molecular weight. The analysis is based on the numerically derived equation for $T_C$ from strong coupling theory for superconductivity by McMillan. The Coulomb pseudopotential $\mu^*$ has been found to be negative for YBa$_2$Cu$_3$O$_y$. The $T_C$ of YBa$_2$(Cu$_{1-x}$Zn$_x$)$_3$O$_7$ decreases linearly from 89 K to the nonsuperconducting state at a rate of about 15 K/at% of Zn substitution. Similar analysis YBa$_2$(Cu$_{1-x}$Zn$_x$)$_3$O$_7$ shows that $\mu^*$ changes sign from negative to positive as $T_c$ reduces. The isotope effect exponent $\alpha$ is found to go through a maximum as $T_C$ decreases and is found to be equal to 1/2 for $x=0.026$ which can be verified experimentally.

V1.00176 Topological Superconductivity in Ferromagnetic Metal Chains: Part II, JIAN LI, Princeton University, RUHAN CHEN, University of Texas at Austin, ILYA DROZDOV, ALI YAZDANI, BOGDAN BERNEVIG, Princeton University, ALLAN MACDONALD, University of Texas at Austin — One most important feature of the Majorana end states observed in the STM experiments is their sharply localized spatial profile. This cannot be explained by a conventional model for the magnetic flux, zero net flux, and non-Abelian states wouldn't be observable in a chain much shorter than the superconducting coherence length. In this second talk we resolve this issue by showing the fundamental difference between the naive 1D model and a proper one, where the 1D-3D hybrid nature of the real experimental structure is taken into account. The strong hybridization between the chain and the higher-dimensional host superconductor introduces long-range (power-law) coupling into the 1D system and significantly modifies the spatial profile of possible Majorana states. As a consequence the superconducting coherence length becomes irrelevant to the decay of the Majorana wavefunctions at a small length scale whereas the Fermi wavelength prevails. We will show concrete examples of eigenstates in a finite-size hybrid system where the Majorana end states are indeed localized within a length scale determined by the Fermi wavelength. This is in good agreement with experimental observations. We will also discuss the implication of this new regime, where the superconducting coherence length is irrelevant by realistic measure, in terms of the coupling energy between Majorana states and the operation time when braiding them.

Research at Hunter was supported by the Sun Harmonics Ltd and by NYSTAR through the Photonics Center for Applied Technology at CUNY.
V1.00177 Magnetic Anisotropy in DyNi2B2C system, W.C. LEE, Dept. of Physics, Sookmyung Women's Univ. Seoul 140-742, Korea — To figure out the magnetic and transport anisotropy in DyNi2B2C which have superconducting critical temperature \( T_c \) lower than the antiferromagnetic Neel temperature \( T_N \) among RNi2B2C (R= rare earth elements) compounds, we have measured the static magnetization curves M(H,T) with the applied magnetic fields parallel and perpendicular to the crystallographic c-axis at various temperatures and applied magnetic fields. We have observed several magnetic transitions only for the applied magnetic field perpendicular to the c-axis and such magnetic transitions have shift sensitively to the higher temperature regions. We compared our results with the Dy\(^{1.1}\) magnetic sublattice structure previously reported from neutron scattering experiments.

V1.00178 ABSTRACT WITHDRAWN —

V1.00179 Anisotropic bias dependent transport property in defective phosphorene Layer, JISANG HONG, M. FAROOQ, Department of Physics, Pukyong National University, Korea — We present the electronic band structure, defect formation energy and bias dependent transport property. Both single and divacancy defects have been considered. We found that the defect formation energy is much less than that in graphene. The defect configuration strongly affects the electronic structure. The band gap vanishes in single vacancy layer, but the band gap reappears in divacancy layers. Interestingly, a single vacancy defect behaves like a p-type impurity for transport property. Unlike the common beliefs, we observe that the vacancy defect can contribute to greatly increasing the current. Along the zigzag direction, both single and divacancy defects contribute to enhancing the current while the I-V characteristics along the armchair direction are dependent on the defect configurations. Despite this defect configuration dependency, we have found that the current along the armchair direction is always greatly larger than that found along the zigzag direction and the anisotropic current ratio of armchair to zigzag direction is an order of \( 10^3 \). This was supported by NRF (No. 2013R1A1A206071) and by the Supercomputing Center/Korea Institute of Science and Technology Information with supercomputing resources including technical support (KSC-2014-C3-052).

V1.00180 Enhanced superconducting properties of Bi2Sr2CaCu2O8+\( \delta \) thin films by incorporating Iridates nanoparticles, JONGHYUN SONG, JEFFREY VERO, INWOONG HWANG, Chungnam Natl Univ, A.C.L. SANTIGO, University of Philipine, JEONGWON JANG, Korea University, JINHEE KIM, Korea Institute of Science and Standards, R.V. SARMAGO, University of Philipine — We incorporated CaIrO\(_2\) (Ca-iridate) nanoparticles at the interface of Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+\delta}\) (Bi-2212) thin films and substrates by pulsed laser deposition and post-growth ex situ annealing. The density of incorporated Ca-iridate strongly affected the superconducting properties and microstructure of the Bi-2212 thin films. For the incorporation of low density Ca-iridate (450 laser pulses) in the Bi-2212, its superconducting properties enhanced (\( T_{c-onset} = 97 \) K, \( T_{c-zero} = 84 \) K) over those of pure Bi-2212 (\( T_{c-onset} = 94 \) K, \( T_{c-zero} = 80 \) K). However, incorporating a higher density (1,800 pulses) significantly reduced \( T_{c-zero} \), to \( \approx 57 \) K. Incorporating a low density of Ca-iridate also decreased the c-axis lattice constant. Films with incorporated Ca-iridate exhibited greater critical current density, \( J_c(90\)K), than the pure Bi-2212 film. These results indicate that incorporating low densities of Ca-iridate nanoparticles into Bi-2212 can improve its superconducting properties.

V1.00181 Dipolar couplings in Li\(_0.9\)Mo\(_6\)O\(_{17}\) purple bronze, GUOQING WU, Yangzhou University, BING WU, Fayetteville State University — We report the study of the internal magnetic field at the atomic scale at the Li site in the quasi-one-dimensional (Q1D) metal Li\(_0.9\)Mo\(_6\)O\(_{17}\) (purple bronze), with theoretical calculations based on the structure of its crystal lattice and the result of our \(^{7}\)Li-NMR measurements on a single crystal sample at an externally applied magnetic field \( B_0 = 6 - 12 \) T. We find that the anisotropic dipolar couplings to the paramagnetic Mo electron spins are the dominant source of the local magnetic field at the lithium site. Other local magnetic field sources such as the dipolar couplings between the \(^7\)Li to \(^{7}\)Li nuclei, isotropic contact hyperfine couplings to the Mo electron spins, and demagnetization and Lorentz fields are also estimated. Significant changes of the distribution of the dipolar couplings are observed at the "metal-insulator" crossover temperature and lower temperatures along the direction of \( B_0 \parallel c \), indicating a significant local magnetic field inhomogeneity due to the spin effect from the Mo electrons. No evidence of charge effect at the "metal-insulator" crossover temperature or lower temperatures is observed.

V1.00182 \(^{11}\)B NMR Study of HoB\(_4\), MOOHEE LEE, KI-HYEOK KANG, JUNG-HOON KIM, Konkuk University, J.Y. KIM, B.K. CHO, Kwangju Institute of Science and Technology — \(^{11}\)B NMR measurements were performed on a single crystal of HoB\(_4\) to investigate disorder induced effects on the 4\(^f\) spin structures and dynamics. The \(^{11}\)B NMR spectrum, shift, linewidth, \( 1/T_1 \), and \( 1/T_2 \), were measured down to 3.5 K at 8 T perpendicular to the c-axis. Above \( T_N = 5.7 \) K, the \(^{11}\)B NMR linewidth is very large and the shift is also large and negative. In addition, both depend on temperature strongly and increase at lower temperature, which is similar to the susceptibility. This fact confirms that the hyperfine field at the boron site originates from the 4\(^f\) spins of Ho. Below \( T_N \), the \(^{11}\)B NMR spectrum shows a single broad shape with an extremely large linewidth. This behavior is an unexpected result compared with usual NMR spectra in an ordered state for a single crystal specimen, where the single broad peak splits into several narrow peaks below \( T_N \), because of the different local magnetic fields at the each boron sites in the AF state. Considering frustration and disorder effects on the NMR data, we conclude that this behavior originates from the magnetic frustration and quadrupole moment disorder effects on the NMR static data. Above \( T_N \), the both rates are very large and then increase toward \( T_N \). Below \( T_N \), the both rates decrease tremendously.

V1.00183 Casimir Levitation: Stabilization of a neutral atom above a dielectric ring, JOHN JOSEPH MARCHETTA, None — Levitation, in popular culture, is the phenomenon of an object rising against gravity by supernatural means. However, levitation is not the work of anything supernatural, nor do you need to have attended Hogwarts School of Witchcraft and Wizardry in order to learn how to achieve it. The goal of my project is to propose a method to levitate a neutral, anisotropically polarizable, atom above a dielectric ring using the Casimir effect. In particular, we have already shown that an anisotropically polarizable atom experiences a repulsive force when it approaches the dielectric ring along the symmetry axis of the ring. But, the atom is not stable on this axis. We are working on the proposal that a spinning anisotropically polarizable atom above a dielectric ring will achieve stability, and thus get trapped. Our goal is to prove this very appealing hypothesis analytically.

V1.00184 RF-sputtered NbN superconducting thin film for the usage as an electrode of graphene FET and a flexible superconducting wire, Jeong-Gyun Kim, Haeyeong Kang, Jong-Gyu Kim, Young Hee Lee, Dongseok Su, CINAP, IBS, DOES, Sungkyunkwan Univ. — Recent report on the usage of NbN as an electrode for two-dimensional electronic system such as graphene encourage the study of noble physical phenomena which makes the injection of superconducting charge carriers into the channel of graphene FET inducing the combination of superconductivity with quantum Hall effect. In this study, we examined NbN thin film deposited by rf-sputtering method in various conditions. We checked the effects of deposition temperature, working pressure, and relative flow-rate ratio between argon and nitrogen gases during sputtering. Structural analysis by XRD and SIMS showed that the NbN film was successfully deposited on the silicon-oxide substrate and the highest T\(_c\) obtained was 10.5K with high Hc2 over 14 T at 5.5K for the film deposited at 600 oC. On the basis of optimal conditions, the change of superconducting properties depending on the deposition temperature was carefully examined for the development of low temperature deposition process that can be applied to the graphene FET fabrication. Additionally we tested the usage of flexible substrate for the deposition of this superconducting material on the purpose of highly flexible superconducting wire with greatly enhanced mechanical properties as reported recently for the MgB\(_2\) superconductor.

1Southern Illinois University
Scanning tunneling microscopy study on new layered superconductor Ta4Pd3Te16 single crystal.

Characterisation of the CDW in the novel superconducting family Na2Ti2X2O7.

Possible importance of charge fluctuation in BiS2 superconductors.

Variable frequency characterization of interaction at nanoscale in linear dynamic AFM.

An ultra-low temperature scanning Hall probe microscope (SHPM) for magnetic imaging below 40 mK.

LF-1mHz/Hz Noise Level Low Temperature Atomic Force & Magnetic Force Microscope (LT-AFM/MFM) in 20mK-300K Temperature Range.
V1.00192 Development of low temperature scanning tunneling microscope and test results at university of ulsan (Korea)1, SANG-UI KIM, JUNGDAE KIM, Department of Physics and EHSRC, University of Ulsan, Ulsan, 680-749, Korea — Thanks to the development of software and electronics in the last few decades along with advanced UHV technology, the scanning tunneling microscope (STM) has made a tremendous impact on various fields of surface science. In order to build an STM system and make it perform as expected, every component of STM needs to serve the others well. Recent progress on the development of low temperature STM at University of Ulsan (Korea) will be discussed. Advantages of our STM system are following: (1) compact design with in-situ sample preparation and tip/sample exchange capability, (2) simple and effective vibration isolation damper, (3) copper-stainless steel welding technique for cryostat, (4) simple liquid helium bath pumping setup for tunneling spectroscopy. Results of recent performance test will be discussed as well. *kimjud@ulsan.ac.kr

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V1.00193 The SQCRAMscope: Scanning Quantum CRyogenic Atom Microscope . RICHARD TURNER, JACK DISCIACCA, SHENGLAN QIAO, BENJAMIN LEV, Stanford University — Microscopy techniques co-opted from nonlinear optics and high energy physics have complemented solid-state probes in elucidating exotic order manifest in condensed matter materials. Up until now, however, no attempts have been made to use modern techniques of ultracold atomic physics to directly explore properties of strongly correlated or topologically protected materials. This poster will present the SQCRAMscope, a novel Scanning Quantum Cryogenic Atom Microscope technique for imaging magnetic and electric fields near cryogenically cooled materials. With our SQCRAMscope, we aim to image inhomogeneous transport and domain percolation in technologically relevant materials whose order has evaded elucidation.


V1.00195 Biological Cell Manipulation by Magnetic Nanoparticles , ALEXANDER KHITUN, FREDERICK GERTZ, University of California Riverside — We report experimental data on biological cells (erythrocytes) manipulation by magnetic (Fe3O4) nanoparticles. The experiments were accomplished on the top of the device consisting of two conducting contours. An electric current flowing through these contours generates a non-uniform magnetic field making magnetic nanoparticles to move towards the magnetic energy minima. In turn, magnetic nanoparticles drag biological cells in the same direction. We present experimental data showing cell manipulation by controlling the electric current. This technique allows us to capture and move cells located in the vicinity (5-10 microns) of the current-carrying wires. One of the most interesting results shows a periodic motion of erythrocytes, which frequency is controlled by the electric circuit. The obtained results demonstrate the feasibility of non-destructive cell manipulation by magnetic nanoparticles with micrometer-scale precision.

V1.00196 The Extended Core Coax: A Novel Nanoarchitecture for Electrochemical Sensing of Infectious Disease Biomarkers1, AMY E. VALERA, MICHELLE M. ARCHIBALD, JEFFREY R. NAUGHTON, TIMOTHY CONNOLLY, MICHAEL J. BURNS, THOMAS C. CHILES, MICHAEL J. NAUGHTON, Boston College — We report the development and fabrication of a novel nanoarchitecture for electrochemical sensing, the extended core coax (ECC). Each ECC is a vertically oriented nanocoax, comprised of an extended inner metal core and an outer metal shield, separated by a dielectric annulus. The inner (gold) and outer (chrome) metals serve as the working and counter electrodes, respectively, with the gold core working electrode, which protrudes ∼200 nm above the shield of the ECC. Additionally, the extended gold core provides a substrate for biofunctionalization, making the ECC an attractive candidate for further development towards electrochemical detection of infectious disease biomarkers such as cholera toxin. [1] B. Rizal, et al., Anal. Chem. 85, 10040 (2013).

1Support from W.M. Keck Foundation and NIH/NIAID (AI100216).

V1.00197 Fabrication and characterization of MoS2 chemiresistor for pH sensing , FENG ZHAO, ALLEN LIM, ZECONG FANG, School of Engineering and Computer Science, Washington State University Vancouver — Chemical and biological sensing is critical in security, driving, navigation and other applications. Development and implementation of sensors with adaptable parameters would provide optimal use of sensing resources. Voltage-tunable, three-dimensional nanoscale profile created by charged quantum dots provides an effective tool to manage nanoscale processes. We experimentally investigate the effects of selective bipolar doping of quantum dot media on the dark current, noise current, photoresponse, and photoelectron lifetime. We also study the redistribution of the built-in dot charge under the voltage bias and tunability of the above characteristics. The preliminary results show a strong effect of nanoscale barriers on noise and photoresponse characteristics of IR nanomaterials.

V1.00198 Adaptable Quantum Dot Nanomaterials for IR Sensing , XIANZHANG, ANDREI SERGEEV, VLADIMIR MITIN, State Univ of NY - Buffalo, KIMBERLY SABLON, U.S. Army Research Laboratory, MICHAEL YAKIMOVA, SERGE OKTYABRYSKAYA, State Univ of NY - Albany, STATE UNIV OF NY - BUFFALO TEAM. U.S. ARMY RESEARCH LABORATORY COLLABORATION, STATE UNIV OF NY - ALBANY COLLABORATION — IR nanomaterials with the effective control of photoelectron processes will strongly enhance sensing technologies for security, driving, navigation and other applications. Development and implementation of sensors with adaptable parameters would provide optimal use of sensing resources. Voltage-tunable, three-dimensional nanoscale profile created by charged quantum dots provides an effective tool to manage nanoscale processes. We experimentally investigate the effects of selective bipolar doping of quantum dot media on the dark current, noise current, photoresponse, and photoelectron lifetime. We also study the redistribution of the built-in dot charge under the voltage bias and tunability of the above characteristics. The preliminary results show a strong effect of nanoscale barriers on noise and photoresponse characteristics of IR nanomaterials.
V1.00199 High performance multilayer surface plasmon sensors, KUNAL TIWARI, SURESH SHARMA, NADER HOZHABRI, University of Texas at Arlington — Though high performance SPR sensors are readily available, it remains desirable to fabricate sensors with enhanced sensitivity, resolution and evanescent fields for numerous applications. Since SPR characteristics of bimetallic (Ag/Au) and bimetallic waveguide coupled (Bi-WC) sensors are known to be better than those of single metal sensors, we have undertaken investigations of the performance of multilayer structures. We employ the transfer matrix method (TMM) for calculating SPR characteristics of such structures as functions of Ag/Au and Si$_3$N$_4$ waveguide thickness. Several quartz/Ag/Si$_3$N$_4$/Au structures were deposited in a class-100 clean room facility. The thicknesses of Ag and Au were fixed at 35 and 28 nm respectively. However, the thickness of the intermediate Si$_3$N$_4$ waveguide layer was varied from 50 - 150 nm. The SPR curves were measured for all these structures by using the Kretschmann configuration system. We observe excellent agreement between the experimental SPR data and computational results. For an optimized 150 nm thickness of Si$_3$N$_4$ waveguide, we observe high sensitivity to changes in the refractive index ($n$, $\approx$ 520/RIU), extremely narrow SPR curves ($FWHM \lesssim 0.28$, yielding high figure-of-merit of 60-180) and increased decay length of evanescent fields ($\delta \approx 258 \text{ nm}$).


V1.00200 Study of parameters for designing Barkhausen noise sensing elements using finite element analysis, NEELAM PRABHU GAUNKAR, ORFEAS KYPRIS, CAJETAN NLEBEDIM, DAVID JILES, Department of Electrical and Computer Engineering, Iowa State University — Barkhausen noise emissions occur in ferromagnetic materials on application of externally varying magnetic field. These emissions primarily occur due to the presence of pinning sites or discontinuities within the material which act as inhibitors to domain wall motion. The emissions can be sensed using an induction coil placed above the sample. This coil senses the variations in magnetic flux which translates to the induced emf. In this study, we optimize the design of the sensing coil with finite element simulations. The selection of optimum number of turns, choice of sensor core material and arrangement will be discussed. The approach to optimization of the sense-coil design will be presented.

V1.00201 Design details of a new positron beam system for materials studies$^1$, Z. H. LIM, R. GLADEN, VARGHESE ANTO CHIRAYATH, P.V. Joglekar, K. Shastery, A.R. Koymen, A.H. Weiss, Univ of Texas, Arlington — We report here the current status of the development of a state of the art high flux variable energy spin-polarized positron beam facility. Monoenergetic positrons are obtained using high efficiency rare gas moderator (RGM-1). This will allow us to collect data 100 times faster than our current beam system. This beam line will include a 2 meters Time-Of-Flight (TOF) tube, which will result in a higher energy resolution for the TOF spectrometer. The design of the beam line also allows for ambient pressure two gamma coincidence measurements. The ultra-high vacuum system for the beam line has been constructed and was tested for a vacuum of ~ 10$^{-8}$ mbar. The magnetic field for the positron transport has been achieved using a combination of Helmholtz and a series of short solenoid coils, and the magnetic field is ~ 40-100 gauss along the beam line. The E x B positron energy filter and the transport magnetic field were successfully tested using an electron beam. We will discuss the installation of the RGM-1 and the 2 meters TOF spectrometer to the beam line and the final beam tuning in conjunction with the SIMION simulation.

$^1$NSF DMR MRI 1338130

V1.00202 Simulation of the positron and electron trajectories for a new Time of flight (TOF) Spectrometer for positron annihilation induced Auger electron spectroscopy (PAES) with high flux positron beam$^1$, R. GLADEN, Z. H. LIM, VARGHESE ANTO CHIRAYATH, P. V. Joglekar, K. Shastery, A. R. Koymen, A. H. Weiss, Univ of Texas, Arlington — A new high flux positron beam line is under construction for TOF-PAES as well as for spin polarized coincidence Doppler broadening spectroscopy for surface characterization at the University of Texas at Arlington (UTA). This beam line has a high efficiency rare gas moderator system and employs a combination of axial and transverse magnetic fields for the selection of positron beam energy. The moderator system feeds the mono-energetic positron beam into the TOF-PAES system where transverse electromagnetic fields (trophoidal analyzer) allow the simultaneous passage of the positron beam and the electrons emitted from the sample. Here we describe the characteristics of the positron beam trajectories from the source to the target through this beam line using SIMION. These simulations have been used to optimize the axial and transverse magnetic field values at the energy selector as well as the electrostatic potentials at the trochoideal energy analyzer. The trajectories of the secondary electrons ejected from the sample as a result of the positron beam interaction are also described for various ejection angles and energies. These later simulations have been utilized to optimize the height of the channel plate used for the detection of electrons.

$^1$NSF DMR MRI 1338130

V1.00203 Anomalous scattering and redirection of sound in narrow liquid channels, ANDRIII BOZHKO, ARKADII KROKHIN, University of North Texas, VICTOR M. GARCIA-CHOCANO, JOSÉ SÁNCHEZ-DEHESA, Universidad Politécnica de Valencia — Propagation of sonic waves through a finite-length channel clad between two identical liquid-immersed metal plates with accounting for excitation of coupled surface Rayleigh waves propagating near metal-liquid interfaces is studied. The transmission coefficient is calculated for the wide range of frequencies of the incident sound wave, $f = 0.2 \pm 1.4 \text{ MHz}$. At discrete frequencies the transmission and reflection is anomalously suppressed that is shown to be accompanied by unusual redirection of sound from the liquid into metal at the edges of the channel. Proposed theory is in excellent agreement with experimental data obtained for water channels formed by Al and Cu plates.

V1.00204 Development and Characterization of Dynamic Light Scattering Instrumentation to Determine Nanoparticle Size$^1$, T.J. SEBASTIAN, J. HARDING, T. VOLPE, J.R. SIMPSON, M. SCHULZE, S.M. LEV, Towson Univ — Dynamic Light Scattering (DLS) provides a high-throughput and quantitative measurement of particle sizes for monodisperse (MD) spherical nanoparticles (NPs). We report on the development and characterization of homebuilt DLS instrumentation to measure the size of MD NPs of gold, polystyrene, and ZnO. HeNe and Ar-ion lasers comprise the excitation sources for the scattering experiment. An avalanche photodiode detects scattered light and an autocorrelation card analyzes the signal to provide a measurement of the translational diffusion coefficient, which for MD and spherical particles allows for the determination of NP radius. We have tested our apparatus using commercially produced gold NPs in the range of 10 nm to 200 nm and synthesized ZnO NPs. DLS measurements were compared to those obtained by Atomic Force Microscopy (AFM). After size characterization, the ZnO NPs will be employed in ongoing toxicity studies.

$^1$T.J.S. and J.H. acknowledge support from Towson University. J.R.S., M.S. and S.M.L. acknowledge support from NSF - CBET #1236083.
V1.00205 Super-resolution imaging using fluorescent soft micro-lens, KEXIN JIAO, PUNIT KOHLI, Department of Chemistry and Biochemistry, Southern Illinois University Carbondale, ANNIE LU, SRINIVASA RAGHAVAN, Department of Chemical & Biomolecular Engineering, University of Maryland, PUNIT KOHLI TEAM, SRINIVASA R. RAGHAVAN COLLABORATION — Spatial resolution of conventional optical microscope is limited by the diffraction of roughly half the wavelength of the incident light. Among strategies of obtaining resolution beyond the diffraction limit, near-field scanning optical microscopy (NSOM) is widely used. In previous work, we performed NSOM using a simple design constituted by attaching a glass micro-lens (MLs) or a liquid MLs on a cantilever. However, NSOM achieves super-high resolution sacrificing its mobility and imaging speed comparing with far-field imaging, especially when the specimen has uneven surfaces. In this work, we showed that a polydimethylsiloxane (PDMS) micro-sized sphere can be used as MLs as well. Images having enhanced contrast resolutions were achieved when the PDMS MLs was mechanically deformed along z-axis. On the other hand, the focal length of PDMS MLs can be tuned when being deformed by the pressure along x-axis. The scanning mobility of the whole device was further improved when attaching PDMS MLs onto a flexible cantilever. We also introduced different fluorophores into PDMS spheres, which resulting fluorescent MLs (FMLs). The advantages of FMLs involve the feasibility of locating MLs during a fluorescent imaging while having tunable focal length.

V1.00206 Compact scanning probe microscope with 3-D positioning capabilities, FERNANDO GARCIA, JORGE OLIVARES, FRANCISCO OLVERA, JULIE GERZINA, ALEX DE LOZANNE, University of Texas at Austin — We developed a new design for scanning probe microscopes (SPM) intended for low temperature operation. The main design philosophy is to make the SPM body compact and rigid, with an outer diameter of one inch. A secondary goal is to make this instrument easier to build, use and repair compared to our previous designs. While all the positioners are based on the stick-slip principle, the motion along the three axes is implemented very differently: motion along Z, or tip-sample approach, is accomplished by two vertical rods running along the length of the body. Motion along X is done by sliding on a single rod, and along Y by sliding the sample stage on top of the tube scanner used for generating images. Initial test results will be presented.

V1.00207 Photon Counting with an Embedded Micro Mojo V3 FPGA, SARA LENTRICCHIA, CARL GROSSMAN, Swarthmore College — We used an inexpensive Field Programmable Gate Array (FPGA) to generate time stamps from a photon counting experiment. The FPGA was configured to receive signals from an avalanche photodiode, latch onto a 32 bit, 400 MHz clock/counter, and transmit the time stamps to a host computer. These time stamps were then analyzed on the host machine in real time to calculate the intensity auto-correlation function of the signal source, in our case a fluorescence correlation spectroscopy experiment. The basic state machines for the system are a clock/counter/trigger, FIFO data buffer, and serial I/O to an onboard processor that handles communication with the host. The trigger state machine is similar to a clock except the cycle is based on the signal positive edge. The trigger cycle stores the counter and initiates data transfer to the FIFO buffer.

V1.00208 Construction for Cryogen free 3He/4He dilution refrigerator integrated with conduction cooled 15T magnet, JUNGHYUN SHIN, SUN-GYU PARK, EUNSEONG KIM, Center for Supersolid and Quantum matter Research and Department of physics, KAIST — We constructed a cryogen-free 3He/4He dilution refrigerator (DR) integrated with a conduction cooled 15T superconducting magnet. The integrated magnet and 3He/4He dilution system is precooled by a commercial two stage pulse tube refrigerator (PTR). 3He/4He mixture gas compressed at 4 Bar is first introduced into the heat exchangers mounted on the first (40K) and the second (2.5K) stage of PTR. The mixture is condensed at the second stage without Joule-Thomson stage due to its high pressure. Once the liquid 3He/4He mixture is obtained, a conventional DR design including a still, counterflow heat exchangers, and a mixing chamber is adopted for the continuous operation. The 15T superconducting magnet is directly connected to the second stage and cooled by conduction cooling down to about 3K after being pre-cooled with liquid N2 flow. The current leads for superconducting magnet up to 120A require careful considerations of low thermal-conductance with high electrical-conductance and robust electrical isolation.

V1.00209 The power of three-dimensional imaging for an unambiguous identification of the ro-vibrational state of H$_2^+$, D$_2^+$, and HD$^{+1}$, J.B. SAUZI, C.I. GUILLEN, A.C. DUOT, V.M. ANDRIANARUADNO, Department of Physics, Pacific Union College, Angwin, CA 94508 — We are presenting a three-dimensional imaging technique that could efficiently measure the ro-vibrational states of small diatomic molecular ions such as H$_2^+$ in two steps. First, the molecular ion is sent toward a jet of alkali atoms to undergo a resonant dissipative charge exchange. Then, the positions of the fragments and their flight time difference are measured with two position sensitive detectors. From these measurements, we obtained the value of the kinetic energy release, which is directly related to the original vibrational excitation of H$_2^+$. This technique scheme was first developed by D. P. de Brujin and J. Los (Rev. Sci. Instrum. 53, 1020, 1982). Details and examples will be presented.

V1.00210 The speed of light is the inflection point matter and dark matter, YONGQUAN HAN, 15811860790 — The gravitational field of the object is due to radiation and rotation. The reason of the objects can radiation is that linear velocity of objects rotation is less than the speed of light. When the linear velocity of object rotation is equal to the speed of light, the object won’t radiate any more, radiate particle(electromagnetic wave particle) rotate by the radius of itself radius, now the state is the inflection point of the matter and dark matter. The rotation of the object’s gravitational field radius equal to the radius of the object, and then continue to change that is dark matter, the velocity of dark matter rotation is faster than the light. Dark matter rotation doesn’t radiate. The gravitational field radius is equal to the radius of the dark matter, that is why dark matter is difficult to be observed also detected. The curvature of the radiation—the the linear velocity of the object divide the speed of the light. The rotation speed of the object—the speed of light multiply the linear velocity and then divide the radius of the object.

V1.00211 Examination of Humidity Effects on Measured Thickness and Interfacial Phenomena of Exfoliated Graphene on SiO$_2$ via AC-AFM, KATHERINE JINKINS, JORGE CAMACHO, LEE FARINA, YAN WU, Univ of Wisconsin, Platteville — Tapping (AC) mode Atomic Force Microscopy (AFM) is commonly used to determine the thickness of graphene samples. However, AFM measurements have been shown to be sensitive to environmental conditions such as adsorbed water, in turn dependent on relative humidity (RH). In the present study, AC-AFM is used to measure the thickness and loss tangent of exfoliated graphene on silicon dioxide (SiO$_2$) as RH is increased from 10% to 80%. We show that the measured thickness of graphene is dependent on RH. Loss tangent is an AFM imaging technique that interprets the phase information as a relationship between the stored and dissipated energy in the tip-sample interaction. This study demonstrates the loss tangent of the graphene and oxide regions are both affected by humidity, with generally higher loss tangent for graphene than SiO$_2$. As RH increases, we observe the loss tangent of both materials approaches the same value. We hypothesize that there is a layer of water trapped between the graphene and SiO$_2$ substrate to explain this observation. Using this interpretation, the loss tangent images also indicate movement and change in this trapped water layer as RH increases, which impacts the measured thickness of graphene using AC-AFM.
V1.00213 Long-range interaction of anisotropic systems. JUN-YI ZHANG, UDO SCHWINGENSCHLÖGL. Division of Physical Science & Engineering, King Abdullah University of Science and Technology — The first-order electrostatic interaction energy between two far-apart anisotropic atoms depends not only on the distance between them but also on their relative orientation, according to Rayleigh Schrödinger perturbation theory. Using the first-order interaction energy and the continuum model, we study the long-range interaction between a pair of parallel graphene sheets. The asymptotic form of the obtained potential density, \( \epsilon(D) \propto -D^{-3} - O(D^{-4}) \), is consistent with the random phase approximation and Lifshitz theory. Accordingly, neglectance of the anisotropy, especially the nonzero first-order interaction energy, is the reason that the widely used Lennard-Jones potential approach and dispersion-corrections in density functional theory give a wrong asymptotic form, \( \epsilon(D) \propto -D^{-4} \).

This work is supported by the King Abdullah University of Science and Technology (KAUST).

V1.00214 Moments and Lanczos Study of the Anisotropic One Dimensional XY Model in a Skewed Magnetic Field, JUN HUI LIANG, ZHI HUA CHENG, YICK HONG CHAN, Kingsborough Community College of CUNY, ERIC ASHENDORF, Brooklyn College, J.D. MANCINI, Kingsborough Community College of CUNY, V. FESSATIDIS, Fordham University, S.P. BOWEN, Chicago State University — Here we wish to study the ground-state and energy gap of the one dimensional spin \( \frac{1}{2} \) anisotropic antiferromagnetic XY Heisenberg model given by

\[
H = \sum_{i=1}^{N} \left[ (1 + \gamma) S_i^x S_{i+1}^x + (1 - \gamma) S_i^y S_{i+1}^y - h (1)^i S_i^z \right]
\]

where \( \gamma \) is the anisotropy parameter and \( h \) is an external magnetic field. We shall investigate the ground-state energy as well as the energy gap as a function of both the anisotropy parameter as well as the number of holes as a function of the external magnetic field.

Authors Liang, Cheng, Chan, and Ashendorf are undergraduate students.

V1.00215 Moments and Lanczos Study of the Anisotropic One Dimensional \( t-J \) Model with Holes, YICK HONG CHAN, JUN HUI LIANG, ZHI HUA CHENG, Kingsborough Community College of CUNY, ERIC ASHENDORF, Brooklyn College, J.D. MANCINI, Kingsborough Community College of CUNY, V. FESSATIDIS, Fordham University, S.P. BOWEN, Chicago State University — In this work we wish to study the ground-state energy as well as the energy gap of the one-dimensional \( t-J \) model given by

\[
H = \sum_{i} \left[ S_{i+1}^x S_i^x + \frac{1}{2} \alpha \left( S_{i+1}^y S_i^y + S_{i+1}^z S_i^z \right) \right]
\]

where \( \alpha \) is the anisotropy parameter. We will investigate both the ground-state energy as well as the energy gap as the number of holes is increased for lattices of length 16 sites.

Authors Chan, Liang, Cheng, and Ashendorf are undergraduate students.

V1.00216 A Variational Moments Approach to the One Dimensional Hubbard Model, ZHI HUA CHENG, YICK HONG CHAN, JUN HUI LIANG, Kingsborough Community College of CUNY, ERIC ASHENDORF, Brooklyn College, J.D. MANCINI, Kingsborough Community College of CUNY, V. FESSATIDIS, Fordham University, S.P. BOWEN, Chicago State University — In this work we shall study the one dimensional Hubbard model

\[
H = t \sum_{i=1}^{N} c_i^\dagger c_i \delta_{ij} + \frac{1}{2} \alpha \left( c_i^\dagger c_{i+1}^\dagger c_i^\sigma c_{i+1} + c_i^\dagger c_{i+1}^\dagger c_{i+1}^\sigma c_{i} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}
\]

using both a connected moments approach as well as a Lanczos triadiagonal scheme. Following the work of Eichenberger and Baeriswyl (PRB 76, 180504(R), 2007) we use a modified variational wavefunction which includes the hopping term of the Hamiltonian. Our results show a marked improvement in our estimation of the ground-state energy in the region of intermediate coupling \( t/U \approx 0.1 \).

Zhi Hua Cheng, Yick Hong Chan, Jun Hui Liang and Eric Ashendorf are undergraduate students.

V1.00217 Quantum Monte Carlo Applied to Binary Transition Metal-Oxides, JUAN A. SANTANA, Oak Ridge Assoc Univ, JARON T. KROGEL, CHANDRIMA MITRA, PAUL R.C. KENT, FERNANDO REBOREDO, Oak Ridge National Laboratory — Materials based on transition metal-oxides (TMO) play a central role in many applications and in the fundamental research of advanced materials. However, this class of materials is one of the most challenging for computation. The standard computational methods to study them are based on Density Functional Theory (DFT), which often fails to provide the required level of accuracy. A natural solution to overcome the intrinsic limitations of DFT approximations is to directly solve the many-body problem in TMO. For large systems, this can be made practical by applying quantum Monte Carlo (QMC) methods. These methods are very expensive computationally, but recent developments in algorithms and computational infrastructures have enabled their application to real materials. We will show that QMC methods, such as diffusion Monte Carlo (DMC), are now practical to study multiple properties of TMO. The application of DMC to study the structural, electronic and ionic defect properties of various binary TMO, including FeO, CoO, NiO, and ZnO will be discussed. We will also outline current limitations in hardware and algorithms.

The work is supported by the Materials Sciences & Engineering Division of the Office of Basic Energy Sciences, U.S. Department of Energy (DOE).
V1.00218 A GPU enhanced approach to identify atomic vacancies in solids materials\textsuperscript{1}. JOAQUIN PERALTA, CLAUDIA LOYOLA, Universidad Andres Bello, SERGIO DAVIS, Universidad de Chile — Identification of vacancies in atomic structures plays a crucial role in the characterization of a material, from structural to dynamical properties. In this work we introduce a computationally improved vacancy recognition technique, based in a previous developed algorithm. The procedure is based in the use of Graphics Processing Unit (GPU) instead of Central Processing Unit (CPU), taking advantage of random number generation as well the use of a large amount of simultaneous threads as available in GPU architecture, improving the spatial mapping in the sample and the speed during the identification process of atomic vacancies. The results show that with this technique, efficiency is improved. Along with the above a reduction of required parameters in comparison with the original algorithm is presented. We show that only the lattice constant and a tunable overlap are enough as input parameters in the process, and are also highly related. A study of those parameters is presented, suggesting how the parameter choice must be addressed. Benchmarks were made using one standard CPU and GPU between the original code and the present work, revealing an improvement in the execution time.

\textsuperscript{1} This work is supported by FONDECYT Iniciacion 2013, 11130501

V1.00219 A Time Parallel Implementation of the Time Decomposition Strategy for the Dirac equation. HYUN LIM, South Dakota State Univ, ARTHUR KURLEJ, University of Massachusetts, Amhrest, JUNG-HAN KIM, South Dakota State Univ — For certain formulations of partial differential equations, proper time-space pre conditioners can be successfully applied in space-time finite element simulations. Such an approach may enable the extraction of more parallelism to better utilize high performance computing resources. In this work, we examine the behavior of the gauge free, low-mass regime Dirac equation using space-time finite elements. The purpose of this research is to present a stable parallel implementation algorithm of the physical system. We discretize space and time together for the entire domain using a finite element space which does not separate space and time basis functions. We also explore the effectiveness of the time decomposition pre conditioner, additive Schwarz preconditioner with KSP (Krylov Subspace Methods) solvers for this problem. We show that proper time parallel implementation allows for physically intuitive boundary conditions, improvement of numerical efficiency, and reduces the overall error of the computed solution

V1.00220 A Multiscale computational approach to predict the elastic deformation fields in Moiré Patterns of 2D van der Waals interfaces and heterostructures. HEMANT KUMAR, VIVEK SHENOY, University of Pennsylvania — Recent technological advancements in isolation and transfer of different 2-dimensional (2D) materials have led to renewed interest in Van der Waals (vdW) heterostructures. We report a multiscale computational method to predict the deformation of vdW heterostructures using density functional theory (DFT) informed continuum simulations. We validate our method by comparing its predictions with all atom atomicistic simulations for the graphene-hBN bilayer system and computing the in-plane strains, local curvature for different misorientation angles between two lattices. We also present closed form solutions for the elastic field as a function of lattice mismatch, relative rotations and predict the deformation fields for MoS2-WSe2, MoSe2-WSe2 systems that have been recently synthesized experimentally.

V1.00221 Atomistic Computational Model of Radiation Damage of Nano-sized Systems in Intense X-ray Pulses\textsuperscript{1}. PHAY HO, CHRISTOPHER KNIGHT, LINDA YOUNG, Argonne National Laboratory — We present a combined Monte-Carlo/molecular- dynamics (MC/MD) computational model that is suitable for monitoring the physics of intense, femtosecond XFEL pulses interacting with complex systems of various sizes, from nanometers to micrometers, and matters of various compositions. In this model, the occurrences of x-ray absorption, ionization, relaxation and electron-impact processes are treated by a MC method, and the subsequent dynamics of the all the electrons, ions and atoms are tracked using an MD method. Our model extends previous MC/MD model and provides new capabilities to probe the impacts of transient states on radiation damage dynamics. Recently, we have added LAMMPS as the driver of MD dynamics. This is a critical addition as now our code can run on Mira, a new petascale supercomputer with 786K core processors at the Argonne Leadership Computing Facility. Also, it can treat micron-sized systems with trillions of particles and both homogeneous and heterogeneous composition. Using our model, we examine the ionization dynamics of Argon clusters in an XFEL pulse as a function of particle sizes and pulse parameters, and we compare our results with the experimental data [S. Schorb \textit{et al.}, \textit{PRL} 108, 233401 (2012)].

\textsuperscript{1} Supported by the Chemical Sciences, Geosciences, and Biosciences Division, Office of Basic Energy Sciences, Office of Science, US Dept of Energy, Contract DE-AC02-06CH11357.

V1.00222 Easy GROMACS: A Graphical User Interface for GROMACS Molecular Dynamics Simulation Package. AYTEN DIZIKIRICI, MUSTAFA TEKPINAR, Yuzuncu Yil University — GROMACS is a widely used molecular dynamics simulation package. Since it is a command driven program, it is difficult to use this program for molecular biologists, biochemists, new graduate students and undergraduate researchers who are interested in molecular dynamics simulations. To alleviate the problem for those researchers, we wrote a graphical user interface that simplifies protein preparation for a classical molecular dynamics simulation. Our program can work with various GROMACS versions and it can be performed essential functions of GROMACS trajectories as well as protein preparation. We named our open source program ‘Easy GROMACS’. Easy GROMACS can give researchers more time for scientific research instead of dealing with technical intricacies.

V1.00223 Calculating Relativistic Transition Matrix Elements for Hydrogenic Atoms Using Monte Carlo Methods. STEVEN ALEXANDER, Southwestern University, R.L. COLDWELL, Retired — The nonrelativistic transition matrix elements for hydrogen atoms can be computed exactly and these expressions are given in a number of classic textbooks. The relativistic counterparts of these equations can also be computed exactly but these expressions have been described in only a few places in the literature. In part, this is because the relativistic equations lack the elegant simplicity of the nonrelativistic equations. In this poster I will describe how variational Monte Carlo methods can be used to calculate the energy and properties of relativistic hydrogen atoms and how the wavefunctions for these systems can be used to calculate transition matrix elements.

V1.00224 Automated discovery of novel solid-state ionic conductors enabled by large-scale molecular dynamics computations. BORIS KOZINSKY, PRATEEK MEHTA, Bosch Research, Cambridge MA — Fast solid-state inorganic Li-ion conductors offer a path toward safer batteries with high energy density, but apart from a few material classes, the inorganic solid-state space remains mostly unexplored. Computational approaches using density functional theory (DFT) have been proven to be successful for the design of electrode materials, but have had few applications for the discovery of electrolytes. This is because the physiochemical factors that regulate ionic conductivity are poorly understood, and conductivity can be very sensitive to small structural and compositional variations. In this work, we present relationships between the ionic conductivity and several potential structural descriptors, like the size and dimensionality of ion-conducting pathways, void fraction, Li-concentration, sensitivity to volume change, etc. We identify these relationships from massive ab-initio molecular dynamics simulations on a comprehensive dataset of approximately 1500 crystalline materials. Our investigation is enabled by computational resources at the Oak Ridge Leadership Computing Facility and the high-throughput automation platform AiiDA.
V1.00225 First Principles Study of Phosphor Host Materials
CLAIRE-ALICE HEBERT, Physics Department, University of California Santa Barbara, RAM SESHADEH, Materials Research Lab, University of California Santa Barbara — Solid state lighting uses light-emitting diodes (LEDs) instead of incandescent filaments. Blue LEDs are combined with an inorganic phosphor consisting of a host lattice doped with Ce$^{3+}$. Electronic transitions between the 4f and 5d levels convert blue light from the diode to light ranging from green (~510 nm) to red (~700 nm) and the combination of yellow with blue creates white light. The most efficient phosphors have been found to have rigid crystal structures, along with band gaps large enough that the 4f to 5d transition of the dopant ion can occur without interference. Using Debye temperature as a proxy for structural rigidity, we use density functional theory (DFT) to calculate and plot $\Theta_D$ versus band gap to give us a prediction of phosphor suitability for forty different materials. PBE functionals and the quasi-harmonic Debye model were used to estimate $\Theta_D$, and band gaps were calculated with a hybrid functional. DFT was also used to probe six potential host materials more closely: AIO$_3$, LaBr$_3$, Ba$_2$SiO$_4$, Sr$_2$SiO$_4$, Sr$_2$Si$_2$N$_8$, and Y$_3$Al$_5$O$_{12}$. The electronic states of these compounds were aligned with vacuum using a supercell slab model and will be compared with the Ce$^{3+}$ levels to determine suitability as host materials.

V1.00226 Transport properties of carbon dioxide and ammonia in water - ethylene glycol mixtures from molecular dynamics simulations
EUGENIYA ISKRENOVA, Air Force Research Laboratory - WPAFB and UES, Inc., SOUMYA S. PATNAIK, Air Force Research Laboratory - WPAFB, OH 45433 — The endothermic decomposition of ammonium carbamate has been proposed as a novel heat sink mechanism for aircraft thermal management (Johnson et al. SAE Technical Paper 2012-01-2190, 2012, doi:10.4271/2012-01-2190). The products of this decomposition are carbon dioxide and ammonia which need to be efficiently removed in order to better control the decomposition reaction. Molecular dynamics simulations can provide insight into the transport properties of carbon dioxide and ammonia in the carrier fluid. In this work, an extensive set of molecular dynamics simulations was performed to better quantify the concentration dependence of solubility and diffusivity of carbon dioxide and ammonia in water, ethylene glycol, and their mixtures at standard temperature and pressure and at elevated temperature. The simulation results confirm the experimental observations that ammonia is more soluble than carbon dioxide in either water or ethylene glycol and that both carbon dioxide and ammonia are more soluble in ethylene glycol than in water. The simulations of water - ethylene glycol mixtures show that increasing the molar fraction of ethylene glycol leads to increased solubility of carbon dioxide and ammonia in the mixture.

V1.00227 A Simple Pythagorean Interpretation of $E^2 = p^2c^2 + (mc^2)^2$
J.A. TOBAR, E.L. VARGAS, V.M. ANDRIANARIJAONA, Department of Physics, Pacific Union College, Angwin, CA 94508 — We are considering the relationship between the relativistic energy, the momentum, and the rest energy, $E^2 = p^2c^2 + (mc^2)^2$, and using geometrical means to analyze each individual portion in a spatial setting. The aforementioned equation suggests that $p$ and $mc^2$ could be thought of as the two axis of a plane. According to de Broglie’s hypothesis $\lambda = h/p$ therefore suggesting that the $p$c-axis is connected to the wave properties of a moving object, and subsequently, the $mc^2$-axis is connected to the particle properties. Consequently, these two axis could represent the particle and wave properties of the moving object. An overview of possible models and meaningful interpretations will be presented.

V1.00228 A Testable Unified Theory That Works
DONALD CHAKERES, The Ohio State University, RICHARD VENTO, Retired, Columbus State Community College — The harmonic neutron hypothesis is a unified theory of a dimensionally consistent harmonic point space defining physical phenomena. It is based on equality-pair transformations (EPTs), of the $n^i$; $e_0^i$; and the Rydberg constant, R, and 3 finite integer sets: $(V_i)$, defined below; the first 12 natural numbers to derive the first generation of particles and bosons; and a finite set of primes for higher generations. All of the derivations/predictions are made using the natural units and the 3 number sets. The purpose is to demonstrate that it is possible to derive, sets of integers, which inter-relate and predict many of the physical constants from Planck time to the Higgs boson starting with just these 4 sets within a harmonic system. All the physical constants are evaluated as frequency equivalent ratios. The fundamental EPT is based on the transformation of electromagnetic energy into matter via the set $(V_i)$, scaled from neutron pair production. Elements $v_i$ in $(V_i)$ are based on the ratio of the annihilation frequency equivalent of the neutron and 1 Hz, $2.271859078 \times 10^{21}$ Hz.

V1.00229 Several notes on physics
XIAO-FAN CHEN, Harbin Institute of Technology — Several notes on physics are presented, which include our views of quantum mechanics, general relativity, special relativity, electric charge, nonlinear electrodynamic, general transformation in hyperspace, solutions to equations of operators, superstring, shapes of particles and statistical mechanics.

V1.00230 SURFACES, INTERFACES AND THIN FILMS

V1.00231 A direct measurement of built-in potential across LaAlO3/SrTiO3(001) heterojunctions
YANG ZHOU, DI WU, Nanjing Univ — The quasi-two-dimensional electron gas (q2DEG) at the oxide interface LaAlO3/SrTiO3 has attracted a lot of attention in recent years due to its rich phenomena. The ?polar catastrophe? model is one of the conducting mechanisms, which relies on the polar potential built-in LaAlO3 layer. Although several experiments have been tried to measure the electrostatic potential in LaAlO3, the magnitude of the polar potential is still under debate.[1][2][3] We present a systematically study on the electronic transport properties of the LaAlO3/SrTiO3 interface capping with several different metals, whose work functions vary from 4.28 to 5.6 eV. The barrier height between the capping layer and the q2DEG estimated by the tunneling resistance shows strong correlation with the metal work function. The carrier density of q2DEG increases as decreasing the capping metal work function. These results strongly suggest the existence of the built-in potential in LaAlO3 and the residual polar potential is estimated to be 1.3 eV. [1]E. Slooten, et al, Phys. Rev. B 87, 085128 (2013). [2]H. Liang, et al, Sci. Rep. 3, 1975 (2013). [3]G. Berner, et al, Phys. Rev. B 88, 115111 (2013).

V1.00232 Surface structures and defect control during epitaxy of crystal
LIXIN ZHANG, Nankai University — In this talk, I will show a few examples in which the surface structures play important roles on the defect incorporation into the crystal lattice. The surface orientations and the atomic structures have strong influence on the solubility, the type, and even the direction of the incorporated defects.

V1.00233 First-principles studies of S-doping and adsorption with hematite $\alpha$-Fe$_2$O$_3$ (0001) film
JIAO AN, PRABATH WANAGURU, QIMING ZHANG, University of Texas at Arlington — Based on spin-polarized density functional theory, we have investigated the atomic, electronic, and magnetic structures of hematite $\alpha$-Fe$_2$O$_3$ (0001) film. An S atom adsorption on the surface of the film has then been studied. The preferred site on the surface has been identified. The changes of the electronic structure of the film have been analyzed when an O atom is substituted by an S atom at different locations inside the film. The change with the concentration of S-doping will also be discussed.

1 The authors gratefully acknowledge the DoD High Performance Computing Centers for computational resources.

2 Authors wish to give special thanks to Pacific Union College Student Senate in Angwin, California, for their financial support.
V1.00234 Revisitation of the frictional properties of Si02 as the LFM (lateral force microscopy) reference1, SUNG HYUN KIM, SUENNE KIM, Department of Applied Physics, Hanyang University — Recently, experimental studies concerning frictional properties at the nanoscale using AFM (atomic force microscopy), specifically with LFM, are made on various kinds of materials including noble 2D graphene sheets and 1D nanotubes. The LFM technique requires calibration of a stable substrate as a reference of importance. Si02 is often used as the standard to calibrate LFM data obtained from a material of interest. However, according to our observation, the friction of cleansed Si02 substrate can change gradually by long-time continuous LFM scanning. The friction increases up to about 1.5 times (50%) in comparison to the initial state while minute topographical difference, at the Å level, is detected. The friction depends on the number of scanning events, and the change follows an inverse exponential function, \( F(t) = A(1-\exp[-Bt]) + F(0) \), where \( F \) is friction, \( t \) means time when continuous measurements are made, and \( A, B, F(0) \) are constants. Here, friction shift accompanied by z-scanner movement has been observed concurrently and corrected for the long-time AFM measurements. In this regard, proper correction for the LFM shift induced by the z-scanner drift will also be introduced.

1This research was supported by Basic Science Research Program through NRF of Korea funded by the ministry of Education(2014R1A1A2056555).

V1.00235 ABSTRACT WITHDRAWN —

V1.00236 Determination of Superlattice Effect on Hafnium nitride/Vanadium nitride Nanostructures, P. PRIETO, CENM Universidad del Valle, J.C. CAICEDO, C. ESCOBAR, Material Department Universidad del Valle, M.E. GOMEZ, CENM Universidad del Valle, MATERIAL DEPARTMENT UNIVALLE TEAM, CENM UNIVALLE TEAM — Binary nitrides multilayers systems were grown on silicon (100) substrates with the aim to study the coherent assembly in HfN/VN material. The multilayers films were grown via reactive r.f. magnetron sputtering technique by systematically varying the bilayer period (\( \Lambda \)) and the bilayer number (\( n \)) while maintaining constant the total coating thickness (\(~2.4 \mu m\)). The multilayers were characterized by High system X-ray diffraction (HA-XRD), low angle X-ray diffraction (LA-XRD), HfN and VN layers were analyzed by X-ray Photoelectron Spectroscopy (XPS) and electron and transmission microscopy (TEM). HA-XRD results showed preferential growth in the face-centered cubic (111) crystal structure for HfN/VN multilayers system with the epitaxial relation (111)[100]HV//\langle200\rangle[100]HV. The maximum coherent assembly was observed with presence of satellite peaks. With this idea, ternary and binary nitrides films have been designed and deposited on Si (100) substrates with bilayer periods (\( \Lambda \)) in a broad range, from nanometers to hundreds of nanometers to study the structural evolution, coherent assembly progress and optical properties like The critical angle, dispersion coefficient, index of refraction for HfN/VN multilayers with decreasing bilayer thickness.

V1.00237 The thickness dependence of surface energy and contact angle of water on ultrathin MoS2 film1, YANHUA GUO, College of Materials Science and Engineering, Nanjing Tech University; Department of Materials Science and Engineering, University of Utah, FENG LIU, Department of Materials Science and Engineering, University of Utah — The properties of ultrathin 2D materials generally show a strong thickness dependence. Using first-principles methods, we have systematically calculated surface energy and surface stress of MoS2 films as a function of thickness from one to 12 layers, using two van der Waals functional based approaches (vdW-DF and DFT-D2). Based on the calculated surface energies, which increases with the increasing thickness, we further analyze the surface contact angle of water droplet on MoS2 film surface using Young’s equation as a function of thickness, in comparison with experiments, from which the water-MoS2 interfacial energy and its MoS2 thickness dependence is derived. These results will be useful for future studies of physical and chemical properties of ultrathin MoS2 films.

1This work is supported by China Scholarship Council (Grant No. 201408320015) and DOE-BES (Grant No. DEFG02-04ER46148).

V1.00238 Integration of a DC magnetron sputtering system into an ultra-high vacuum chamber for fabrication of Schottky diodes1, NICHOLAS Pieniazek, CHRISTOPHER DURCAN, ROBERT RALSON, VEINCENT LABELLA, The College of Nanoscale Science and Engineering — A DC magnetron sputtering system was installed into a UHV chamber for sputtering of metal thin films with little contamination. Control of the DC power, chamber pressure and deposition time is crucial to deposit metal films with reproducible thicknesses and topographies. A graphical user interface was created to efficiently control all potential process variations. Thin films of tungsten were deposited on both n-Si and p-Si using Argon as the ionizing gas. Scanning tunneling microscopy was used in situ to analyze the surface roughness. Ballistic electron emission microscopy was utilized to provide nanometer scale insight into the homogeneity of the tungsten-silicon Schottky barrier.

1Schottky Diode UHV Deposition and Analysis Processes

V1.00239 Depth-Resolved X-Ray Reciprocal Space Mapping for Surface Microstructure Measurements, FRANCES WILLIAMS, Norfolk State University, KELI HU, QIGUANG YANG, UltraHighScore LLC, XIN ZHAO, Vertical Carbon Technologies, Inc. ANNE-MARIE VALENTE-FELICIANO, CHARLES REECE, Thomas Jefferson National Accelerator Facility — A depth-resolved X-ray reciprocal space mapping technology has been developed to investigate crystal microstructures from top of the surface to few micrometers under the surface. The depth-dependent microstructures were successfully used to reveal structure evolution occurred in both crystal-growth process and post growth treatments in few different thin films and/or crystals. Our results show that depth-resolved reciprocal space mapping is a powerful tool to monitor thin film and/or crystal microstructures and provide important information for optimization of the crystal-growth process and post-growth treatments.

V1.00240 Depth of origin of sputtered atoms and isotopic angular distribution of atoms sputtered from metal alloys, NARESH DEOLI, KARL HASENSTEIN, LOUIS HOUSTON, Univ of Louisiana, DUNCAN WEATHERS, Univ of North Texas, LOUISIANA ACCELERATOR CENTER TEAM, ION BEAM MODIFICATION AND ANALYSIS LABORATORY COLLABORATION — Angular distribution of atoms sputtered from the surface and the near surface region under ion bombardment provides critical information about the sputtering mechanism. In the present study Monte-Carlo based SRIM simulation is used to explore the depth dependent energy and angular distribution of the sputtered atoms from liquid metal alloys, Ga:In and Ga:Bi, using normally incident keV Ar ions. These alloys are known to exhibit Gibbvsan segregation where lightly bound species tend to segregate on the top of the alloy. The isotopic distributions of sputtered atoms from the alloy are also presented.
the thermal conductivity $\kappa$ showed that the conductivity and thermoelectric power are conveyed by electrons with different effective masses in the Brillouin zone. In point of view masses contribute to different transport phenomena in the crystal. The discrepancy between the effective mass for the conductivity and the thermoelectric mechanism behind the high power factor from calculation about the transport properties. The key to understanding the power factor is that different effective calculation about layered oxychalcogenides. In addition, we calculated thermoelectric properties Blotch-Boltzmann equation, semi-classically. We indicate the for new type thermoelectric materials. Firstly, from DFT and DFPT calculations, we performed the electronic structure calculation and the thermal structure FUNASHIMA, Osaka Univ — In order to restrain global warming and realize a sustainable global energy system, the researches of various energy resources are

thin 2D crystals, including graphene, hexagonal boron nitride (hBN), molybdenum disulphide (MoS$_2$) etc.; at the same time pristine graphene and other 2D materials are impermeable to molecules and atoms including helium. Protons represent somewhat intermediate case, which, together with the fact that hydrogen technologies are extremely important nowadays, motivated us to study proton permeation through thin 2D crystals. Employing both liquid and solid proton conducting electrolytes we demonstrate that monolayers of graphane and hBN are permeable to protons at ambient conditions, while MoS$_2$, bilayer graphene and multilayer hBN show no proton conduction. Temperature dependence confirms the thermionic nature of the proton permeation with the activation energies of 0.3, 0.6 and 0.8 eV for monolayer hBN, monolayer graphene and bilayer hBN, respectively. Our findings suggest that atomically thin crystals can be promising for various hydrogen technologies, for instance, as proton exchange membranes for fuel cells.

Visualization of Exciton Transport in Molecular and Quantum Dot Solids, GLEB AKSELROD, PARAG DEOTARE, FERRY PRINS, NICHOLAS THOMPSON, LISA POULIKAKOS, ELIZABETH LEE, MARK WEIDMAN, JOLENE MORK, JIYE LEE, ADAM WILLARD, MARCO BALDO, Center for Excitons, Center of Materials Science, Massachusetts Institute of Technology, VINOD MÉNON, City College of New York, WILLIAM TISDALE, VLADIMIR BULOVIC, Center for Excitons, Massachusetts Institute of Technology — Transport of nanoscale energy in the form excitons is at the core of the operation of a wide range of nanostructured optoelectronic devices such as solar cells, light emitting diodes and excitonic transistors. Particularly important is the relationship between exciton transport and nanoscale disorder, the defining characteristic of molecular and nanostructured materials. Here we report a spatial, temporal, and spectral visualization of exciton transport in molecular crystals and quantum dot solids. Using tetracene as an archetype molecular crystal, the imaging reveals that exciton transport occurs by random walk diffusion, with a transition to subdiffusion as excitons become trapped. By controlling the morphology of tetracene, we show that the transition to subdiffusive transport occurs at earlier times as disorder is increased. In colloidal quantum dot films, we show that diffusion does not occur by a random-walk process; instead, energetic disorder causes the exciton diffusivity to decrease over time. Our findings demonstrate that the mechanism of exciton transport depends strongly on the nanoscale morphology and disorder.

Self-consistent theory of helium atom scattering by a thermally excited monolayer solid, L.W. BRUCH, Dept. of Physics, Univ of Wisconsin-Madison, F.Y. HANSEN, Dept. of Chemistry, Technical University of Denmark — The inelastic scattering of a helium atom beam by an incommensurate monolayer solid of Xe/Ph(111) for incident energies in the range 4 – 16 meV and monolayer temperatures of 25 – 75 K is evaluated self-consistently (SC) in the one-phonon approximation. The target is very corrugated and the final scattering state comprises strong diffraction and inelastic terms. At 50 and 75 K, the atom energy gain (phonon annihilation) processes have strength comparable to the energy loss (phonon creation) processes; there are pervasive and large departures from expectations based on weak-coupling detailed balance ratios. The SC results are compared to experimental data and to results from a simpler non-self-consistent approximation (NSC) that relies on harmonic approximations to the Debye-Waller attenuations of elastic and inelastic strengths. There are major differences in the trends seen in the SC and NSC results.

EN能, RESEARCH AND APPLICATIONS

Transient Heat Conduction in Strongly Correlated Systems, RITA AGHJAYAN, ARTHUR LUNIEWSKI, KAMIL WALCZAK, Department of Chemistry and Physical Sciences, Pace University, 1 Pace Plaza, New York, NY 10038, NANOscale PHYSICS DIVISION TEAM — We examine the electronic heat transport phenomena in nanoscale junctions composed of organic molecules weakly coupled to two heat reservoirs of different temperatures. The electronic heat flux and its dynamical noise properties are calculated within the scattering (Landauer) formalism with the transmission probability determined by using non-equilibrium Green’s functions technique. The perturbative computational scheme is used to determine nonlinear corrections to the electronic heat flux and its noise power spectral density with up to the second order terms in relation to the temperature difference. Our results show the limited applicability of ballistic Fourier’s law and the fluctuation-dissipation relations to nanoscale heat flow carried by electrons. Further, we discuss the influence of quantum interference and dimensionality of heat reservoirs onto the transport characteristics and shot noise spectra related to molecular systems under consideration. Importantly, the nonlinear transport theory developed by us may be extended to higher order terms to address a huge variety of problems associated with nonlinear thermal effects, which may occur at nanoscale.

Nonlinearities and Noise Properties of Electronic Heat Transfer in Molecular Junctions, ARTHUR LUNIEWSKI, RITA AGHJAYAN, KAMIL WALCZAK, Department of Chemistry and Physical Sciences, Pace University, 1 Pace Plaza, New York City, NY 10038, NANOscale PHYSICS DIVISION TEAM — We examine the electronic heat transport phenomena in nanoscale junctions composed of organic molecules weakly coupled to two heat reservoirs of different temperatures. The electronic heat flux and its dynamical noise properties are calculated within the scattering (Landauer) formalism with the transmission probability determined by using non-equilibrium Green’s functions technique. The perturbative computational scheme is used to determine nonlinear corrections to the electronic heat flux and its noise power spectral density with up to the second order terms in relation to the temperature difference. Our results show the limited applicability of ballistic Fourier’s law and the fluctuation-dissipation relations to nanoscale heat flow carried by electrons. Further, we discuss the influence of quantum interference and dimensionality of heat reservoirs onto the transport characteristics and shot noise spectra related to molecular systems under consideration. Importantly, the nonlinear transport theory developed by us may be extended to higher order terms to address a huge variety of problems associated with nonlinear thermal effects, which may occur at nanoscale.

Theoretical Study of Layered Oxychalcogenides as Thermoelectric Materials, HIROKI FUNASHIMA, Osaka Univ — In order to restrain global warming and realize a sustainable global energy system, the researches of various energy resources are done. In these various energy resources, attracted technology is thermoelectric technology. Recently Layered oxychalcogenides has interesting properties useful for new type thermoelectric materials. Firstly, from DFT and DFPT calculations, we performed the electronic structure calculation and the thermal structure calculation about layered oxychalcogenides. In addition, we calculated thermoelectric properties Blotch-Boltzmann equation, semi-classically. We indicate the mechanism behind the high power factor from calculation about the transport properties. The key to understanding the power factor is that different effective masses contribute to different transport phenomena in the crystal. The discrepancy between the effective mass for the conductivity and the thermoelectric power showed that the conductivity and thermoelectric power are conveyed by electrons with different effective masses in the Brillouin zone. In point of view the thermal conductivity $\kappa$, we discuss the electronic part $\kappa_e$ from Bloch-Boltzmann equations, and $\kappa_{ph}$ from DFT calculations.
V1.00248 Separating Lattice and Electronic Thermal Conductivity Contributions in Bi$_2$Se$_3$ and Bi$_2$Te$_3$ Single Crystals, CYRIL OPEIL, MENGLIANG YAO, Boston College, Chestnut Hill, MA 02467, STEPHEN WILSON, University of California, Santa Barbara, CA 93106, MONA ZEBARIJADI, Rutgers University, Piscataway, NJ 08854 — Nanostructured materials are an effective approach in reducing lattice thermal conductivity and improving overall thermoelectric efficiency. A challenge for experimental measurements of thermal conductivity is separating the contributions from both carriers and phonons. Building on the work of K. Lukas et al., Phys. Rev. B 85, 205410 (2012), we report measurements of thermal and electrical conductivity of single crystal thermoelectrics: Bi$_2$Se$_3$ and Bi$_2$Te$_3$ in a transverse magnetic field up to 9 Tesla. Our experiments provide a separation of the lattice/electronic components and make possible a better theoretical model of the lattice portion of the thermal conductivity in materials.

V1.00249 Computational screening of organic materials towards improved photovoltaic properties, SHUO DAI, Dept. Physics, Oklahoma State Univ, ROBERTO OLIVARES-AMAYA, Dept. Chemistry, Princeton Univ, CARLOS AMADOR-BEDOLLA, Dept. Chemistry, UNAM, ALAN ASPURU-GUIZIK, Dept. Chemistry, Harvard Univ, MARIO BORUNDA, Dept. Physics, Oklahoma State Univ — The world today faces an energy crisis that is an obstruction to the development of the human civilization. One of the most promising solutions is solar energy harvested by economical solar cells. Being the third generation of solar cell materials, organic photovoltaic (OPV) materials is now under active development from both theoretical and experimental points of view. In this study, we constructed a parameter to select the desired molecules based on their optical spectra performance. We applied it to investigate a large collection of potential OPV materials, which were from the CEPDB database set up by the Harvard Clean Energy Project. Time dependent density functional theory (TD-DFT) modeling was used to calculate the absorption spectra of the molecules. Then based on the parameter, we screened out the top ten performing molecules for their potential OPV usage and suggested experimental efforts toward their synthesis. In addition, from those molecules, we summarized the functional groups that provided molecules certain spectrum capability. It is hoped that useful information could be mined out to provide hints to molecular design of OPV materials.

V1.00250 First-principles study of amorphous carbon: a promising candidate for Na-ion batteries, KONSTANTINOS KOTSIS, FLEUR LEGRAIN, SERGEI MANZHOS, National University of Singapore — The perspective of a widespread use of clean but intermittent sources of electricity (wind and solar) as well as that of hybrid electric vehicles calls for alternatives to Li-ion batteries as Li resources are limited. Na being abundant, cheap, and a relatively light and small atom, Na-ion batteries have attracted a lot of interest the past few years. However, while most of the Na-ion batteries studies focus on the positive electrode, the negative electrode remains little investigated and an efficient anode providing all a good capacity, a high cycle life, and a decent rate of charge/discharge, is still not available. The efficient electrode materials for Li, in particular diamond Si and graphite C, have been shown to not allow the intercalation of Na [1, 2]. Computational studies report positive intercalation energies [3, 4] and therefore suggest that the insertion of Na into the crystalline framework (C and Si) is thermodynamically not favored: Na atoms prefer to gather into Na clusters rather than to intercalate into the crystalline phase. Amorphization of Si was found to be a valid strategy to improve the interaction between Si and Na [3]. We investigate here the effects of amorphization of C on its storage properties vis-à-vis Na (as well as Li for reference).

V1.00251 First-Principles Density Functional Theory Modeling Study on the Redox Chemistry of Graphene Oxides Affected by Placement Geometry of Oxygen Functional Groups, SUNGHEE KIM, KI CHUL KIM, SEUNG WOO LEE, SEUNG SOON JANG, Georgia Inst of Tech — To date, lithium-ion batteries have been extensively gained attention due to their promising potential in the industry. Despite their promising properties, improving their poor power density is still needed for practical applications. In addition, sustaining the high redox potential in the lithium-ion batteries is prerequisite for exhibiting the high energy and power densities. Recently, layered carbon materials including graphene and carbon nanotubes have been paid special attention as promising electrode materials with high power densities due to their exceptionally high surface area and active oxygen functional groups on their surfaces. However, the lack of reliable information on the redox chemistry of the candidates is the obstacle to be uncovered for practical applications. In this study, we investigated the redox chemistry of graphene oxides cluster models with well-controlled hydroxyl functional groups at the edge. First-principles density functional theory approach was employed to understand the geometric effect of the incorporated hydroxyl functional groups on the redox chemistry. Our study will provide an insight on the strategy for improving the redox potentials of graphene-based electrode candidates.

V1.00252 Temperature dependent study of impurities in LiFePO$_4$/C nanoparticles and their impact on electrochemical performance, KULWINDER SINGH DHINDSA, KHADJUE BAZZI, Gholam-Abbas NAZRI, Wayne State University, Detroit, MI, US, VAMAN M.NAIK, University of Michigan-Dearborn, Dearborn, Michigan, US, VIJAYENDRA K. GARG, Universidade de Brasilia, Instituto de Fisica, Brasilia – DF, Brazil, ADERBAL C. OLIVEIRA, Unidade Universitaria De Ciencias Exatas E Tecnologicas, Universidade, PREM VAISHNAVA, Kettering University, Flint, Michigan, US, RATNA NAIK, ZHIXIAN ZHOU, Wayne State University, Detroit, MI, US — We have synthesized LiFePO$_4$/C nanoparticles using a simple sol-gel method followed by calcination at various temperatures from 600 °C to 900 °C. X-ray diffraction shows that samples annealed at 600°C are phase pure while those treated at higher temperatures contain Fe$_2$P and Li$_3$PO$_4$ impurity phases, which increase with increasing annealing temperature. Mossbauer spectroscopy and magnetic measurements were used to quantify the amount of Fe$_2$P impurity phase. Scanning electron microscopy measurement reveals a noticeable increase in particle size as the annealing temperature increases from 700 °C to 900 °C. Optimal results are obtained in LiFePO$_4$/C samples annealed at 700 °C, which show the lowest charge transfer resistance, highest Li-ion diffusion coefficient, the highest specific capacity of 166 mAh/g at a rate of 1C and the best rate capability and cycling stability among all samples.

V1.00253 Porous MnO$_2$ prepared by sol-gel method for electrochemical supercapacitor, K. BAZZI, A. KUMAR, Wayne State University, O.D. JAYAKUMAR, Bhabha Atomic Research center, G.A. NAZRI, Wayne State University, V.M. NAIK, University of Michigan-Dearborn, R.A. NAIK, Wayne State University — MnO$_2$ has attracted great attention as material for electrochemical pseudocapacitor due to its high theoretical specific faradic capacitance (∼ 1370 F g$^{-1}$), environmental friendliness and wide potential window in both aqueous and nonaqueous electrolytes. However, the MnO$_2$ has a low surface area which depresses its electrochemical performance. The amorphous α-MnO$_2$ composite was synthesized by sol gel method in the presence of the tri-block copolymer P123. Our aim is to investigate the role of P123 on the electrochemical performance of MnO$_2$. The samples with and without P123 were prepared and characterized by x-ray diffraction (XRD), SEM, TEM and Brunauer–Emmett–Teller (BET) method. The electrochemical performances of the amorphous MnO$_2$ composites as the electrode materials for supercapacitors were evaluated by cyclic voltammetry and AC impedance measurements in a 1M Na$_2$SO$_4$ solution. The results show that the sample prepared without P123 exhibited a relatively low specific capacitance of 28F g$^{-1}$, whereas the porous MnO$_2$ prepared with P123 exhibited 117 F g$^{-1}$ at 5 mV/s. The results of crystalline MnO$_2$ composites will also be presented.

The authors acknowledge the support from the Richard J. Barber Foundation for Interdisciplinary Research.
V1.00254 Synthesis and electrochemical characterization of mesoporous Li$_2$FeSiO$_4$/C composite cathode material for Li-ion batteries, AJAY KUMAR, Wayne State University, O.D. JAYAKUMAR, Bhabha Atomic Research Centre, KHADIE BAZZI, GHOULAM-ABBAS NAZRI, Wayne State University, VAMAN M. NAIK, University of Michigan Dearborn, RATNA NAIK, Wayne State University — Lithium iron silicate (Li$_2$FeSiO$_4$) has the potential as cathode for Li ion batteries due to its high theoretical capacity (∼330 mAh/g) and improved safety. The application of Li$_2$FeSiO$_4$ as cathode material has been challenged by its poor electronic conductivity and slow lithium ion diffusion in the solid phase. In order to solve these problems, we have synthesized mesoporous Li$_2$FeSiO$_4$/C composites by sol-gel method using the tri-block copolymer (P123) as carbon source. The phase purity and morphology of the composite materials were characterized by x-ray diffraction, SEM and TEM. The XRD pattern confirmed the formation of ∼12 nm size Li$_2$FeSiO$_4$ crystallites in composites annealed at 600 °C for 6 h under argon atmosphere. The electrochemical properties were measured using the composite material as positive electrode in a standard coin cell configuration with lithium as the active anode and the cells were tested using AC impedance spectroscopy, cyclic voltammetry, and galvanostatic charge/discharge cycling. The Li$_2$FeSiO$_4$/C composites showed a discharge capacity of ∼240 mAh/g at a rate of C/30 at room temperature. The effect of different annealing temperature and synthesis time on the electrochemical performance of Li$_2$FeSiO$_4$/C will be presented.

V1.00255 Synthesis of Nanostructured Graphene/Metal-oxides Hybrid for High-performance Supercapacitors, JUN-BO SIM, Department of Nuclear and Quantum Engineering, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Republic of Korea, SUNDAR MAVAYAN, Division of Corrosion & Materials Protection, Central Electrochemical Research Institute, Karaikudi-630006, Tamil Nadu, India, SUNG-MIN CHOI, Department of Nuclear and Quantum Engineering, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Republic of Korea — Graphene has been considered as promising material for supercapacitor electrodes due to their large surface area, good chemical stability and excellent electrical conductivity. However, until now, conventional graphene-based supercapacitors cannot provide enough energy storage ability due to irreversible restacking behavior of graphene sheets. Various methods have been explored to solve this problem, but most of methods require complex and multi-step process, which will prevent scalable synthesis. Here, we present an easy and scalable synthesis method for nanostructured graphene/metal-oxides hybrid starting from graphene-oxide. The hybrid material prepared in this method provides high specific capacitance with high electrochemical stability. The sample characterization using XRD, XPS, FE-SEM, FE-TEM and Cyclic-Voltammetry will be presented.

V1.00256 Superstructured Carbon Nanotube/Porous Silicon Hybrid Materials for Lithium-Ion Battery Anodes, JUN-KI LEE$^1$, SHIN-HYUN KANG$^2$, SUNG-MIN CHOI$^3$, KAIST — High energy Li-ion batteries (LIBs) are in great demand for electronics, electric-vehicles, and grid-scale energy storage. To further increase the energy and power densities of LIBs, Si anodes have been intensively explored due to their high capacity, and high abundance compared with traditional carbon anodes. However, the poor cycle-life caused by large volume expansion during charge/discharge process has been an impediment to its applications. Recently, superstructured Si materials were received attentions to solve above mentioned problem in excellent mechanical properties, large surface area, and fast Li and electron transportation aspects, but applying superstructures to anode is in early stage yet. Here, we synthesized superstructured carbon nanotubes (CNTs)/porous Si hybrid materials and its particular electrochemical properties will be presented.

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V1.00257 Charge Transport and Structural Dynamics in Deep Eutectic Mixtures, TYLER COSBY, ADAM HOLT, LOGAN TERHEGGEN, University of Tennessee, Knoxville, PHILIP GRIFFIN, University of Pennsylvania, ROBERTO BENSON, JOSHUA SANGORO, University of Tennessee, Knoxville — Charge transport and structural dynamics in a series of imidazole and carboxylic acid-based deep eutectic mixtures are investigated by broadband dielectric spectroscopy, dynamic light scattering, $^1$H nuclear magnetic resonance spectroscopy, calorimetry, and Fourier transform infrared spectroscopy. It is found that the extended hydrogen-bonded networks characteristic of imidazoles are broken down upon addition of carboxylic acids, resulting in an increase in dc conductivity of the mixtures. These results are discussed within the framework of recent theories of hydrogen bonding and proton transport.

V1.00258 Understanding Iron-based catalysts with efficient Oxygen reduction activity from first-principles calculations, HASNAH HAFIZ, B. BARBIELLINI, Q. JIA, Northeastern U., U. TYLUS, Northeastern U. and LANL, K. STRICKLAND, A. BANSIL, S. MUHERJEE, Northeastern U. — Catalysts based on Fe/N/C clusters can support the oxygen-reduction reaction (ORR) without the use of expensive metals such as platinum. These systems can also prevent some poisonous species to block the active sites from the reactant. We have performed spin-polarized calculations on various Fe/N/C fragments using the Vienna Ab initio Simulation Package (VASP) code. Some results are compared to similar calculations obtained with the Gaussian code. We investigate the partial density of states (PDOS) of the 3d orbitals near the Fermi level and calculate the binding energies of several ligands. Correlations of the binding energies with the 3d electronic PDOS’s are used to propose electronic descriptors of the ORR associated with the 3d states of Fe. We also suggest a structural model for the most active site with a ferrous ion (Fe$^{2+}$) in the high spin state or the so-called Doublet 3 (D3).

V1.00259 Plasmon Enhanced Hetero-Junction Solar Cell, GEN LONG, LEVINE CHING, MOSTAFA SADOQI, HUIZHONG XU, Department of Physics, College of Liberal Arts and Sciences, St John’s University, 8000 Utopia Parkway, Jamaica, NY 11439 — Here we report a systematic study of plasmon-enhanced hetero-junction solar cells made of colloidal quantum dots (PbS) and nanowires (ZnO), with/without metal nanoparticles (Au). The structure of solar cell devices was characterized by AFM, SEM and profilometer, etc. The power conversion efficiencies of solar cell devices were characterized by solar simulator (OAI TriSOL, AM1.5G Class AAA). The enhancement in the photocurrent due to introduction of metal nanoparticles was obvious. We believe this is due to the plasmonic effect from the metal nanoparticles. The correlation between surface roughness, film uniformity and device performance was also studied.
V1.00260 Local Structure and Electrical Performance of Pulsed Laser Deposited CdTe/CdS Thin-Film Solar Cells¹. ARYA NABIZADEH, DARREN LESINSKI, LUIS CERQUEIRA, MEHMET SAHINER, Seton Hall Univ, SAHINER-AMSC Team — The photovoltaic thin films of CdS/CdTe were prepared by pulsed laser deposition (PLD) on indium tin oxide (ITO) coated glass. The local structural variations in the thin films around Cd atom upon variations in the thin film growth parameters were investigated by X-ray absorption near-edge spectroscopy (XANES) and extended X-ray absorption fine-structure spectroscopy (EXAFS) and X-ray diffraction. X-ray absorption spectroscopy measurements were performed at the National Synchrotron Light Source of Brookhaven National Laboratory. The effect of the thicknesses of the CdS and CdTe layers, laser energy and the substrate temperature on the local crystal structure and coordination around the Cd atoms were investigated through quantitative multiple scattering analysis and modeling of the x-ray absorption spectroscopy data. The induced local structural modifications upon varying synthesis conditions are correlated with the electrical performance of these photovoltaic thin-films. The quantitative multiple scattering analyses and modeling of X-ray absorption spectroscopy data revealed the local environment around the Cd atoms are highly sensitive to thin film deposition parameters and the variations of the Cd local structure influences interface quality consequently, affect the electrical performance of these photovoltaic thin films.

¹This work is supported by NSF Award #:DMI-0420952 and Research Corporation Award #:CC6405 and New Jersey Space Grant Consortium.

V1.00261 Electrowetting-Controlled Dual Liquid Prism for Adaptive Beam Steering, JIANGTAO CHENG, University of North Texas — The use of concentrating photovoltaic (CPV) technology has been the most promising method of harvesting solar radiation. These CPV systems often require motor-driven tracking devices to steer the sun's beams onto solar cells. The cost of maintaining these tracking systems is the primary inhibitor for widespread application. We aim to overcome the need for mechanical trackers through the use of an electrowetting-driven solar tracking system. The electrowetting-driven solar tracking system consists of an array of novel electrowetting-controlled dual liquid prisms, which are filled with immiscible fluids that have large differences in refractive indices. The naturally formed meniscus between the fluids can function as a dynamic optical prism. Via the full-range modulation of the liquid prisms, incident sunlight can be adaptively tracked, steered, and focused onto CPV cells through a fixed optical condenser. Furthermore, unlike the conventional and cumbersome motor-driven tracking systems used today, the liquid prism system would be suitable for rooftop applications. The results of this project reveal that the EWST system has the potential to generate ~ 70% more green energy at 50% of the conventional capital cost.

V1.00263 A possibility as a new type of thermoelectric application on organic-inorganic hybrid perovskite ABI3 system: A density functional theory study¹. CHANGHOON LEE, JISOOK HONG, JJ HOON SHIM, Pohang Univ of Sci & Tech, MYUNG-HWAN WHANGBO, NC State Univ, POSTECH Team — The electronic structures of organic-inorganic hybrid systems ABI₃ (A = CH₃NH₃, NH₂CHNH₂; B = Sn, Pb; X = I) in the distorted phase from their patent cubic phase are systematically studied using the first-principles calculations. Here, we examine thermoelectric properties for ABI₃ compounds based on the DFT electronic structures of their optimized crystal structures. The ABI₃ compounds should be considered for good thermoelectric application. We reveal that good thermoelectric performance of ABI₃ systems originate from large Seebeck coefficients and low thermal conductivities. As a consequence, we predict that ABI₃ system is a promising material for new thermoelectric application compared to thermoelectric properties of well-known thermoelectric material Bi₂Te₃.

¹This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education(2013R1A1A200341)

V1.00264 Graphene oxide as a candidate material for natural gas storage: A first principles study¹. RAJIV KUMAR CHOIHOUN, KANCHAN ULMAN, TSU, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore, India, SHOBHANA NARASIMHAN, TSU, and Sheikh Saqr Laboratory, ICMS, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore, India — Alternative sources of clean energy will be much in demand in the coming days. To store methane (CH₄) in sorbent materials at ambient conditions for on-board vehicular usage, minimum adsorption energy of 18.8 KJ/mol is desirable. In this work, we have investigated methane adsorption on graphene oxide using first principles calculations. To accurately capture the weak interactions between CH₄ and the substrate we have included van der Waals interactions in our calculations. We show that the adsorption energy falls within the target range. Careful analysis of the various contributions to the binding shows that the enhancement in adsorption energy on going from graphene to graphene oxide arises from a subtle synergy between various effects.

¹Funding agencies CSIR, India, DST Nanomission and JNCSAR. Computational facilities provided by TUE-CMS, JNCSAR.

V1.00265 Solar photocatalytic conversion of CO2 to fuels by nanostructured oxides, OOMMAN VARGHESE¹, IVY AHIABU², GIWAN KATIUWAL³, MAGGIE PAULOSE¹. University of Houston — Converting the carbon dioxide and water vapor to hydrocarbon fuels through photocatalytic processes using sunlight is a promising route for limiting the CO2 accumulation in the atmosphere. This CO2 recycling process facilitates the unabated use of hydrocarbon fuels as well. Nevertheless, the photocatalytic CO2 conversion process has not yet demonstrated a reasonable light-to-fuel energy conversion efficiency for it to be considered as a viable technology. Nanostructured oxide semiconductors have recently shown potentials for efficiency enhancement. Appropriate band gap and band alignment, sufficient surface area for light absorption and low loss transfer of photocarriers to the surface are important criteria for the selection of photocatalysts. We will present the results of study on solar photocatalytic conversion of CO2 and water vapor using three oxide nanostructured materials, TiO2, ZnO and Cu2O, with different band gaps and flat band positions in converting CO2 to fuels. We will compare the quantum efficiencies and discuss possible reaction routes studied by using isotopic form of water for the reaction.

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**V1.00266 Vacuum force**, YONGQUAN HAN, 15611860790 — To study on vacuum force, we must clear what is vacuum, vacuum is a space do not have any air and also ray. There is not exist an absolute the vacuum of space. The vacuum of space is relative, so that the vacuum force is relative. There is a certain that vacuum vacuum space exists. In fact, the vacuum space is relative, if the two spaces compared to the existence of relative vacuum, there must exist a vacuum force, and the direction of the vacuum force point to the vacuum region. Any object rotates and radiates. Rotate bend radiate—centripetal, gravity produced, relative gravity; non gravity is the vacuum force. Gravity is centripetal, is a trend that the objects who attracted wants to Centripetal, or have been do Centripetal movement. Any object moves, so gravity makes the object curve movement. That is to say, the radiation range curve movement must be in the gravitational objects, gravity must be existed in non vacuum region, and make the object who is in the region of do curve movement (for example: The earth moves around the sun), or final attracted in the form gravitational objects, and keep relatively static with attract object. (for example: objects on the earth moves but can’t reach the first cosmic speed).

**V1.00267 Using Simple Circuits as Thermal Models for your Home**, ADELE POYNOR, Allegheny College — One of the most cost effect ways to improve the energy efficiency of your home is to increase your home’s insulation. But would it be better to insulate your walls or by new windows? Not all options are equally effective, nor do they have equal costs. So how can you determine which option improves your homes insulation the most? I present an analogy to simple resistor circuits that can be used by introductory students to answer these questions.

**V1.00268 Anisotropic O vacancy formation and diffusion in LaMnO3**, OMOTAYO SALAWU, LIYONG GAN, UDO SCHWINGENSCHLOGL, King Abdullah Univ — Anisotropy effects in solid oxide fuel cells are typically not considered because of the high operating temperatures. Focusing on the prototypical perovskite LaMnO3, we apply first-principles calculations to demonstrate that this approximation is no longer valid when the operating temperature is reduced and discuss the consequences for the material properties. In addition, we show that strain and Sr doping can be used to further increase the anisotropy. Tensile strain promotes both the O formation and diffusion in pristine and Sr doped LaMnO3, while Sr doping enhances the O vacancy formation but not the diffusion barrier. Both in LaMnO3 and La0.75Sr0.25MnO3 the O diffusion is found to be favorable in the [011] and [01$ar{1}$] directions.

**V1.00269 Electronic structure and vacancy formation in La(1-x)B(x)CoO3 (B=Mg,Ca,Ba and x=0.125)**, OMOTAYO SALAWU, LIYONG GAN, UDO SCHWINGENSCHLOGL, King Abdullah Univ — The LaCoO3 class of materials is of interest for cathodes of solid oxide fuel cells. Spin-polarized density functional theory is applied to cubic La0.75(Mg/Ca/Ba)0.125CoO3. The effect of this cation doping on the electronic and magnetic properties as well as oxygen vacancy formation energy is studied. Oxygen vacancies with proximity to the dopant are energetically favourable in most cases. We discuss the effect of distortions of the CoO6 octahedron on the electronic structure and the formation energy of oxygen vacancies. The order of formation oxygen is found to be Mg > Ca > Ba. Cation doping incorporates holes to the Co-O network which enhances the oxygen vacancy formation.

**V1.00270 Thin Film Evaporation of Receding Meniscus within Micro Pillar Arrays**, MOHAMED H. ALHOSANI, AMMAR A. ALSHEGHRI, AMAL ALGHAFERI, TIEJUN ZHANG, Masdar Institute of Science and Technology — Evaporation is a key process in power generation, water desalination, and thermal management applications. It has been proved that hydrophilic micro structured surfaces can enhance the convection heat transfer by promoting high-performance thin film evaporation and enlarging the total heat transfer surface area. When depositing a water droplet on hydrophilic structured surfaces, two distinct regions can be observed, a) central region with water level higher than the micro pillar height (droplet region), b) thin film region as a result of liquid meniscus receding among micro structures. In this study, we are able to probe the physics of thin film evaporation of receding liquid meniscus among micro pillar arrays with different pillar heights, spacings and diameters. Heat transfer is systematically studied in the droplet and thin film region for each sample. Also, Young-Laplace equation and kinetic theory of mass transport are used to model the thin film evaporation around micro pillars. With the proposed model, the shape of meniscus around micro pillars and the diameter of droplet extended thin film region can be predicted and compared with the experimental measurement. The model can also be extended to model thin film evaporation of meniscus within nano structured surfaces.

1 Supported by cooperative agreement between Masdar Inst and MIT

**V1.00271 Positron Annihilation Spectroscopy of Common Mineral Constituents of Shale**, JOAH CHUN*, Colorado College, JAMES BUFKIN*, Angelo State University, HELGE ALSLEBEN, TCU Department of Geology, FNU AMEENA, C.A. QUARLES, TCU Department of Physics and Astronomy — Recent investigation of positron lifetime and Doppler broadening in Barnett Shale samples have shown a small intensity of positronium (Ps) formation. The samples studied have XRF information on 35 elements, XRD information on mineral constituents, and chemical information on total organic carbon (TOC). It is not known where Ps is formed in the shale. Previous research has shown that Ps is not formed in quartz-rich sandstone, calcite-rich limestone or dolomite-rich rocks, which contain minerals that also constitute a significant part of most shale samples. No information about Ps formation in clay minerals, which are often dominant in shale, has been available. The purpose of the present study is to determine which clay minerals form Ps. Twenty-five different common rock-forming minerals have been studied. Hydration of some of the minerals has also been varied. As a result of this work, a better idea of where Ps is formed in the shale samples has been obtained, but there still remains some uncertainty regarding the hydration in the shale and the possibility of direct Ps formation in the organic carbon itself. *Participant in the summer 2014 TCU REU program in Physics and Astronomy funded by the National Science Foundation under grant PHY-1358770.

**V1.00272 METALS AND METALLIC ALLOYS —**

**V1.00273 Effect on stabilities of self-Interstitials in HCP-Zirconium**, QING PENG, WEI JI, JIE LIAN, Rensselaer Polytechnic Institute, XIAO-JIA CHEN, Chinese Academy of Sciences, HANCHEN HUANG, Northeastern University, FEI GAO1, Pacific Northwest National Laboratory, SUVRANU DE, Rensselaer Polytechnic Institute — The self-interstitial atoms (SIAs) mediate the evolution of micro-structures which is crucial in understanding the instabilities of hexagonal close packed (HCP) structures. Taking zirconium as a prototype, we investigate the pressure effect on the stabilities of SIAs using first-principles calculations based on density-functional theory. We found that the pressure greatly affects the stability of the SIAs. The SIAs in basal planes are more stable under pressure. The SIA configuration of the lowest formation energy changes from basal octahedral (BO) to octahedral (O) at a pressure of 21 GPa. The lowest formation enthalpy configuration switches from BO to S (split-dumbbell) at the pressure of 30 GPa. The formation volumes of SIAs decrease monotonically in response to an increase in pressure. Our results reveal that it is important to take pressure effects into account when predicting the micro-structural evolution of HCP structures. (Scientific Reports, 4, 5735)

1 now in University of Michigan
**V1.00274 Electrical Properties of the Ln$_{3-x}$Y$_x$TaO$_7$ (Ln=Dy, Gd) solid solution.** JOSE FRANCISCO GOMEZ-GARCIA, Facultad de Química, ALEJANDRO DURAN, Centro de Nanociencias y Nanotecnología, PABLO DE LA MORA$^1$, Facultad de Ciencias, GUSTAVO TAVIZON, Facultad de Química, Universidad Nacional Autónoma de México — Systems with the formula Ln$_{3-x}$Y$_x$TaO$_7$ (Ln=Dy, Gd) crystallizing in the website related structure (SG C222, No. 20) were synthesized by the solid-state reaction method. Structural characterization through Rietveld reflections indicates that a solid solution in the whole range 0<x<3 exist in both Gd and Dy systems. Structural cell parameters as a function of the rare-earth content are shown in this work, as well as the AC electrical properties in the 30-700°C range. We have performed impendence (400-600°C) and electric polarizability measurements (at room temperature); the results indicate that the polarizability reaches its maximum values at $x=0.67$, 1.67 and 2.33 for the Gd samples, meanwhile these values were $x=0.67$ and 2.0 for the Dy samples. In intermediate composition values, the Ln$_{3-x}$Y$_x$TaO$_7$ samples exhibit null polarization.

$^1$On sabbatical leave at the University of Texas at Austin

**V1.00275 The 4f multipole ordering effect on core-level spectroscopies of Ce intermetallics.** NORIMASA SASABE, HIRONORI TONAI, TAKAYUKI UOZUMI, Osaka Prefecture Univ — The 3d transition metal compounds and 4f rare earth compounds show attractive phenomena, such as superconductivity and Kondo effect, due to strong electron correlations among localized 3d and 4f electrons. Especially, multipole ordering of orbital and/or spin in 4f and 5f compounds is attracting much attention these years. For example, CeB$_6$ is known to show antiferro-quadrupolar (AFQ) ordering below 3.2K. X-ray core-level spectroscopy is an efficient technique to investigate the electronic states of strongly correlated systems. Recent years, experimental techniques have been rapidly developing and, especially, the progress in experimental resolution has enabled us to observe fine spectral features, which were not formerly observed. These advantages will enable us to observe spectral fine features related with the multipole ordering. In this study, we discuss multipole ordering effects on X-ray spectra for CeB$_6$, especially paying attention on the polarization dependence. In order to simulate the electronic state of CeB$_6$ with the multipole ordering, we use an impurity Anderson model including a simplified RKKY interaction.

**V1.00276 Low temperature heat capacity of Uranium-Plutonium MOX single crystals.** JEAN-CHRISTOPHE GRIVEAU, ERIC COLINEAU, RACHEL ELOIRDI, ROBERTO CACIUFFO, European Commission, Joint Research Centre (JRC), Institute for Transuranium Elements (ITU), Postfach 2340, D-76125 Karlsruhe, Germany — The establishment of the basic properties of actinides based materials is crucial for the understanding of conventional and advanced nuclear fuels. Accessing ground state properties at very low temperature for these systems gives a direct overview of their fundamental features. Moreover, when these materials can be produced as single crystals, side effects due to the presence of grains and impurities phases are drastically reduced, giving a very powerful add-in for theoretical and industrial oriented studies. This clearly ensures the reliability of the parameters determined while existing models of these strategic materials can be probed especially in the purpose of applications/developments and safety concerns. Here we report on heat capacity measurements performed on U-Pu MOX in single crystal form. Tiny crystals with mass of 2 to 15 mg have been produced by solid-solid chemical vapour transport technique with several different compositions ranging from pure UO$_2$ to PuO$_2$. Compositions close to UO$_2$ (U rich) present a persistent signature similarly to the magnetic transition reported for the pure phase $T_N \sim 31$ K while plutonium rich concentrations do not show any hint of the magnetic transition down to the minimum temperature achieved.

**V1.00277 Thermodynamics of plastic flow of BCC metals from atomistic studies of isolated screw dislocations.** ROMAN GRÖGER, Institute of Physics of Materials and CEITEC IPM, Academy of Sciences of the Czech Republic, VACLAV VITEK, Department of Materials Science and Engineering, University of Pennsylvania. — The thermodynamic description of dislocation glide in BCC metals depends crucially on the shape of the Peierls barrier that 1/2⟨111⟩ screw dislocations have to overcome when moving in the lattice. While the height of this barrier can be obtained unequivocally using saddle-point search algorithms such as the Nudged Elastic Band (NEB) method, its exact shape depends on the chosen approximation of the transition pathway of the system. We formulate a procedure that allows to identify the position of the dislocation directly from the displacements of atoms in its core. We investigate the performance of this model by calculating curved paths of a 1/2⟨111⟩ screw dislocation in tungsten from a series of images obtained recently using the NEB method at zero applied stress and for positive/negative shear stresses perpendicular to the slip direction. The Peierls barriers plotted along these curved paths are shown to be quite different from those obtained previously by assuming a straight dislocation path. We demonstrate how these results can be utilized to develop a new thermodynamic model of plasticity of BCC metals that is systematically linked to the atomic-level properties of isolated 1/2⟨111⟩ screw dislocations.

**V1.00278 Temperature Dependence of the Dielectric Function of Ni near the Curie Temperature.** STEFAN ZOLLNER, DENNIS TRUJILLO, LAURA PINEDA, LINA ABDALLAH, New Mexico State Univ — Onstein et al. (Physica V, 1938) observed a discontinuity in the normal-incidence reflectance of Ni at the Curie temperature. A similar phenomenological observation of a temperature related slope change in resistivity versus temperature in Ni was made by Litschel et al. (J. Phys. Chem. Solids, 1985). To follow up on these observations we carried out measurement of the dielectric function $\epsilon$ as a function of temperature for a magnetized thin film Ni sample (1000 Å Ni on SiO$_2$) and bulk polycrystalline Ni via ellipsometric measurement at a fixed photon energy (1.9 eV). For a magnetized sample, we observe a discontinuity in the dielectric function versus temperature just below the Curie temperature for both thin film and bulk polycrystalline Ni. In an unmagnetized Ni sample (obtained by heating above the Curie temperature), this continuity is not present. We believe that this observation is due to a change in the on-diagonal dielectric tensor elements for Ni in the magnetized samples, not due to the off-diagonal elements related to the Koofer effect.

$^1$NSF (DMR-1104934)

**V1.00279 GENERAL —

**V1.00280 A theoretical investigation of the origins of atoms and sub-atomic particles.** CATHERINE DEROW, No Company Provided — It seems the universe was at some very early stage shortwave energy. When the universe cooled some of this became matter, others delved into particles of sub-atomic parts. The positive charge and motion of the negative charge of the atom keep them from merging and yet the attractive forces stop them from parting, apart from when radiation activity is observed. The neutral charge may add a motion which loosens the attraction of the positive protonic attractive force for the negative electronic force. It seems thus the atom is relatively immobilized negative, positive and neutral waves held in confined motion. These waves can be loosed into travelling as waves by forces which break the balance of intra-atomic attractive forces and thus cause the emission of sub-atomic “particles” as waves. Thus the attractive forces in normal circumstances balance the “wave motion” forces, keeping stable atomic structure intact.
V1.00282 Democracy is a historical urgency. MIROSLAV SYNEK, No Company Provided — Survival of humanity, on this planet, may depend, heavily, on coping with advancing technology of nuclear missiles. Let us consider critical alternatives of powerful governments: democracy, as an alternative to dictatorship. Democracy is based on free elections, as a government of the people, by the people, and for the people. Democracy is a historical urgency, in the age of inter-continental nuclear missiles, computerized on a push-button, conceivably controllable by a very powerful, miscalculating and/or insane, dictator, capable of producing global nuclear holocaust, on our entire planet. Diplomacy, together with supporting activities, should be utilized, to help, in important steps, at this time, for achieving democracy in critical areas.

V1.00283 Geometric Implications of Maxwell’s Equations. FELIX T. SMITH, None — Maxwell’s synthesis of the varied results of the accumulated knowledge of electricity and magnetism, based largely on the searching insights of Faraday, still provide new issues to explore. A case in point is a well recognized anomaly in the Maxwell equations: The laws of electricity and magnetism require two 3-vector and two scalar equations, but only six dependent variables are available to be their solutions, the 3-vectors E and B. This leaves an apparent redundancy of two degrees of freedom (J. Rosen, AJP 48, 1071 (1980); Jiang, Wu, Povineili, J. Comp. Phys. 125, 104 (1996)). The observed self-consistency of the eight equations suggests that they contain additional information. This can be sought as a previously unnoticed constraint connecting the space and time variables, r and t. This constraint can be identified, It distorts the otherwise Euclidean 3-space of r with the extremely slight, time dependent curvature &kappa;= k(t) = Rcrit/r(t) of the 3-space of a hyperspace whose radius has the time dependence dRcrit/dt = ±ic nonrelativistically, or dRcrit/dt = ±ic relativistically. The time dependence is exactly that of the Hubble expansion. Implications of this identification will be explored.

V1.00284 Prof. Jakob Narkiewicz-Jodko’s Discoveries and his Laboratory. VLADIMIR SAMUILOV, State University of NY at Stony Brook, LARRISA SAMUILOVA, Department of Mathematics, SCCC — Prof. Jakob Narkiewicz-Jodko (1947–1995) major discoveries are: Electrography — the method of the visualization of electric discharge from the bodies due to the application of high strength and high frequency electric fields [3,4], and the first observation of the propagation of the electromagnetic waves for information transfer over the distances [5,6]. They were made in his laboratory located at his manor home Nadniemen. We describe these experiments and the Lab equipment used for the discoveries. Unfortunately the Nadniemen manor designed and built in Neogothic style was destroyed at the WWII. Our goal is to restore the Lab of Prof. Jakob Narkiewicz-Jodko as a museum. We also introduce our hypothesis regarding architectural design of the manor home Nadniemen. [1] Decrespe M. La vie et les oeuvres de M. de Narkiewicz-Jodko, member et collaborateur de l’Institut imperial de medecineexperimentale de Saint-Petersburg, member of correspondant de la Societe de Medecine de Paris, etc./ Marius Decrespe.- Paris, Chamuel, 1896, 51p. [2] Annalen der Physik.- Leipzig, 1896. – Bd 293, 132 [3] Electrography// The Photographic news for amateurs.- 1896.- vol. 40, p.450 [4] Maack F. Elektrographie. Mit besonderer Berucksicht-tigung der Versuche Narkiewicz-Jodko/ Ferdinand Maack// Wissenseschaltliche Zeitschrift. – 1898.- Bd 1, 8-22; 1898.- Bd 1, 2/3, 89-99. [5] Séances de la societe francaise de physique/ Societe francaise de physique. – Paris, 1898, p. 77-79. [6] Present condition of wireless telegraphy// Consular reports: Commerce, manufacturers, etc. of their consular districts. Bureau of Foreign Commerce of United States.- Washington 1901, v.66. p. 44.

V1.00285 Relativistic Navier-Stokes Equation, (Navier-Stokes Equation with Estakhr’s Correction). AHMAD REZA ESTAKHR1, Researcher — At relativistic speeds Navier-Stokes equation is incorrect unless Estakhr’s correction is included. This equation relates energy flux as vector at relativistic speeds. (-1/c²) (ωf) = at low speeds Estakhr’s relativistic correction vanishes. ργv(ωf) = ργv(ωf + v·∇v) = −∇p + f, T = −1/c² (ωf) + f, where v is the flow velocity, ρ is the fluid density, p is the pressure, T is the (deviatoric) component of the total stress tensor, which has order two, f represents body forces (per unit volume) acting on the fluid, V is the del operator, γ is the Lorentz factor.

1This is corrected version of my previous abstract: (MAR15-2014-000047)

V1.00286 The Crisis in Scholarly Communication, Open Access, and Open Data Policies: The Libraries’ Perspective. RACHEL BESARA, Florida State University Libraries — For years the cost of STEM databases have exceeded the rate of inflation. Libraries have reallocated funds for years to continue to provide support to their scientific communities, but they are reaching a point at many institutions where they are no longer able to provide access to many databases considered standard to support research. A possible or partial alleviation to this order of inflation. Libraries have reallocated funds for years to continue to provide support to their scientific communities, but they are reaching a point at many institutions where they are no longer able to provide access to many databases considered standard to support research. A possible or partial alleviation to this dilemma is the open access movement. However, this shift challenges the current model of publishing and data management in the sciences. This talk will discuss these topics from the perspective of research libraries supporting physics and the STEM disciplines.

V1.00287 Climate Change & Social Justice: Why We Should Care1. NATHAN T. NESBITT, Boston College — In the past several years the global impacts brought about by climate change have become increasingly apparent through the advent of numerous natural disasters. In these events the social costs of climate change have materialized demonstrating high costs in lives, livelihoods, and equity. Due to geographic bad-luck many of the countries most affected by climate change are those that contributed least, a challenge that’s exacerbated by a lack of robust infrastructure in these countries. Wealthy nations remain at risk themselves and incidents such as Hurricanes Sandy & Katrina have demonstrated that in times of crisis even institutions like the Red Cross will abandon the poor to their deaths. As necessary action on climate change would cost the fossil fuel industry $20 trillion, money in politics has stymied action. Recently, however, a groundswell grassroots movement (e.g. People’s Climate March in NYC) and great strides in energy technology and policy have begun to create necessary change. Reports quantifying the impacts of climate change will be discussed, as well as an update on the current state of the global climate justice movement. The important contributions from scientists to this movement will be highlighted.

1This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. (DGE-1258923).

V1.00288 The Evolution of Carbon Burning Flames Inside Super-Asymptotic Giant Branch Stars. CARL FIELDS, ROBERT FARMER, FRANCIS TIMMES, Arizona State University, SPIDER COLLABORATION — We explore how carbon burning impacts the bifurcation region separating stars whose final fate is a massive white dwarf from stars whose final fate is a massive star supernova. A dense grid of models with initial mass (Mini) from 6.0 M⊙ to 11.0 M⊙ are evolved from pre-main-sequence to the end of nuclear burning using the open-source toolkit, Modules for Experiments in Stellar Astrophysics (MESA). For stars between 7.0 M⊙ ≤ Mini ≤ 9.0 M⊙, energy losses at the center of the core due to neutrino cooling causes a temperature inversion resulting in off-center ignition. First ignition occurs where the minimum temperature of 7.1010 K, and a density (ρcrit) of 2·106 g/cm³ is met. We conclude that for stars within this range, the location of first ignition decreases as a function of initial mass. Moreover, we show that there exist a unique ignition density of 2·106 g/cm³.
V1.00289 A Type of Dark Matter May be found by Neutron Emissions, RICHARD KRISKE, University of Minnesota — This author has previously suggested that Neutrons in Neutron Stars are arranged in a Quasi-Crystal Structure and when they are ejected at Relativistic Velocities maintain some of that structure in forming Very large Nuclei of many Neutrons. When the Neutrons are ejected a Nuclear Electron and a Neutroino are emitted, making Neutron Stars Neutroino Sources, both from the Surface and from the Ejected matter. Likewise large collections of the Ejected matter form Dark Matter in Outer space as they are Super Heavy Hydrogen and sometimes just large Collections of Neutrons. As time passes the Large Collections of Neutrons break apart and form many Super Heavy Hydrogen Nuclei, but of smaller mass. Each breaking produces Neutroino emissions. The Super Heavy Hydrogen combines with Oxygen to produce Super Heavy water, which collects in Comets, on Planets like Earth and on moons such as Europa. Europa should be emitting Neutrinons, as there should be some emissions from the Earth itself and from the Earth’s Atmosphere. The Neutrinons emitted from around Black Holes and Neutron stars should be particularly easy to detect, as there should be a lot of them.

V1.00290 A Synchrotron Radiation Research Facility for Africa, HERMAN WINICK, SLAC National Accelerator Lab — Africa is the only habitable continent without a synchrotron light source. Dozens of African scientists use facilities abroad. Although South Africa has become a member of ESRF, the number of users is limited by distance and travel cost. A light source in Africa would give thousands of African scientists access to this tool. Momentum is now building for an African light source, as a collaboration involving several sub-Saharan African countries. An interim Steering Committee has been formed. SESAME, now nearing completion in Jordan as a collaboration of 9 countries in the Middle East (www.sesame.org.jo) may be the example followed. UNESCO became the umbrella organization for SESAME at its Executive Board 164th session, May 2002, as it did in the case of CERN in the 1950s. UNESCO’s Executive Board described SESAME as “a quintessential UNESCO project combining capacity building with vital peace-building through science” and “a model project for other regions”. It is likely that UNESCO, if asked, would play a similar role as a facilitator for an African light source.

V1.00291 Analytical Model for the Diffusion Process in a In-Situ Combustion Tube, PATRICIA GUTIERREZ, ADRIAN REYES, Universidad Nacional Autónoma de México — The in-situ combustion process (ISC) is basically an air or oxygen enriched gas injection oil recovery process, inside an extraction well. In contrast to a conventional gas injection process, an ISC process consists in using heat to create a combustion front that raises the fuel temperature, decreasing its viscosity, making extraction easier. The oil is taken toward the producer by means of a vigorous gas thrust as well as a water thrust. To improve and enhance this technique in the field wells, it has been widely perform experimental laboratory tests, in which an in-situ combustion tube is designed to simulate the extraction process. In the present work we propose to solve analytically the problem, with a parabolic partial differential equation associated to the convection-diffusion phenomenon, equation which describes the in-situ combustion process. The whole mathematical problem is established by completing this equation with the correspong boundary and initial conditions, the thickness of the combustion zone, flow velocity, and more parameters. The theoretically obtained results are compared with those reported in literature. We further, fit the parameter of our model to the mentioned data taken from the literature.

V1.00292 Flexo-Opto-Electric Studies of fullerene (C$_{60}$) nano-colloids in namatic liquid crystal, JON FOUST, ANGELO VISCO, KEVIN SOBCZAK, RIZWAN MAHMOOD, Slippery Rock University — We have explored the effects of fullerene (C$_{60}$) nano colloids on the elastic, dielectric and optical properties of thermotropic liquid crystal in nematic phase as a function of C$_{60}$ concentration and temperature. Data suggest softening of elastic behavior and divergence of dielectric properties as the temperature approaches to the isotropic phase. We will also report critical concentration and the critical exponent as extracted by fitting data to a model equation. These studies are important because of the potential applications in liquid crystal devices, drug delivery vehicles, and solar energy systems.

V1.00293 Metallicities of Low Mass Inefficient Star Forming Dwarfs in S4G: Testing the Closed Box Paradigm, MYLES MCKAY, South Carolina State University, SABRINA STIREWALT, University of Virginia, KARTIK SHETH, National Radio Astronomy Observatory, BONITA DE SWARDT, Square Kilometre Array South Africa, DONALD WALTER, South Carolina State University — Low mass dwarf galaxies are the most numerous extragalactic population in the Local Universe. Many gas-rich dwarfs appear to be forming stars less efficiently than normal, massive disk galaxies and are therefore important laboratories for the study of star formation. Here we present new observations using the Palomar Double Spectrograph for 19 dwarf galaxies from the S4G Survey with the lowest stellar to HI mass ratios. Preliminary analysis of the data indicate a wide range of metallicities which vary by as much as 0.5 dex in a single galaxy in different star forming regions. Such a dispersion in metallicities favors an open box model and the results suggest a varid star formation history, possibly induced via minor mergers and accretion.

V1.00294 A phenomenological model for tunneling rate of nonequilibrium quasiparticles in superconducting qubits, MOHAMMAD ANSARI, Kavli Institute for Nanoscience, Delft University of Technology — In superconducting qubits the lifetime of quantum states cannot be prolonged arbitrarily by decreasing temperature. At low temperature quasiparticles tunneling between electromagnetic environment and superconducting islands takes the condensate state out of equilibrium due to charge imbalance. We obtain tunneling rate from a phenomenological model for non-equilibrium, where a fixed non-equilibrium quasiparticle density leads to a temperature-dependent chemical potential shift. This deduces a non-monotonic behavior of the relaxation rate as function of temperature. As a result electromagnetic environment can dramatically influence qubit transitions. This leads to crucial fabrication hints for improvement in quantum control of superconducting qubits.

V1.00295 Simulation of a Solid-Solid Transition in Confined Colloidal Hard Spheres, WEIKAI QI, Soft Condensed Matter, Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands, YI PENG, YI-HONG HAN, Department of Physics, Hong Kong University of Science and Technology, Hong Kong, China, RICHARD BOWLES, Dept. Chemistry, University of Saskatchewan, Canada, MARJOLEIN DIJKSTRA, Soft Condensed Matter, Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands — Recent experiments on a system of colloidal particles confined between two flat plates showed a two-stage nucleation process involving the transition of a solid, consisting of n-1 crystalline layers with a square symmetry (n=1 s-phase), to another solid consisting of n triangular layers (n t-phase), via an intermediate metastable liquid droplet [1]. Using event-driven molecular dynamics and Monte Carlo simulations, we study the 5s → 4t solid-solid transition in colloidal hard spheres confined between two planar hard walls. The 5s solid initially melts, forming a liquid droplet, within which the 4t solid nucleates. Calculations of the free-energy landscape confirm that the optimal kinetic pathway is a two-stage nucleation process with a critical nucleus consisting of liquid-like and t-solid-like particles. In addition, we find that the t-solid-like cluster nucleates near the planar hard walls, and contains both face-centered-cubic and hexagonal-close-packed ordered particles.


3 Current Address: Dept. Chemistry, University of Saskatchewan, Canada
V1.00296 A Pseudopotential Approach to Compute Thermodynamic Properties of Liquid Semiconductors, ANAND PRAJAPATI, PANKAJ THAKOR, Department of Physics, Veer Narmad South Gujarat University, Surat 395 007, Gujarat, India, YOGESH SONVANE, Department of Applied Physics, S. V. National Institute of Technology, Surat 395 007, Gujarat, India — This paper deals with the theoretical approach for calculating the thermodynamical properties viz. Enthalpy(E),Entropy(S) and Helmholtz free energy(F) of some liquid semiconductors (Si, Ga, Ge, In, Sn, Ti, Bi, As, Se, Te and Sb). The Gibbs-Bogoliubov(GB) variational method is applied to compute the thermodynamical properties. Our well established model potential is used to define the electron-ion interaction. Charged Hard Sphere (CHS) reference system is used to describe the structural contribution to the Helmholtz free energy in the liquid phase. Local field correction function proposed by Farid et al is adopted to see the screening effect. Lastly, our newly constructed model potential is an effective one to produce the data of thermodynamical properties of some liquid semiconductor.

V1.00297 Electronic and Optical Properties of Core/Shell Pb16X16/Cd52S52 (X=S, Se, Te) Quantum Dots, PATRICK TAMUKONG, North Dakota State University, MICHAEL MAYO, Retired, SVETLANA KILINA, North Dakota State University — The electronic and optoelectronic properties of semiconductor quantum dots (QDs) are mediated by surface defects due to the presence of dangling bonds producing trap states within the HOMO-LUMO energy gap, and contributing to fluorescence quenching. Surface capping ligands are generally used to alleviate this problem and increase the quantum yields of QDs. An alternative way is to synthesize core-shell QD structures, i.e., a QD due to the shell composition of another semiconductor material. We have investigated the effects of Cd52S52 shells on the photoexcited dynamics of Pb16X16 (X=S, Se, Te) QDs. The thin (≈ 0.50 nm) shells were found to result largely in type I core/shell structures and a blue shift of the absorption spectra. Our studies revealed fairly strong core-shell hybridization in the electronic states close to the conduction band (CB) edge for Pb16S16 and Pb16Se16 cores, whereas for the Pb16Te16 core, such CB states were largely shell-like in nature. Nonadiabatic DFT-based dynamics, coupled with the surface hopping method, was used to study the effects of the core and shell compositions on energy relaxation rates in these systems.

V1.00298 Role of Radio Frequency Power in the Plasma Enhanced Chemical Vapor Deposition, SUDIP SEN, Claflin University, SC and College of William & Mary, VA — PECVD. Plasma Enhanced Chemical Vapor Deposition, is used to deposit thin films from a gas state to a solid state on a substrate. Experimental study from the X-ray diffraction spectra of Silicon-Oxide films deposited as a function of radio frequency (rf) power apparently indicates that RF power might be playing a stabilizing role and produces better deposition. The results show that the rf power results in smoother morphology, improved crystallinity, and lower sheet resistance value in the PECVD process. The PECVD processing allows deposition at lower temperatures, which is often critical in the manufacture of semiconductors. In this invited talk we will address two aspects of the problem, first to develop a model to study the mechanism of how the PECVD is affected by the RF power, and second to actually simulate the effect of rf power on PECVD. As the PECVD is a very important component of the plasma processing technology with many applications in the semiconductor technology and surface physics, the research proposed here has the prospect to revolutionize the plasma processing technology through the stabilizing role of the rf power. Recent results obtained after the abstract submission will also be included.

V1.00299 Magnetoelastic coupling in superconducting Sr2VO3FeAs revealed by scanning tunneling microscopy, SEOKHWAN CHOI, HYUNWOO CHOI, HYUN-JUNG LEE, JIN-OH JUNG, DONGHYON SON, Department of Physics, KAIST, Daejeon 305-701, Korea, JUN SUNG KIM, JONG MOK OK, Department of Physics, POSTECH, Pohang 790-784, Korea, JHINHWAN LEE, Department of Physics, KAIST, Daejeon 305-701, Korea — Sr2VO3FeAs is known to exhibit high Tc (~ 37K) superconductivity with no magnetic ordering in the FeAs layer but weak magnetic moment in the V sublattice. From the density functional theory study, there is found to be a band gap between the electronic levels of V 3d orbitals. We have studied on Sr2VO3FeAs single crystal using spectroscopic imaging scanning tunneling microscopy (SI-STM) with variable temperature from 4.6K to 100K, and magnetic field up to 7T. Our results show that Sr2VO3FeAs has charge density wave (CDW) modulation in the V sublattice with the same wave vector observed in the neutron scattering experiment. The modulation strength is reduced with applying magnetic field. An electronic Fermi surface with largest V 3d character shows suppressed superconductivity possibly due to strong V-site correlation. However the multi-orbital nature of FeAs allows overall unsuppressed superconductivity at high Tc.

V1.00300 Carbon Nanotube Charge Collectors in Doped Hybrid Perovskite Solar Cells, ZANE OLDS1,2, ROSS HAROLDSON2, KAMIL MIELCZAREK, ANVAR ZAKHIDOV1, Univ of Texas - Dallas — Hybrid organo-metallic solar cells based on perovskite crystals have had steadily improved power conversion efficiencies over the past two years, and within this period have achieved efficiencies over 19%. We show that additions of Metal-Halide dopants, such as Cobalt (II) Iodide or Indium and Bismuth materials, can cause substitutional doping at the Lead atom. This may result in structural distortions (as in isovalent Co-doping) from the lattice causing change in the spatial distribution of charge carriers. We show that Co-doping results in an increased open circuit voltage upon light soaking due to possible higher charge accumulation. We also have investigated effects of p-doping the hole transport layer. We also incorporate composite sheets of MW carbon nanotubes and silver nanowires as charge collectors. These sheets provide a transparent and flexible electrode with lower sheet resistance due to integration of Ag nanowires. This has an effect on the work function of the sheet, p-doping the hole transport layer. We also incorporate composite sheets of MW carbon nanotubes and silver nanowires as charge collectors. These sheets provide a transparent and flexible electrode with lower sheet resistance due to integration of Ag nanowires. This has an effect on the work function of the sheet, p-doping the hole transport layer.

V1.00301 Pressure-induced magneto-structural transition in iron via a modified solid-state nudged elastic band method, NIKOLAI A. ZARKEVICH, DUANE D. JOHNSON2, Ames Laboratory, U.S. Department of Energy at Iowa State University, Ames, Iowa 50011-3020 — Materials under pressure may exhibit critical electronic and structural transitions that affect equation of states, as known for superconductors and the magneto-structural transformations of iron with both geophysical and planetary implications. While experiments often use constant-pressure (diamond-anvil cell, DAC) measurements, many theoretical results address a constant-volume transitions, which avoid issues with magnetic collapse but cannot be directly compared to experiment. We establish a modified solid-state nudged elastic band (MSS-NEB) method to handle magnetic systems that may exhibit moment (and volume) collapse during transformation. We apply it to the pressure-induced transformation in iron between the low-pressure body-centered cubic (bcc) and the high-pressure hexagonal close-packed (hcp) phases, find the bcc-hcp equilibrium coexistence pressure and a transitional pathway, and compare to shock and DAC experiments.

V1.00302 POSTDEADLINE ABSTRACTS —
V1.00303 Theoretical Investigation Optical Properties of Si$_{12}$C$_{12}$ Clusters and Oligomers having Potential as Excitonic Materials$^1$, XIAOFENG DUAN, Air Force Research Laboratory, AFRL RCM, LARRY BURGGRAF, Air Force Inst of Tech - WPAFB — SIC clusters may have potential in 2-D exciton circuits. We determined the most stable Si$_n$C$_m$ isomer structures ($n \leq 12$) out of hundreds to thousands isomers using a method combining Stochastic Potential Surface Search and Pseudopotential Plane-Wave Density Functional Theory Car-Parinello Molecular Dynamics simulated annealing (PSWP-CPMD-SA). Four low-energy Si$_{12}$C$_{12}$ isomer structures are discussed to illustrate the varying optical properties of clusters with structures: i) cage type with C- and Si- segregations, ii) symmetric type formed having n-stacked C aromatic rings and exterior Si regions, iii) nearly planar bowl with C fullene fragment surrounded by Si atoms, and iv) symmetrical SIC cluster having alternate SiC bonding in the structure. We employed B3LYP and PBE0 functionals and both cc-pVTZ and aug-cc-pVTZ basis sets to perform TDDFT calculations of excitation energies and photo-absorption spectra to show how structure and bonding patterns affect photo excitations in different types of SIC clusters. The electron and the hole charge distribution patterns in excitation were calculated for major photoabsorption transitions, reported for the most stable isomer, closo Si$_{12}$C$_{12}$. To understand electric field effects we also calculated dynamical polarizabilities for all the four structures using Coupled Perturbed Hartree-Fock (CPHF) at B3LYP/aug-cc-pVTZ and PBE0/aug-cc-pVTZ level of theory.

$^1$We gratefully acknowledge support from the Air Force Office of Scientific Research in a program managed by Dr Michael Berman.

V1.00304 Use of atomic hydrogen source in collision: technological challenges$^2$, R.T. HOVEY, E.L. VARGAS, D.I. PANCHENKO, D.A. RIVAS, V.M. ANDRIANARIJAONA, Department of Physics, Pacific Union College, Angwin, CA 94508 — Atomic hydrogen was extensively studied in the past due to its obvious fundamental aspect. Also, quite few investigations were dedicated to atomic hydrogen sources because the results of experimental investigations on systems involving H would provide very rigorous tests for theoretical models. But even if atomic hydrogen sources are currently widespread in experimental physics, their uses in experiments on collisions are still very challenging mainly due to threefold problem. First, there is the difficulty to create H in the laboratory in sufficiently large number densities. Second, there is the strain to adjust the velocities of the produced atomic hydrogen. And third, there is the toll to control the internal energies of these atomic hydrogens. We will present an outline of different techniques using atomic hydrogen sources in collisions, which could be found in the libraries, such as merged-beam technique, gas cell technique, and trap, and propose an experiment scheme using a turn-key atomic hydrogen source that experiments such as charge transfer could benefit from.

$^2$This work is supported by the National Science Foundation under Grant No. PHY-1068877.

V1.00305 Spatially and temporally resolved exciton dynamics and transport in single nanostuctures and assemblies, LIBAI HUANG, Purdue University — The frontier in solar energy conversion now lies in learning how to integrate functional entities across multiple length scales to create optimal devices. To address this new frontier, I will discuss our recent efforts on elucidating multi-scale energy transfer, migration, and dissipation processes with simultaneous femtosecond temporal resolution and nanometer spatial resolution. We have developed ultrafast microscopy that combines ultrafast spectroscopy with optical microscopy to map exciton dynamics and transport with simultaneous ultrafast time resolution and diffraction-limited spatial resolution. We have employed pump-probe transient absorption microscopy to elucidate morphology and structure dependent exciton dynamics and transport in single nanostructures and molecular assemblies. More specifically, (1) We have applied transient absorption microscopy (TAM) to probe environmental and structure dependent exciton relaxation pathways in sing-walled carbon nanotubes (SWNTs) by mapping dynamics in individual pristine SWNTs with known structures. (2) We have systematically measured and modeled the optical properties of the Frenkel excitons in self-assembled porphyrin tubular aggregates that represent an analog to natural photosynthetic antennae. Using a combination of ultrafast optical microscopy and stochastic exciton modeling, we address exciton transport and relaxation pathways, especially those related to disorder.

V1.00306 Pressure-induced magnetic quantum critical point in the itinerant helimagnet MnP, JINGUANG CHENG, Institute of Physics, Chinese Academy of Sciences, KAZUYUKI MATSUBAYASHI, ISSP, University of Tokyo, WEI WU, FUKUN LIN, JIANPING SUN, JIANLIN LUO, Institute of Physics, Chinese Academy of Sciences, YOSHIYA UWATOKO, ISSP, University of Tokyo, JIAQIANG YAN, MASAAKI MATSUDA, Oak Ridge National Laboratory — manganese monophosphide, MnP, is an interesting magnetic material that has been investigated since 1960s in the context of rich magnetic phase diagram, Lifshitz multicritical point, and magnetocaloric effect [1-4]. It adopts in the orthorhombic B31-type structure derived from the hexagonal NiAs-type structure. At ambient pressure, MnP is ferromagnetic below $T_c = 291$ K and $T_c \approx 50$ K, below which the magnetic structure changes into a screw-type order with Mn spins rotating in the a-b plane and propagating along the c axis [1,2]. We have performed comprehensive high-pressure studies on MnP single crystals up to 10 GPa with a suite of experimental probes, including resistivity, ac magnetic susceptibility, and stochastic exciton modeling, we address exciton transport and relaxation pathways, especially those related to disorder.

V1.00307 On The Nature Of Spacetime, ASEEM GUPTA$^3$, None — While Einstein made spacetime relative for observers and an active player in physical phenomena he tacitly assumed that all observers experience spacetimes that are always synchronized We propose extension of concept of spacetime by considering possibility of an observer experiencing spacetimes that cannot synchronize with that of a system due to impossibility of transfer of any information between them. This coupled with fundamental premise of quantized action leads to increasing desynchronisation between spacetime experienced by observer and that of system leading to only probability distribution functions connecting spacetime coordinates of two. This desynchronisation of spacetimes is postulated as the root cause of fundamental probabilistic nature of Quantum Physics. It is shown that Schrodinger’s equation models space desynchronization but not that of time inclusion of which leads to Quantum Field Theory. Desynchronization explains fundamental difference in quantum statistics and classical statistics and also existence of dynamic symmetry in addition to geometric symmetry. Nested desynchronized spacetime model of our Universe is proposed. It is shown how desynchronization can allow modeling of elementary particles as extended systems and not point-like explaining why these may be modeled as representations of Lie groups.

$^3$This is a study to discern one fundamental premise of spacetime conception in classical physics and demonstrating how this premise does not hold in quantum physics. Desynchronization is presented as fundamental aspect of ontology of quantum theory.
V1.00308 Coexistence of three-wave, four-wave and five-wave mixing processes and Autler-Townes splittings in a superconducting artificial atomic system

GUO-QIN GE, HAICHAO LI, Huazhong University of Science and Technology — We present a theoretical study of multi-wave mixing in a driven superconducting quantum qubit (artificial atom) with \( \Delta \)-type three-level structure. We first show that three-wave mixing (TWM), four-wave mixing (FWM) and five-wave mixing (FWM) processes can coexist in the microwave regime in such an artificial system due to the absence of selection rules. Because of electromagnetically induced transparency suppression of linear absorption in a standard ladder-type configuration, the generated FWM is enhanced greatly and its efficiency can be as high as \(0.1\%\) for only a single artificial atom, which is comparable to or even larger than that of many previous schemes in atomic systems. Moreover, it is possible to obtain a more higher conversion efficiency by using an array of such artificial atoms. We also show that quantum interference between TWM and FWM signals has a significant impact on the total signal intensity being a coherent superposition of these two signals. Our scheme for the generation of microwave signals may have potential applications in solid-state quantum information processing.

This work was supported in part by the National Natural Science Foundation of China under the Grant No. 11274132 and the Hubei Provincial Natural Science Foundation of China.

V1.00309 Highly Ordered and Highly Aligned Two-Dimensional Binary Superlattice of a SWNT/Cylindrical-Micellar System

SUNG-HWAN LIM, HYUNG-SIK JANG, JAE-MIN HA, KAIST, TAE-HWAN KIM, KAERI, PAWEL KWASNIEWSKI, THEYENCHERI NARAYANAN, ESRF, KYEONG SIK JIN, POSTECH, SUNG-MIN CHOI, KAIST — The synthesis of binary nanoparticle superlattices, which may provide new properties through synergetic coupling between different types of nanoparticles, are of great interest for various potential applications as well as its own scientific merit. While existing progress has been made in the fabrication of binary spherical-nanoparticle superlattices with various symmetries by using an interplay of entropic and enthalpic interactions, systematic experimental studies on the formation of binary 1D nanoparticle superlattices have been very rare. Here, we report a highly ordered intercalated hexagonal binary superlattice of hydrophobically functionalized single-walled carbon nanotubes (p-SWNTs) and surfactant (C12E5) cylindrical micelles. When p-SWNTs (with a diameter slightly larger than that of the C12E5 cylinders) were added to the hexagonally packed C12E5 cylindrical-micellar system, p-SWNTs positioned themselves in such a way that the free-volume entropies for both p-SWNTs and C12E5 cylinders were maximized, thus resulting in the intercalated hexagonal binary superlattice. The binary superlattice can be highly aligned in one direction by an oscillatory shear field and remains aligned after the shear is removed.

This research was supported by NRF grants funded by the MEST of the Korean government (No. 2014R1A2A1A05007109 and 2011-0031931) and the BK21.

V1.00310 Optical studies of photoactive states in mixed organic-inorganic hybrid perovskites stabilized in polymers

BEATA KARDYNAL, LIFEI XI, PGI 9, Forschungszentrum Jülich, Germany, TEDDY SALIM, MSE, NTU, Singapore, SVEN BORGHARDT, TOMA STOICA, PGI 9, Forschungszentrum Jülich, Germany, YENG MING LAM, MSE, NTU, Singapore — Mixed organic-inorganic hybrid perovskites \( \text{MAX-PbY}_2(X,Y=\text{I, Br, Cl}) \) have been demonstrated as very attractive materials for absorbers of solar cells and active layers of light emitting diodes and optically driven lasers. The bandgap of the perovskites can be tuned by mixing halogen atoms in different ratios. In this presentation we study mixed \( \text{MAX-PbY}_2(X,Y=\text{I, Br, Cl}) \) particles synthesized directly in protective polymer matrices as light emitters. Both, time integrated and time resolved photoluminescence have been used to study the materials. So synthesized \( \text{MAX-PbX}_2 \) are very stable when measured at room temperature and in air with radiative recombination of photogenerated carriers as the main decay path. In contrast, \( \text{MAX-PbY}_2 \) with mixed halogen atoms display luminescence from sub-bandgap states which saturate at higher excitation levels. The density of these states depends on the used polymer matrix and increases upon illumination. We further compare the \( \text{MAX-PbY}_2 \) synthesized in polymers and as films and show that these states are inherent to the material rather than its microstructure.

This work has been supported by EU NWs4LIGHT grant.

V1.00311 Phase Transition Study of Ammonia Borane/Polymer Composites: Potential Hydrogen Storage Systems

OZGE GUNAYDIN-SEN, RAMESH SUVVARI, Lamar University — Ammonia Borane \((\text{NH}_3\text{BH}_3)\), a potential hydrogen storage material exhibits a phase transition at \( T_P \sim 223 \text{ K} \) but the underlying mechanism is unclear. Ammonia borane \((\text{AB})\) blended with polymers (e.g. polyacrylamide) significantly improves the dehydrogenation kinetics and suppression of byproducts/impurities. We carried out heat capacity measurements over a temperature range of 180–300 K, and detected an anomaly at around 223 K, indicating a first-order transition. The change in enthalpy and entropy was calculated for \( \text{AB} \) as well as the composites and compared. The transition enthalphy and entropy revealed a decrease by increasing the polymer content and the transition temperature showed a small shift to lower temperatures for \( \text{AB}/\text{Polymer} \) composites both of which could be due to the interaction between polyacrylamide and \( \text{AB} \) after blending. This phenomena was also supported by infrared measurements.

This work was supported by Lamar University and Welch Foundation.

V1.00312 Pure spin current transport in Alq3 by spin pumping

SHENWEI JIANG, PENG WANG, ZHONGZHI LUAN, XINDE TAO, HAIFENG DING, DI WU, Nanjing University — The use of organic semiconductors (OSCs) in spintronics has aroused considerable interests, owing to their much longer spin-relaxation times of OSCs than those of inorganic counterparts. The most studied example is the organic spin valve (OSV), in which magnetoresistance (MR) effect is frequently reported. However, studies on pure spin current injection and transport in OSCs are scarce. Recently, the pioneering work by Watanabe et al. demonstrated that pure spin current can be pumped into and propagates in semiconducting polymers \([1]\). In the present work we extend the study to small molecule OSCs, and demonstrate that pure spin current can be injected into Alq3 from the adjacent magnetic insulator \( Y_2\text{Fe}_5\text{O}_3 \text{(YIG)} \) by spin pumping. The pure spin current is detected by inverse spin Hall effect (ISHE) in Pd after propagation through Alq3. From the ISHE voltage \( V_{\text{ISH}} \) as a function of the Alq3 thickness, the spin diffusion length is determined to be \( \sim 50 \text{ nm} \) and does not depend on temperature. This result indicates the MR decrease as increasing temperature in OSVs is not due to the reduced spin diffusion length.

V1.00313 Second-harmonic rotational anisotropy and circular dichroism of a Sb$_2$Te$_3$ topological insulator nanoplate, YONG AN, ROBIN JACOBS-GEDRIM, AVERY GREEN, SAMUEL O'MULLANE, ALAIN DIEBOLD, SUNY College of Nanoscale Science and Engineering — Topological insulators are an exotic class of materials that are electrically insulating in the bulk but conducting at the surface due to the presence of topological surface states. Spin-momentum locking of the surface states makes topological insulators potential candidates for spintronic applications. Experimental detection of the surface states and their spin polarization due to spin-momentum locking remains difficult because of the lack of surface-specific analytical techniques. Optical second-harmonic generation (SHG) is a surface-specific probe and thus it should probe the topological surface states preferentially over the bulk states. Here we present an experimental study of SHG from a Sb$_2$Te$_3$ topological insulator nanoplate, which is a 30-µm wide, hexagonal-shaped, and (001)-faced single crystal grown via chemical vapor deposition on an oxidized Si(001) substrate. We show that SHG rotational anisotropy can identify the crystalline symmetry of the nanoplate and also probe spin-polarized currents excited by circularly polarized light. Furthermore, by measuring SHG circular dichroism (the differential SHG of left- and right-handed circularly polarized excitation), we show that a non-zero SHG circular dichroism signal when the incident plane lies in the mirror symmetry plane of the nanoplate corresponds to time reversal symmetry breaking due to photo-induced spin polarization.

V1.00314 ABSTRACT WITHDRAWN —

V1.00315 Trapping and manipulating single nano-objects with dynamic temperature fields, FRANK CICHOS, MARCO BRAUN, ANDREAS BREGGULLA, University Leipzig, Germany, MOLECULAR NANOPHOTONICS GROUP TEAM — One of the challenges of single molecule experiments in solution is the ability to trap and manipulate one or even multiple molecules against the erratic Brownian motion. The Brownian fluctuations are fueled by thermal energy and increase in strength with increasing temperature. Therefore, it is at first glance counterintuitive to confine Brownian fluctuations with the help of elevated temperatures. In thermal nonequilibrium, however, temperature gradients induce thermo-phoretic and thermo-osmotic drifts, which provide the means for single particle manipulation in solution. Here we describe experiments which use optically heated metal nanostructures to create dynamical temperature profiles in solution. These temperature profiles induce thermo-phoretic drift fields that act as effective potentials for objects suspended in liquids. Combined with optical feedback mechanisms, such effective potentials can be shaped to store and manipulate single or even well-defined number of multiple objects in a small observation volume. The developed thermophoretic trapping system therefore paves the way for extended single molecule studies in solution or even well controlled bi- or multi molecular interaction studies.

V1.00316 Large Chern number topological superfluids in bilayer system, MING GONG, BEIBING HUANG, The Chinese University of Hong Kong, GONG TEAM — We investigate the topological phase transition with large Chern number in a coupled layer system. The topological transitions between different topological superfluids can be realized by controlling the binding energy, interlay tunneling and layer asymmetry etc. These topological phase transitions can be characterized by energy gap closing and reopening at the critical points at zero momentum, where the Pfaffian and Chern number undergo a discontinuous change. The bulk-edge correspondence ensures that the number of edge modes exactly equals the Chern number. However, all these edge modes localized at the same edge have the same chirality and propagate along the same direction. These topological phases can be detected by spin texture at or near zero momentum, which changes discontinuously across the phase transition point due to band inversion. This model can be easily generalized to multilayer system in which the Chern number equals any positive integer — similar to that in integer quantum Hall effect — can be realized. This work paves a new way in the realization of topological superfluids with large Chern number.

V1.00317 Two distinct superconducting fluctuation diamagnetisms in Bi$_2$Sr$_{2-x}$La$_x$CuO$_{6+y}$, H. XIAO, Institute of Physics, Chinese Academy of Sciences — Superconducting fluctuations were studied through the angular dependent torque measurements on a series of Bi$_2$Sr$_{2-x}$La$_x$CuO$_{6+y}$ (BSCCO) single crystals. Two distinct superconducting fluctuation diamagnetisms were observed: one is the superconducting thermal fluctuation, with a boundary close to the superconducting phase boundary; while another one, up to the temperature as high as about 180 K, showing maximum signal in the sample with hole carrier density $p = 0.125$, could be due to preformed pairs. In addition, we observed linearly temperature dependent paramagnetic torque signals in BSCCO samples, possibly a result of quantum criticality from a quantum critical point at the optimal doping.

3We acknowledge support from the MOST of China, Projects No. 2011CBA00107 and No. 2012CB210302 and NSFC, project No. 11104335.

V1.00318 Straining graphene with low-temperature compatible electrostatic comb-drive actuators, TYMOFYI KHODKOV, MATTHIAS GOLDSCHE, JARA-FIT and II. Institute of Physics A, RWTH Aachen, SVEN REICHARDT, II. Institute of Physics A, RWTH Aachen, CHRISTOPH STAMPFER, JARA-FIT and II. Institute of Physics A, RWTH Aachen — Graphene holds great promises as an active element in future nano electromechanical systems. Therefore, thorough study of electromechanical properties of this 2D material is a crucial step towards its applications in flexible electronics. We present the fabrication and characterization of silicon-based electrostatic comb-drive actuators made for integrating individual graphene sheets. The micromachined comb-drive actuators are designed such that they can induce significant mechanical forces for straining graphene allowing to systematically investigate mechanical and electromechanical properties of high-quality graphene. By using highly doped silicon the comb-drive actuators become compatible with low temperatures, i.e. cryogenic temperatures allowing for quantum electromechanical experiments. Further device functionality is introduced by a local gate that enables the tunability of the chemical potential of the graphene. This approach makes possible a detailed study of the graphene under controlled high strain allowing simultaneous and independent tuning of other external parameters, i.e temperature, charge density, magnetic field. With Raman spectroscopy we measure and characterize mono and bilayer graphene samples at room temperature under applied strains up to 1%. A detailed analysis of data allows clear separation of strain and doping. It is demonstrated that with this technique graphene sheet reproducibly experiences only strain while operating the comb-drive actuator.

V1.00319 Fragmentation, vortices and phantom vortices in rotating Bose-Einstein Condensates, MARIOS C. TSATSOS, University of Sao Paulo, STORM WEINER, University of California at Berkeley, AXEL LODE, University of Basel — Superfluids are a superfluid subject to external rotation. In this work we study a trapped ultracold Bose gas of $N = 100$ atoms in two spatial dimensions that is either stirred by a rotating beam or by a rotating anisotropy. We extend the time-dependent multiconfigurational Hartree method for bosons, that extends the mainstream mean-field theory, to calculate the dynamics of the gas in real time. As the gas is rotated the wavefunction of the system changes symmetry and topology. Fragmentation accompanies the resonances and change of symmetry of the wavefunction of the gas. We see a series of resonances as the rotating frequency is increased and a variety of different excitations. Most importantly, we identify a novel type of topological defect as a phantom vortex. A phantom vortex cannot be seen in the density of the gas but it leaves its signature in the correlation function. We conclude that fragmentation of the gas appears hand-in-hand with resonant absorption of energy and angular momentum from the external agent of rotation.
V1.00320 Influence of $^{13}$C isotopic labeling location of $^{13}$C DNP of acetate using TEMPO free radical. CHRISTOPHER PARISH, PETER NIEBDSALSKI, LLOYD LUMATA, University of Texas System — Dynamic nuclear polarization (DNP) via the dissolution method enhances the liquid-state magnetic resonance (NMR or MRI) signals of insensitive nuclear spins by at least 10,000-fold. The basis for all these signal enhancements at room temperature is the polarization transfer from the electrons to nuclear spins at cryogenic temperature and high magnetic field. In this work, we have studied the influence of the location of $^{13}$C isotopic labeling on the DNP of sodium acetate at 3.35 T and 1.4 K using a wide ESR linewidth free radical 4-oxo-TEMPO. The carbonyl $[^{1-^{13}}]$Cacetate spins produced a polarization level that is almost twice that of the methyl $[2-^{13}]$Cacetate spins. On the other hand, the polarization of the methyl $^{13}$C spins doubled to reach the level of $[1-^{13}]$Cacetate when the methyl group was deuterated. Meanwhile, the solid-state nuclear relaxation of these samples are the same and do not correlate with the polarization levels. These behavior implies that the nuclear relaxation for these samples is dominated by the contribution from the free radicals and the polarization levels can be explained by a thermodynamic picture of DNP.

V1.00321 Dynamic nuclear polarization of carbonyl and methyl $^{13}$C spins in acetate using trityl OX063. PETER NIEBDSALSKI, CHRISTOPHER PARISH, LLOYD LUMATA, Univ of Texas - Dallas — Hyperpolarization via dissolution dynamic nuclear polarization (DNP) is a physics technique that amplifies the magnetic resonance signals by several thousand-fold for biomedical NMR spectroscopy and imaging (MRI). Herein we have investigated the effect of carbon-13 isotopic location on the DNP of acetate (one of the biomolecules commonly used for hyperpolarization) at 3.35 T and 1.4 K using a narrow ESR linewidth free radical trityl OX063. We have found that the carbonyl $^{13}$C spins yielded about twice the polarization produced in methyl $^{13}$C spins. Deuteration of the methyl group, beneficial in the liquid-state, did not produce an improvement in the polarization level at cryogenic conditions. Concurrently, the solid-state nuclear relaxation of these samples correlate with the polarization levels achieved. These results suggest that the location of the $^{13}$C isotopic labeling in acetate has a direct impact on the solid-state polarization achieved and is mainly governed by the nuclear relaxation factor.

V1.00322 Key to formation of two-dimensional electron gas and two-dimensional superconductivity at LaAlO$_3$/SrTiO$_3$. YINLONG HAN, SHENCHUN SHEN, CHENGJIAN LI, ZHONGZHANG LIOU, GUOSHANG QI, JIACAI NIE, Department of Physics, Beijing Normal University, JIACAI NIE TEAM — In this report, we systematically studied the band alignment and interfacial atomic structure of (110) LaAlO$_3$/SrTiO$_3$ (LAO/STO) interfaces. We show that for both (110) and (001) LAO/STO heterojunctions, the intrinsic or extrinsic coexistence of La and Ti in ABO$_3$ perovskite unit cells at the interface reduces the valence of Ti, generating a local field and further leading to band bending of the STO. The free electrons would be trapped in the bended conduction band forming 2DEG. This opens new insights of band engineering for controlling the behavior of complex oxide heterojunctions. Besides, the two-dimensional superconductivity of (110) LAO/STO samples is demonstrated based on the systematical transport measurements. The two dimensional characteristics of the superconductivity is confirmed by analyzing the Berezinskii-Kosterlitz-Thouless transition. The estimated superconductivity thickness is about 18 nm. This discovery may inspire a new round of upsurge on study of LAO/STO interfaces.

V1.00323 Nontrivial anomalous Hall effect in ultrathin Pt/permalloy bilayers. YANQING ZHANG, RONG SHAN, Tongji Univ — Anomalous Hall effect of Pt (2.5 nm)/permalloy bilayers with the thickness $t_{Py}$ = 0.6–10 nm; Pt/permalloy (2.2 nm) bilayers with the thickness $t_{Py}$ = 1.5–10 nm and Pt (2.5 nm)/permalloy (2.2 nm) bilayers with the post-annealing temperature $100\text{–}500^\circ$C grown on MgO (001) substrates are investigated. The Pt/permalloy bilayer showed distinguished performance from the single permalloy layer due to the interfacial influence. Effective magnetic anisotropy of the bilayer with $t_{Py}$ <2.2 nm turns to be perpendicular to the film plane and it increases with decreasing measured temperature. More interestingly, the anomalous Hall effect is also greatly enhanced in these Pt/permalloy bilayers, comparing with that in bulk permalloy. The parameters presenting skew scattering, side jump and intrinsic contribution become extremely large, indicating a strong influence of spin orbit coupling coming from Pt/permalloy interface on the anomalous Hall effect.

V1.00324 Evolution of Anomalous Hall Behavior in Pt/Co/ Pt Trilayers. NIU YI SUN, RONG SHAN, Tongji University — A series of Pt (t nm)/Co (0.5 nm)/Pt (5–t nm) trilayers with various thickness were prepared and post annealed for changing the proportions among the skew scattering (a), side jump and intrinsic contributions (b), which dominate the anomalous Hall effect in these films from a general point of view. The shape of Hall angle curve ($\rho_{xx}/\rho_{xy}$ versus $\rho_{xx}$) is expected, turned from bending to linear and then bending again with raising the annealing temperature. The conventional scaling expression $\rho_{xx}/\rho_{xy} = a + b\rho_{xx}$ is not adequate for the analysis of anomalous Hall effect, especially in those very thin films since side jump is suppressed by surface roughness and the skew scattering is enhanced by the interfacial scattering. The evolution of anomalous Hall behavior with temperature demonstrates the reliability of identifying the skew scattering as a cooperation of a residual resistance of impurities and a phonon scattering. Likewise, the thermal treatment can also tune the side jump contribution, so as to the ratio between the side jump scattering and the skew scattering, leading to a change of the shape of Hall angle curve. The distinct physical image was exhibited by 3D maps of correlation coefficient for $\rho_{xx}/\rho_{xy}$ and $\rho_{xx}$, which may help to build a proper synergy between theory and experiment on the research of anomalous Hall effect.

V1.00325 Proton transfer along water bridges in biological systems with density-functional tight-binding. KRYSLE REISS, ABIAGAIL WISE, JAMES MAZZUCA, Alma College — When examining the dynamics of charge transfer in high dimensional enzymatic systems, the exact chemical mechanism of electrons increases exponentially with the size of the system. As a semi-empirical method, density-functional tight-binding aids in shortening these calculation times, but can be inaccurate in the regime where bonds are being formed and broken. To address these inaccuracies with respect to proton transfer in an enzymatic system, DFTB is being used to calculate small model systems containing only a single amino acid residue donor, represented by an imidazole molecule, and a water acceptor. When DFTB calculations are compared to B3LYP geometry calculations of the donor molecule, we observe a bond angle error on the order of 1.2 degrees and a bond length error on the order of 0.011 Å. As we move forward with small donor-acceptor systems, comparisons between DFTB and B3LYP energy profiles will provide a better clue as to what extent improvements need to be made. To improve the accuracy of the DFTB calculations, the internuclear repulsion term may be altered. This would result in energy profiles which closely resemble those produced by higher-level theory.

V1.00326 The Effect of Isotopic Substitution on Quantum Proton Transfer Across Short Water Bridges in Biological Systems. JACOB BLAZEJEWSKI, CHASE SCHULTZ, JAMES MAZZUCA, Alma College — Many biological systems utilize water chains to transfer charge over long distances by means of an excess proton. This study examines how quantum effects impact these reactions in a small model system. The model consists of a water molecule situated between an imidazole donor and acceptor group, which simulate a fixed amino acid backbone. A one dimensional energy profile is evaluated using density functional theory at the 6-31G*/B3LYP level, which generates a barrier with a width of 0.6 Å and a height of 20.7 kcal/mol. Quantum transmission probability is evaluated by solving the time dependent Schrödinger equation on a grid. Isotopic effects are examined by performing calculations with both hydrogen and deuterium. The ratio of hydrogen over the deuterium shows a 130-fold increase among the skew scattering (a), side jump and intrinsic contributions (b), which dominate the anomalous Hall effect in these films from a general point of view. The distinct physical image was exhibited by 3D maps of correlation coefficient for $\rho_{xx}/\rho_{xy}$ and $\rho_{xx}$, which may help to build a proper synergy between theory and experiment on the research of anomalous Hall effect.

1 Alma College Provost’s Office

2 Alma College Provost’s Office
V1.00327 Selective Label-free Electrokinetic Cell Tracker (SELECT): a novel liquid platform for cell characterization. RAJESHWARI TARUVAI KALYANA KUMAR, IZABELLE DE MELLO GINDRI, DAVID KINNAMON, PRADYOTHA KANCHUSTAMBH, DANIELI RODRIGUES, SHALINI PRASAD, University of Texas at Dallas, BIOMATERIALS FOR OSSEOINTEGRATION AND NOVEL ENGINEERING LAB COLLABORATION — Characterization and analysis of rare cells provide critical cues for early diagnosis of diseases. Electrokinetic cell separation has been previously established to have greater efficiency when compared to traditional flow cytometry methods. It has been shown by many researchers that buffer solutions in which cells are suspended in, have enormous effects on producing required dielectrophoretic (DEP) forces to characterize cells. Most commonly used suspension buffers used are deionized water and cell media. However, these solutions exhibit high level of intrinsic noise, which greatly masks the electrokinetic signals from cells under study. Ionic liquids (ILs) show promise towards the creation of conductive fluids with required electrical properties. The goal of this project is to design and test ILs for enhancing DEP forces on cells while creating an environment for preserving their integrity. We analyzed two methylimidazolium based ILs as suspension medium for cell separation. These dicationic ILs possess slight electrical and structural differences with high thermal stability. The two ILs were tested for cytotoxicity using HeLa and bone cells. The effects of electrical neutrality, free charge screening due to ILs towards enhanced electrokinetic signals from cells were studied with improved system resolution and no harmful effects.

V1.00328 Designing the bandgap of ZnO via Alloying of Magnesium and Sulfur1. JESSE HUSO, DINESH THAPA, HUI CHE, AMRAH CANUL, Department of Physics, University of Idaho, CALEB COROLEWSKI, M.D. MCCLUSKEY, Department of Physics, Washington State University, LEAH BERGMAN, Department of Physics, University of Idaho — ZnO is emerging as one of the materials of choice for UV applications. It has a benign chemical nature, a deep excitonic energy level, and a direct bandgap of 3.4 eV. The latter two properties make ZnO a highly efficient light-emitter at and above room temperature. Alloying ZnO with magnesium and sulfur creates the Mg$_x$Zn$_{1-x}$O$_2$ alloy systems which can tune the bandgap by design and add new optical and electronic functionalities to ZnO. In Mg$_x$Zn$_{1-x}$O$_2$, annealing studies were performed to overcome the phase segregation tendency, reduce intrinsic defects, and enhance the UV luminescence. It was found that annealing under an argon environment significantly improved the material and optical properties of the films due to the removal of intrinsic defects and completion of alloying. In Mg$_x$Zn$_{1-x}$O$_2$, phase segregation is expected to occur during growth due to the various crystal structures of end members and large difference in anion radii of S and O. However, this alloy system may form intermediate compounds such as zinc sulfate (ZnSO$_4$) which significantly impact material and optical properties. The removal of undesirable compounds will be discussed in terms of the growth conditions.

1This work is supported by the National Science Foundation under Grant No. DMR-1202532.

V1.00329 Correlation between local crystal structure and physical properties in BiS$_2$-based superconductors1. YOSHIKAZU MIZUGUCHI, JOE KAIJITANI, TAKAFUMI HIROI, OSUKE MIURA, Tokyo Metropolitan University, NAURANG SAINI, Sapienza University of Rome — Recently, layered superconductors with BiS$_2$ conduction layer have been discovered. Since the layered structure and low-dimensional electronic states are similar to cuprates and Fe-based superconductors, studies on exploration of new superconductors and discussion of superconductivity mechanisms of the BiS$_2$-based superconductors have got attention of researchers in the field of condensed matter physics. To understand the mechanisms of induced superconductivity in the BiS layer, we have investigated the physical properties and established superconductivity phase diagrams of various series of RE01-xFxBiS$_2$. To understand these phase diagrams, powder x-ray diffraction and x-ray absorption fine structure were carried out. It was found that optimization local crystal structure and reduction of in-plane disorder should be correlating with the physical properties of BiS$_2$-based compounds. We will discuss how superconductivity is induced and the Tc is enhanced, on the basis of local crystal structure such as atomic coordinates, atomic distances and in-plane disorder.

1This work was partly supported by Grant-in-Aid for Scientific Research (KAKENHI).

V1.00330 Critical anomalous Hall behavior in Pt/Co/Pt trilayers grown on paper with perpendicular magnetic anisotropy. WENRU CHE, XIAOFEI XIAO, NIUYI SUN, YANQING ZHANG, RONG SHAN, ZHENGANG ZHU. None — Perpendicular magnetic anisotropy was observed in Pt/Co/Pt trilayers prepared on three kinds of paper substrates with conspicuous difference of roughness by sputtering. Anomalous Hall effect exhibits well magnetic transport properties for partial samples. The trends of Hall resistivity over longitudinal resistivity ($\rho_{Hall}/\rho_{xx}$) versus $\rho_{xx}$ are bending instead of a traditional linear relationship for thick single-layer Co films. Further, study reveals that this behavior strongly depends on ratios among contributions from the skew scattering induced by residual resistance and phonons, the side jump and the intrinsic parts in anomalous Hall effect. A 3D map of correlation coefficients ($R$) of $\rho_{Hall}/\rho_{xx}$ and $\rho_{xx}$ shows the ratios locate at a critical and ultra-narrow area for our trilayers. This study may throw new light on the understanding of anomalous Hall effect as well as lead to an economical and practical method to fabricate Hall devices on flexible substrates.

V1.00331 ABSTRACT WITHDRAWN —

V1.00332 The origin of the UV Luminescence and its Enhancement in nanocrystalline ZnO film1. DINESH THAPA, JESSE HUSO, HUI CHE, AMRAH CANUL. Department of Physics, University of Idaho, CALEB COROLEWSKI, M.D. MCCLUSKEY, Department of Physics, Washington State University, LEAH BERGMAN, Department of Physics, University of Idaho — ZnO is an excellent luminescent material in the UV range with a potentially wide range of applications. However, many as-grown films are observed to contain some intrinsic defects which can diminish UV-emission efficiency, limiting their practical usefulness. This study presents a route to enhance UV luminescence from ZnO sputtered films. The photoluminescence (PL) spectra of the as-grown film exhibits prominent visible PL attributed to zinc interstitial (Zn$_i$) related defects, and a weak UV PL peak. To understand the route toward enhanced UV PL, one set of as-grown films were annealed in O$_2$ atmosphere and another set in Ar atmosphere. PL spectra of O$_2$-annealed samples revealed enhanced UV PL and elimination of the Zn$_i$-related defect emission, however, an O$_2$-related defect emission was evolved. In contrast, Ar annealed films showed significantly enhanced UV emission with nearly completely quenched visible emissions. The origin of UV PL was studied by low temperature measurements which indicate that an emission related to structural defects is dominant in the UV region.

1We acknowledge the US Department of Energy, Office of Basic Energy Science, Division of Materials Science and Engineering under Grant No. DE-FG02-07ER46386.

V1.00333 Leveraging zinc interstitials and oxygen vacancies for sensitive biomolecule detection through selective surface functionalization. NANDHINEE RADHA SHANMUGAM, SRIRAM MUTHUKUMAR, SHAJEE CHAUDHRY, SHALINI PRASAD, The University of Texas at Dallas, Richardson, TX 75080 — In this study, functionaly engineered EIS technique was implemented to investigate the influence of surface functionalization on sensitivity of biomolecule detection using nanostructured ZnO platform. Organic molecules with thiol and carboxylic functional groups were chosen to control biomolecule immobilization on zinc and oxygen-terminated 2D planar and 1D nanostructured ZnO surfaces. The amount of functionalization and its influence on charge perturbations at the ZnO-electrolyte interface were studied using fluorescence and EIS measurements. We observed the dependence of charge transfer on both the polarity of platform and concentration of cross-linker molecules. Such selectively modified surfaces were used for detection of cortisol, a major stress indicator. Results demonstrated preferential binding of thiol groups to Zn terminations and thus leveraging ZnO interstitials increases the sensitivity of detection over larger dynamic range with detection limit at 10fg/mL.
V1.00334 Spin transport of the frustrated quasi-two-dimensional Heisenberg antiferromagnet

, LEONARDO DOS SANTOS LIMA, Centro Federal de Educacão Tecnológica de Minas Gerais — We use the Self Consistent Harmonic Approximation together with the Kubo formalism of the Linear Response Theory to study the spin transport in the quasi-two-dimensional frustrated Heisenberg antiferromagnet in a square lattice with easy-plane ion single anisotropy at zero temperature. The regular part of the spin conductivity $\sigma^{reg}(\omega)$ is determined for several values of the critical ion single parameter $D_D$, that separates the low $D$ region from the large $D$ quantum paramagnetic phase. We have obtained an abrupt change in the spin conductivity in the point of phase transition indicating a strong influence of frustration on the spin transport properties.

V1.00335 The Vibrational Dynamics of 3D HOCl Above Dissociation1, YI-DER LIN, LINDA REICHL, University of Texas at Austin, CHRISTOF JUNG, Universidad Nacional Autonoma de Mexico — We have analyzed the vibrational dynamics of HOCl above dissociation using a 3D energy surface which governs the vibrational dynamics of HOCl above dissociation. The dynamics is dominated by an invariant manifold which is transversally unstable for small spacing between Cl and HO complex, and stable for large spacing. Above dissociation, the inM separates two mirror image periodic orbits, embedded in a large chaotic sea, that can hold a large number of quantum states. These periodic orbits have the capability of forming significant quasibound states of the molecule above dissociation.

1Welch Foundation

V1.00336 Development of Micro-Four-Point Probe Compatible with an Scanning Tunneling Microscope, CANHUA LIU, Shanghai Jiao Tong Univ — As miniaturization of electronic devices goes on, while more attention has to be paid to the influence of the existence of surfaces and interfaces on the electronic and/or magnetic properties of the electronic materials, some researchers have proposed to use the intrinsic surface properties for the development of future devices. On the other side, the existence of crystal surface and interface may reduce the spatial degrees of freedom of the carriers, and thus results in various novel quantum phenomena related to the reduction of dimensionality. It is highly desirable to obtain the electronic structure, morphology information and transport property of a material in situ, since they are strongly related. Based on a commercial apparatus equipped with STM and MBE systems, we developed an electronic transport measurement system that is compatible with the STM. A micro-four-point probe (MFPp) is utilized to increase the surface sensitivity in the transport measurement, which can be conducted at low temperature ($T_{min}$=1 K) and high magnetic field ($B_{max}$=11 T). With this system, we succeeded in detecting superconductivity above 100 K in a single unit-cell layer of FeSe film grown on an Nb-doped strontium titanate.

V1.00337 Coherent single-spin source based on topological insulators1, YANXIA XING, ZHONG-LIU YANG2, Beijing institute of technology, QING-FENG SUN, Peking University, JIAN WANG, HongKong University — We report on the injection of quantized pure spin current into quantum conductors. In particular, we propose an on-demand single-spin source generated by periodically varying the gate voltages of two quantum dots that are connected to a two-dimensional topological insulator via tunneling barriers. Due to the nature of the helical states of the topological insulator, one or several spin pairs can be pumped out per cycle giving rise to a pure quantized alternating spin current. Depending on the phase difference between two gate voltages, this device can serve as an on-demand single-spin emitter or single-charge emitter. Again, due to the helicity of the topological insulator, the single-spin emitter or charge emitter is dissipationless and immune to disorder. The proposed single-spin emitter can be an important building block of future spintronic devices.

1We gratefully acknowledge the financial support from from NSF-China under Grant (Nos. 11174032 and 11374246), NBRP of China (2012CB921303), and a RGC Grant (HKU 705212P) from the Government of HKSAR.

2Beijing institute of technology

V1.00338 Thermoelectric properties of bulk nanowire-nanoparticle composites, VENKATA VASIRAJU, Materials Science and Engineering Department, Texas &M University, LANCE BROCKWAY, Artie McFerrin Department of Chemical Engineering, Texas A&M University, SREEJAM VADDIRAJU, Artie McFerrin Department of Chemical Engineering, Materials Science and Engineering Department, Texas A&M University — Towards realizing highly efficient bulk thermoelectrics based on nanowire-nanoparticle composites, the effect of microstructure and composition on thermoelectric properties of an illustrative composite system composed of copper nanoparticles and zinc phosphate ($Zn_3P_2$) nanowires is studied. Here, the intent is to extend high efficiencies achieved in individual nanowire devices to bulk nanowire assemblies. To study these effects of microstructure, thermoelectric performances of compositionally non-uniform copper nanoparticle- unfuctionalized $Zn_3P_2$ nanowire pellets (composite-I) were compared against those of compositionally uniform copper nanoparticle-benzenedithiol functionalized $Zn_3P_2$ nanowire pellets (composite-II). These results indicated that compositional non-uniformity, coupled with copper doping of $Zn_3P_2$ nanowires, offers more room for optimizing the thermoelectric performances of the composites. Overall, a high thermoelectric figure of merit of 0.23 at 770K was achieved in composite-I. This is two orders of magnitude higher than any achieved to date in $Zn_3P_2$ system. This study indicates that tuning the microstructures and composition of materials is a route for enhancing their thermoelectric efficiencies.

V1.00339 Quantum phase transition of light in the resonator array, CHUN-WANG WU, MING GAO, ZHI-JIAO DENG, HONG-YI DAI, PING-XING CHEN, CHENG-ZU LI, College of Science, National University of Defense Technology, Changsha 410073, China, QUANTUM COMPUTATION GROUP OF NUDT TEAM — We give a concrete experimental scheme for engineering the insulator-superfluid transition of light in a one-dimensional (1-D) array of coupled superconducting stripline resonators. In our proposed architecture, the on-site interaction and the photon hopping rate can be tuned independently by adjusting the transition frequencies of the charge qubits inside the resonators and at the resonator junctions, respectively, which permits us to systematically study the quantum phase transition of light in a complete parameter space. By combining the techniques of photon-number-dependent qubit transition and fast read-out of the qubit state using a separate low-Q resonator mode, the statistical property of the excitations in each resonator can be obtained with a high efficiency. An analysis of the various decoherence sources and disorders shows that our scheme can serve as a guide to coming experiments involving a small number of coupled resonators.

V1.00340 Frustrated spin-spin interactions between trapped ions using longitudinal and transverse phonon modes1, YANLI ZHOU, College of Science, National University of Defense Technology — We present a scheme of quantum simulation of many-body interactions with trapped ions via the exchange of virtual phonons, where the motion from both the longitudinal and the transverse directions is considered. By tuning the detunings of Raman lasers, the long-range and locally tunable interaction is easily obtained between different spins. We show that the competing spin-spin couplings mediated by all motion modes can give rise to higher levels of frustration and richer phase transitions than the conventional approaches based on the longitudinal or the transverse phonon modes alone.

1This work is supported by NSFC Grants No.11304390.
V1.00341 Single laser beam photothermal microscopy, ANDRE HEBER, MARKUS SELMKE, MARCO BRAUN, FRANK CICHO; Leipzig University — Fluorescence microscopy provides a tool to study dynamics in soft matter materials on a molecular level. However, the observation time for fluorescent objects is limited due to bleaching. One way to overcome this limitation is the use of gold nanoparticles as labels. They are chemically inert under typical situations. These particles are selectively imaged using a modulated heating laser and a non-absorbed detection laser even in the presence of background scatterers. The absorbed power results in a localised temperature profile and to a refractive index change which only occurs for absorption. For finite thermal diffusivities the temperature profile does not instantly follow temperature changes present on the nanoparticle’s surface. This results in an out-of-phase modulation of the detection laser. By exploiting the limited thermal diffusivity we show that a single laser beam being intensity modulated is enough to selectively image and quantify absorption. The use of a single laser makes photothermal microscopy easier to implement into existing microscopy setups

V1.00342 Quantum Computational Resource Quality of a Symmetry-Protected Topologically Ordered Phase, JACOB MILLER, AKIMASA MIYAKE, University of New Mexico — Symmetry-protected topologically ordered (SPTO) states are many-body quantum states invariant under an on-site symmetry group, which can be grouped into distinct SPTO phases based on their non-local entanglement structure. While originally arising in the context of condensed matter physics, SPT states have also attracted interest in quantum information for their ability to be used as resource states for quantum computation. We investigate entanglement naturally present in the 1D SPTO phase associated with on-site octahedral symmetry and show that, as long as certain characteristic lengths are finite, all its ground states can be used to efficiently implement any one-qubit gate operation with arbitrary accuracy. This feature is an intrinsic property of the entire phase, and we show that it can also be probed by means of a particular string-order parameter. Our approach may pave the way toward a novel program to classify quantum many-body systems based on their operational use for quantum information processing.

V1.00343 Thermal and laser induced sintering in Pt nanoparticles studied by conventional and synchrotron x-ray diffraction, BRIAN KELLY, AARON LOETHER, Department of Physics and Astronomy, University of Delaware, RONALD CICHOCKI, Department of Chemistry and Biochemistry, University of Delaware, GERALD Poirier, Delaware Environmental Institute, University of Delaware, MATTHEW DECAMP, KARL UNRUH, Department of Physics and Astronomy, University of Delaware — The thermal and laser induced sintering behavior of 5 – 6 nm Pt nanoparticles self-assembled into 50 nm diameter spherical aggregates has been studied by conventional and synchrotron-based x-ray diffraction (XRD) measurements. In the first instance, the aggregated Pt nanoparticles were solution annealed at temperatures between 120 and 215 °C over time periods from 10s to 100s of minutes. In each case the linewidth of the conventionally measured diffraction pattern consisted of a single component which systematically narrowed suggesting an increase in the size of the as-prepared nanoparticles. In a second set of experiments, the aggregated Pt nanoparticles were exposed to about 10,000 laser pulses, each with a duration of about 1 ps and an energy density of 250 mJ/cm². XRD spectra were acquired after each 100 lasers pulses corresponding to 100 ps of sample irradiation. A narrow line component was observed in the diffraction pattern after the first 100 laser pulses and dominated the lineshape after a few thousand laser pulses. These measurements reflect the effects of long term, low temperature atomic transport in comparison with high energy, short time transport.

V1.00344 Single file diffusion in microtubules, ANDREW RUTENBERG, SPENCER FARRELL, AIDAN BROWN, Dalhousie University — We investigate the single file diffusion (SFD) of large particles entering a confined tubular geometry, such as luminal diffusion of proteins inside microtubules or flagella. While single-file effects have no effect on particle density, we report significant single-file effects for individually-tracked tracer particle motion. Both exact and approximate ordering statistics of particles entering semi-infinite tubes agree well with our stochastic simulations. Considering initially empty semi-infinite tubes, with particles entering at one end starting from an initial time t = 0, tracked particles display super-diffusive effective exponents just after they enter the system and trends towards diffusive exponents at later times. Equivalently, if diffusive exponents are assumed the effective diffusivity is reduced at early times and enhanced at later times through a logarithmic factor \( \log N \), where \( N \) is the number of particles in the tube. When we number each particle from the first (\( n = 1 \)) to the most recent (\( n = N \)), we find good scaling collapse of the effective diffusivity for all \( n \). Techniques that track individual particles, or local groups of particles, such as photo-activation or photobleaching, will exhibit single-file effects.

V1.00345 Temperature dependent thermal conductivity of single- and bi-layer MoS\textsubscript{2} and MoSe\textsubscript{2}, XIAN ZHANG, DEZHENG SUN, YILEI LI, Columbia University, GWAN-HYOUNG LEE, Yonsei University, YUMENG YOU, TONY HEINZ, JAMES HONE, XU CUI, Columbia University, JAMES HONE TEAM, TONY HEINZ TEAM — Thin layer transition metal dichalcogenide (TMDC) materials have received extensive interests in recent years. In this work, for the first time we systematically investigated and compared the thermal transport properties of two TMDC materials, MoS\textsubscript{2} and MoSe\textsubscript{2}, and in single-layer (1L) and bi-layer (2L) forms. The optothermal Raman technique is used in the measurement process. With an improved and more robust experimental data processing protocol, we discovered the thermal contact resistance and the interfacial thermal conductance of the four materials for the first time. These factors provide boundary conditions and are crucial in generating the final thermal conductivity for the suspended materials. For 1L MoS\textsubscript{2} and MoSe\textsubscript{2}, the room-temperature thermal conductivities are (80 ± 17) W/mK and (72 ± 19) W/mK, respectively. For 2L MoS\textsubscript{2} and MoSe\textsubscript{2}, we obtain values of (73 ± 25) and (39 ± 13) W/mK. The thermal conductivity of suspended 1L MoS\textsubscript{2} decreases to (66 ± 16) W/mK upon heating to 500K.

V1.00346 Substrate-Phonon-Mediated Plasmon Hybridization in Coplanar Graphene Nanoribbons, QING DAI, XIAOXIA YANG, XIAN-TIAN KONG, BING BAI, ZHENJUN LI, HAI HU, XIAOHUI QIU, National Center for Nanoscience and Technology — Mode hybridization between adjacent graphene nanoribbons determines the integration density of graphene-based plasmonic devices. Here we demonstrate this plasmon hybridization by characterizing the temperature dependence of plasmons in graphene nanoribbon arrays in terms of graphene Fermi level and inter-ribbon spacing. Both experimental and computational results showed that the plasmon coupling is strongly mediated by the substrate phonons. For polar substrate, the plasmon coupling strength was limited by the plasmon-phonon interaction. In contrast, nonpolar substrate affects neither the energy distribution of original plasmon modes in graphene nanostructures nor their plasmon interactions, which increase exponentially as the inter-ribbon spacing decreases. To further explore the potential of graphene broadband plasmonics on nonpolar substrate, we propose a scheme that uses a metal-dielectric heterostructure to preserve the overlap of plasmons between neighboring graphene nanoribbons. The device structures retain the plasmon resonance frequency of the graphene ribbons and maximally isolate the plasmonic components from the surrounding electromagnetic environment, allowing modular design in integrated plasmonic circuits.

1Supported by National Natural Science Foundation of China (No. 51372045)
V1.00347 New Method for Storing Information based on the Magnetic Permeability, ALAN EDELSTEIN, JONATHAN PETRIE, KRISTOPHER WIELAND, RAYMOND MENCIA, US Army Research Laboratory, SY-HWANG LIOU, Physics Dept., University of Nebraska, GEORGE NEWBURGH, US Army Research Laboratory, CORY CRESS, Naval Research Lab, JOHN TIMMERWILKE, US Army Research Laboratory, SERGEI URAGHINDIN, Dept. of Physics, Emory University — We present a new approach for storing information based on bits with different values for their magnetic permeability. Unlike present magnetic recording, information stored in this way should be ideal for archiving since it is unaffected by exposure to a magnetic field or moderate changes of temperature. Using heating with laser pulses as short as 100 ns, we have decreased the permeability of micron sized bits of an amorphous ferromagnet, Metglas, by crystallizing them. The permeability of micron sized bits of Cu/permalloy bilayers was decreased by using ohmic heating to cause the Cu to diffuse into the permalloy (80% Ni 20% Fe). This occurs because Ni is no longer ferromagnetic if the Ni atoms have too many Cu neighbors. The changes in the permeability are read by using either a magnetic tunnel junction or a spin transfer oscillator to measure whether the flux lines of a probe field are affected by the bits. The permeability of Cu/permalloy bilayers is not affected by 10 mega rads of gamma radiation from Co 60. Using heat assisted recording (HAMR) will permit writing permeability bits on a nm scale.

V1.00348 Thermal stability of organic-inorganic hybrid perovskite structures from first principles, AMIR FARAJIAN, Department of Mechanical and Materials Engineering, Wright State University — Organic-inorganic hybrid perovskites are currently the focus of intense research owing to their impressive efficiency as photovoltaic devices. Specifically, methylammonium lead tri-halides are of interest in this regard, however, some of their basic properties are not completely known yet. We investigate structural stability of organic-inorganic hybrid perovskites of methylammonium lead tri-halide type (MAPb\(_{1-x}\)Cl\(_x\), n = 0-3) at different temperatures, using ab initio structure optimization, energy calculations, and molecular dynamics. Different crystal structures and free energies are compared, and effects of temperature change are discussed. The results provide insight toward understanding stable methylammonium lead tri-halides for photovoltaic applications.

V1.00349 Multiple sharp lattice plasmon modes in 2D Au nanoparticle superlattices, DANQING WANG, ANKUN YANG, ALEXANDER HRYN, GEORGE SCHATZ, TERI ODOM, Northwestern Univ, ODOM GROUP TEAM — Periodic metal-nanoparticle (NP) 1D chains and 2D arrays can produce sharp lattice plasmon modes due to the coupling between the diffraction mode of the periodic lattice and the localized surface plasmon resonance of the metal NPs. 2D Au NP superlattices, new structures that combine multiple length scales, have the potential for new optical properties such as mode coupling. They differ from periodic 2D arrays in that the spacing between NP patches introduces an additional microscale patch periodicity while the sub-microscale NP periodicity is maintained within one patch. In the reciprocal space, the small periodicity corresponds to a large wavevector while the large periodicity corresponds to a small one. For 2D NP superlattices, the two wavevectors sum together and show additional, satellite diffraction modes at higher and lower energies than the modes for periodic 2D arrays. We found that multiple sharp lattice plasmon modes exist in the 2D Au NP superlattices as the satellite diffraction modes couple with the localized surface plasmon mode. Multiple peaks with narrow linewidths in the transmission spectrum were observed in both numerical calculations and experiments. 2D Au NP superlattices provide flexibility in tuning the lattice plasmon mode through changing the microscale periodicity of the patches. The multiple sharp lattice plasmon modes can also serve as potential cavity modes for surface-emitting lasing.

V1.00350 Modularity Enhances the Rate of Evolution in a Rugged Fitness Landscape, DONG WANG, RICE UNIVERSITY, JEONG-MAN PARK, RICE UNIVERSITY AND THE CATHOLIC UNIVERSITY OF KOREA, MAN CHEN, MICHAEL DEEM, RICE UNIVERSITY — Biological systems are modular, and this modularity affects the evolution of biological systems over time and in different environments. We here develop a theory for the dynamics of evolution in a rugged, modular fitness landscape. We show analytically how horizontal gene transfer couples to the modularity in the system and leads to more rapid rates of evolution at short times. The model, in general, analytically demonstrates a selective pressure for the prevalence of modularity in evolution. We use this model to show how the evolution of the influenza virus is affected by the modularity of the proteins that are recognized by the human immune system. A modular model of the fitness landscape of the virus better fits the observed virus evolution data.

1This research was supported by the US National Institutes of Health under grant 1 R01 GM 10046801. JMP was also supported by the National Research Foundation of Korea Grant (NRF-2013R1A1A2006983).


V1.00352 Magnetic properties of MnF\(_3\), BAEKSOON CHO, KAIST, CHANGSOO KIM, KBSI, SEJUN PARK, SOONCHIL LEE, KAIST — MnF\(_3\) which is A-type antiferromagnetic material has been reported to show the negative thermal expansion (NTE) below Neel temperature. In this work, the temperature and magnetic field dependence of the magnetization of MnF\(_3\) was measured to find the spin order. The M(T) curve measured by NMR fits well with the theory for antiferromagnet with anisotropy, T^2 e^{−(J/κ_a)}1, and the measured energy gab(E_G) is about 30 K. The M(H) curve shows that the ferromagnetic phase is mixed with the antiferromagnetic phase below the transition temperature. From the comparison of the M(H) curve at 30 K with theory, the relation between K_a and J_1 was obtained which is given by K_a ∼ 1.9 J_1 + 10.3 in absolute temperature unit.

V1.00353 Excitonic Josephson effect in \(E \ell = 1\) quantum Hall bilayer effect, YA-FEN HSU, Department of Electrophysics, National Chiao Tung University, Hsinchu 300, Taiwan — The many similarities between exciton condensates and cooper pairs have driven intense interests to search for exciton-superfluidity effect. The Josephson-like tunneling conductance peak in a single quantum Hall (QH) has been viewed as a strong signature of exciton superfluidity. However, in fact, the Josephson-like effect is not an exact analogy of Josephson effect in superconducting junctions. Therefore, we study three kinds of excitonic Josephson junctions (JJs) composed of QH bilayers: SS, SNS, and SS’S junctions in a pseudospin picture. By solving the Landau-Lifshitz-Gilbert equations, we find, in contrast with superconducting JJs, interlayer single-particle tunneling raises spatial inhomogeneity in supercurrent and system-size dependent current-phase-relation. In addition, under the effect of the tunneling, the supercurrent could not flow through the normal metal via Andreev reflection. Interestingly, anomalous supercurrents occur in SNS junctions even in absence of Josephson interference: the tunneling would set the phase to zero at NS interfaces, which will lead to a phase bias across a Josephson-like junction (i.e. single condensate system) with a nonzero ground state phase, and hence induces the anomalous supercurrent.
V1.00354 Screening effect on electronic and field-emission properties of graphene nanoribbons

WAN-SHENG SU, National Center for High-performance Computing, HAN HU, TSAN-CHIEN LEUNG, Department of Physics, National Chung Cheng University — The electronic and field-emission properties of zigzag graphene nanoribbons (ZGNRs) influenced by manipulated nanostructure width (Lw) and nanostructure-to-nanostructure separation (Dx) are investigated using first-principles calculations. The corresponding characteristics, including band gap, magnetic moment, field enhancement factor and work function are explored and presented. It is found that the behavior of those properties under saturation versus Dx is observed, and the corresponding values approach their limits as Dx increases to a certain value. In addition, the electric-field-induced changes in band gaps of the ZGNRs with and without separated gaps are much more significant than that of ZGNRs with little separation. These phenomena can be attributed to physical origins such that the greater the separation between ZGNRs, the less significant the screening effect becomes. Finally, the altered magnetic moment of the ZGNRs due to the presence of an external electric field is analyzed and discussed.

V1.00355 Controlling magnetic order and quantum disorder in molecule-based magnets

SAMAN GHANNAZADEH, High Field Magnet Laboratory, Netherlands, TOM LANCASTER, Durham University, UK, PAUL GODDARD, STEPHEN BLUNDELL, FRANCESCA FORONDA, ISABEL FRANKE, University of Oxford, UK, JOHANNES MÖLLER, ETH Zürich, Switzerland, LINGEN HUANG, JOACHIM WOSNITZA, High Magnetic Field Laboratory, Germany, JAMIE MANSON, Eastern Washington University, USA — Metal-organic coordination polymers are materials in which transition metal ions are linked via organic molecules into chain or plane-like structures. Strong hydrogen bonds enable these units to form three-dimensional lattices, while the underlying anisotropy causes low-dimensional magnetism to evolve. Here the magnetic properties of a number of these compounds are investigated through high-field magnetization, heat capacity, and magnetic susceptibility measurements. It is shown that [Cu(pyz)H2O(gly)]ClO4 is a highly one-dimensional antiferromagnet, whilst the compounds [Cu(pyz)(gly)]ClO4 and Cu(H2O)VCF3 are dimerized with a non-magnetic singlet ground state and behave as zero-dimensional disordered magnets at zero field. Furthermore, these two materials are shown to undergo a field-induced transition through a quantum critical point into an XY ordered phase, which in the case of [Cu(pyz)(gly)]ClO4, is reminiscent of Bose-Einstein condensation of triplons.

V1.00356 ABSTRACT MOVED TO Q8.00008

V1.00357 The Structural Bases for Polymer Glass-Transition Temperatures

JIALONG SHEN, ALAN TONELLI, North Carolina State Univ — The glass-transition temperatures (Tgs) observed for chemically distinct polymers range over several hundred K, and the molecular bases for this wide variability are largely unknown, though the following three factors are often mentioned as being pivotal: 1. Their inherent conformational flexibilities; 2. The sizes or steric bulk of their side-chains; and 3. Their inter-chain interactions. These three factors are generally interdependent, making it difficult to predict or even rationalize the Tgs of polymers. Structurally analogous aliphatic copolymers, copolymides, and copoly(ester/amide)s can be synthesized to produce amorphous samples with Tgs that are unaffected either by crystallinity or polymer chain lengths. Their conformations are virtually identical, and each can be synthesized with or without side-chains, so we can begin to evaluate the relative importance of the above three factors. The Tgs of un-branched analogous samples should differ solely due to factor 3, while analogous samples with singly-branched repeat units should provide a measure of the relative importance of factors 1 and 2.

V1.00358 Optically Excited Graphene - Non - Equilibrium Many Body Theory

REGINE FRANK, Institut für Theoretische Physik, Eberhard-Karls University Tübingen, Germany, ANDREAS LUBATSCH, Georg-Simon-Ohm University of Applied Sciences, Nuremberg, Germany — A generalized non-equilibrium dynamical mean field theory (DMFT) for graphene is presented. The NE-DMFT describes graphene in the presence of an external field coupling to the electrons and thus changing in a severe but controllable way the electronic properties of graphene. The non-equilibrium DMFT derives properties such as electronic density of states (LDOS) and occupation numbers of the optically driven system. It fully characterizes the system in its time dependent state. It is demonstrated, how such a setup may be employed in order to realize all-optical switching processes. Results for relevant time scales in setups as well as wave-mixing influences are presented.

Thursday, March 5, 2015 2:30PM - 5:30PM
Session W1*DMP: Focus Session: Graphene: Nanostructures 001A - An-Ping Li, Oak Ridge National Laboratory

2:30PM / W1.00001 Semiconductor half-metal transition in zigzag-graphene-nanoribbons/graphene

MINGXING CHEN, MICHAEL WEINERT, Department of Physics, University of Wisconsin-Milwaukee — Magnetic and electronic properties of H-terminated zigzag graphene nanoribbons supported by graphene substrate are investigated using first-principles calculations. A critical width of 3 nm is found for the onset of electron-electron interactions between the edges. Weak edge magnetism of the nanoribbons is well preserved upon the presence of the graphene substrate due to the weak interaction between them, which on the other hand drives a size-dependent spin splitting of the edge states. As a result of the interaction, a semiconductor-halfmetal transition is observed. Our findings not only are of fundamental interest but also have practical implications in potential applications of graphene-based nanoelectronics.

2:42PM W1.00002 Observations of superlattice Dirac points in one-dimensionally-ripped graphene on hexagonal BN using scanning tunneling spectroscopy

WON-JUN JANG, MIN WOOK LEE, SOON-HYEONG LEE, Department of Physics, Korea University, MIN WANG, SUNG KUYO JANG, MINWOO KIM, SUNCJOO LEE, SANG-WOO KIM, YOUNG JAE SONG, SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University (SKKU), SE-JONG KAHNG, Department of Physics, Korea University — It has been predicted that superlattice potentials in graphene would induce new Dirac points due to lattice-induced chirality of charge carriers. In this talk, we present our experimental observations of new Dirac points in one-dimensionally-ripped graphene on hexagonal BN using scanning tunneling microscopy and spectroscopy. The ripples, formed by thermal cycles, showed two new Dirac points of which energy levels were proportional to 1/L, where L was the period of a ripple. The agreement with theoretical predictions. Our study shows that one-dimensional periodic potential is an accessible component for controlling electronic properties of graphene.

2:54PM W1.00003 Imaging coherent transport in a mesoscopic graphene ring

DAMIEN CABOSART, SEBASTIEN FANIEL, FREDERICO R. MARTINS, Université catholique de Louvain (UCL), IMCN/NAPS, BORIS BRUN, Institut Neel et Université Joseph Fourier, ALEXANDRE FELTEN, Université de Namur (Unamur), VINCENT BAYOT, BENOIT HACKENS, Université catholique de Louvain (UCL), IMCN/NAPS — Mesoscopic graphene devices often exhibit complex transport properties, stemming both from the peculiar electronic band structure of graphene, and from the high sensitivity of transport to local disorder in this two-dimensional crystal. To disentangle contributions of disorder in the different transport phenomena at play in such devices it is necessary to devise new tools in physics of metals, and to establish links between transport and the microscopic structure of the devices. Here, we present a spatially-resolved investigation of coherent transport inside a graphene quantum ring (QR), where Aharonov-Bohm conductance oscillations are observed. Thanks to scanning gate microscopy, we firstly identify spatial signatures of Coulomb blockade, associated with disorder-induced localized states. We then image resonant states which decorate the QR local density of states (LDOS). Simulations of the LDOS in a model disorder graphene QR confirm the presence of such scarred states.
3:06PM W1.00004 Electronic Transport in Hexagonal Boron Nitride Encapsulated Graphene Nanoribbon. WON JONG YOO, DAEYOUNG LEE, EUYHEON HWANG, Sungkyunkwan Univ, PHILIP KIM, Harvard Univ — The electronic transport properties of the hexagonal boron nitride (hBN) encapsulated graphene nanoribbon (GNR) are studied. We find that the transport gap of the hBN encapsulated GNR is almost identical to that of the same size GNR on silicon dioxide (SiO₂) substrate in spite of their quantitatively different physical parameters, indicating that the transport gap of the hBN encapsulated GNR is affected mainly by edge disorders rather than surface disorders. The relatively lower density of Coulomb diamonds (20/√4m), larger charge island diameter (80 nm), longer hopping length (200 nm), and other results obtained from electrical and temperature dependent measurements show that the hBN encapsulated GNR has the less degree of disorder than the surface disorder. The insulating behavior within the transport gap of the hBN encapsulated GNR is maintained up to temperatures and evolves with magnetic field. We comment on the implication of our observations with respect to the electronic properties of sidewall EGNRs.

3:18PM W1.00005 Semiconducting Graphene Ribbons Grown on Nitrogen-Seeded SiC. FENG WANG, Georgia Inst of Tech, GANG LIU, Rutgers University, SARA ROTHWELL, University of Minnesota, MERIDITH NEVIUS, MATTHEW CONRAD, Georgia Inst of Tech, PHILIP COHEN, University of Minnesota, LEONARD FELDMAN, Rutgers University, EDWARD CONRAD, Georgia Inst of Tech — A wide band gap semiconducting form of graphene can be produced by growing a buckled form of graphene from a SiC(0001) surface randomly seeded with nitrogen. In this work, we show that the disorder observed in this form of graphene can be substantially reduced by pre-patterning the nitrogen seeded SiC surface into trenches. The result of the patterning is highly improved film thickness variations, orientational epitaxy, domain size, and electronic structure. In addition, the ordering induced by this patterned growth offers a way to take advantage of the extremely high mobilities and switching speeds in C-face graphene devices while having the thickness uniformity and fabrication scalability normally only achievable for graphene grown on the SiC(0001) Si-face.

3:30PM W1.00006 Surface-assisted formation of graphene nanoribbons on Au surfaces. CLAUDIA CARDOSO, DEBORAH PREZZI, ELISA MOLINARI, ANDREA FERRETTI, S3 Center, Istituto Nanoscience, CNR via Campi 213/A, 41125, Modena, Italy — The formation of graphene nanoribbons (GNRs) on Au(110) and Au(111), as based on the surface-mediated reaction of 10,10'-dibromo-9,9' bithiophene (DBBA) molecules was investigated by means of first-principles calculations. The study was done in direct collaboration with experimental groups performing structural and spectroscopic characterization by means of STM, XPS/UPS, NEXAFS. Comparison between the Au(110) and Au(111) surfaces unveils the delicate interplay between surface atomic corrugation, molecular mobility, and adsorption energies, that drive the GNR growth. Concerning the Au(110) surface, we have studied the molecule/surface interaction at different stages of the GNR formation. The role of different reconstructions has been investigated, showing that both precursors and GNRs interact differently with different surfaces. Calculations for the precursor molecules showed that initial stages of the reaction crucially determine the final configuration and orientation of the GNRs. In the specific case of Au(111) we have also studied the evolution of the Au Shockley surface state as a function of GNR bonding state. We show that the GNR/Au interaction results in an upshift of the Shockley surface state of Au(111) by 0.2 eV, together with an increased electron effective mass.

3:42PM W1.00007 Ballistic nanostructures for epitaxial graphene nanoelectronics. VALT DE HEER, Georgia Institute of Technology — Epitaxial graphene nanoelectronics [1] was inspired by carbon nanotube electronics. While carbon nanotubes demonstrated advantageous electronic properties, like room temperature ballistic transport, immunity to electromigration and significant bandgaps, manufacturability remains a problem. Independent of other graphene work research at Georgia Tech evolved from the premise that epitaxial graphene on silicon carbide could serve as a viable platform for graphene based electronics. Epitaxial graphene (EG), known since the 1970's, is produced by sublimation of Si from the SiC surface. The 2D electronic and structural properties of EG are significantly superior to transferred graphene, EG is scalable[2]. Nanopatterning is achieved by selective high temperature graphene growth on the sidewalls of structures that are etched in the SiC. These annealed graphene nanostructures demonstrate a host of remarkable properties. Recently 10 μm scale single channel room temperature ballistic transport (R = h/e² ≈ 26 kOhm) has been observed in neutral graphene sidewall nanoribbons [3] (in contrast, similarly sized exfoliated graphene ribbons are insulators due to disorder). These ballistic nanoribbons, as well as other nanostructures are readily and reliably produced using optical lithography. Remarkably, the ballistic transport does not depend on the microstructure of the ribbon edges, thereby precluding current models for the effect. These ballistic ribbons can be used as quantum wires in graphene based nanoelectronics. This high mobility has been observed in neutral graphene sidewall nanoribbons. These devices are promising candidates for graphene transistors, because of the ability to control structural parameters of GNRs, such as their width, edge structure and termination, with atomic precision. These properties of the GNRs can also be modified by their doping with heteroatoms, such as nitrogen, resulting in nitrogen-doped GNRs or N-GNRs. These graphene nanoribbons are promising materials for future electronics and photovoltaics. The ability to control structural parameters of silicon nanowires, such as their width, edge structure and termination, with atomic precision is the key for practical realization of these intriguing nanoscale properties. Physical properties of GNRs can also be modified by their doping with heteroatoms, such as nitrogen, resulting in nitrogen-doped GNRs or N-GNRs. In this talk I will demonstrate that large quantities of narrow atomically precise N-GNRs can be synthesized via Yamamoto coupling of molecular precursors containing nitrogen atoms followed by cyclohydrogenation using Scholl reaction. Several types of N-GNRs with different doping levels have been synthesized and systematically studied by means of spectroscopic, microscopic and transport methods. Incorporation of nitrogen atoms in graphene lattice is shown to be an effective route to affect GNRs' band gap, doping level as well as aggregation behavior.


4:18PM W1.00008 Atomically precise nitrogen-doped graphene nanoribbons1. ALEXANDER SINITSKII, University of Nebraska - Lincoln — There is a considerable interest in graphene nanoribbons (GNRs), few-nm-wide strips of graphene with high aspect ratios, because of their intriguing physical properties. For example, GNRs with zigzag edges are predicted to exhibit low-dimensional magnetism, while GNRs with armchair edges can possess large energy band gaps, making them promising materials for future electronics and photovoltaics. The ability to control structural parameters of GNRs, such as their width, edge structure and termination, with atomic precision is the key for practical realization of these intriguing nanoscale properties. Physical properties of GNRs can also be modified by their doping with heteroatoms, such as nitrogen, resulting in nitrogen-doped GNRs or N-GNRs. In this talk I will demonstrate that large quantities of narrow atomically precise N-GNRs can be synthesized via Yamamoto coupling of molecular precursors containing nitrogen atoms followed by cyclohydrogenation using Scholl reaction. Several types of N-GNRs with different doping levels have been synthesized and systematically studied by means of spectroscopic, microscopic and transport methods. Incorporation of nitrogen atoms in graphene lattice is shown to be an effective route to affect GNRs’ band gap, doping level as well as aggregation behavior.

1This work was supported by the Nebraska Center for Energy Sciences Research (#12-00-13), the Nebraska Research Initiative and the NSF through Nebraska MRSEC (DMR-0820521) and EPS-0904994.

4:30PM W1.00009 Superconducting Proximity Effect in Sidewall Graphene Nanoribbons. OWEN VAIL, JOHN HANKINSON, School of Physics, Georgia Tech, CLÉMENT BOUVIER, CLAIRE BERGER, Gatech - School of Physics, CNRS-Institut Neel, WALT DE HEER, ZHIGANG JIANG, School of Physics, Georgia Tech — Epitaxial graphene nanoribbons (EGNRs) grown on sidewall SiC have recently emerged as a novel material system enabling single channel room temperature ballistic transport over micrometer distance. In this work, we fabricate Al-EGNR-Al junctions and study the electronic transport as a function of bias voltage, temperature, and magnetic field. We show that although the measured resistance across the junction is dominated by the EGNR, spectral features associated with superconductivity of Al electrodes are evident. These features are fully developed at low temperatures and evolve with magnetic field. We comment on the implication of our observations with respect to the electronic properties of sidewall EGNRs.
4:42PM W1.00010 Spin orbit coupling and electron pairing instabilities in superconductors1. ARMEN KOCHARIAN, California State University, Los Angeles, CA, GAYNATH FERNANDO, KUN FANG, University of Connecticut, Storrs, CT, ALEXANDER BALATSKY, Nordic Institute for Theoretical Physics, Stockholm, Sweden — Exact diagonalization, Lanczos and variational cluster approximation (VCA) have been used for accurate studies of Rashba spin-orbit effects in the presence of electron correlations. These have been carried out in order to address current challenging problems in superconductivity, magnetism, topological insulators and spin dependent transport associated with numerous interfaces and heterostructures. The modeled spin-orbit coupling in assembled nano-ribbons (as arrays of clusters) in various two-dimensional square and topological honeycomb structures (generated by periodically repeated Betts lattices) provide an ideal playground for understanding various competing phases, electron pairing and phase separation instabilities in conventional and unconventional superconductors. Our models allow us to calculate the spectral functions and accurately extract electronic, magnetic properties including spin transport and electron pairing in these systems. The results also highlight important aspects of the interplay of the spin-orbit coupling with magnetic fields in graphene-like systems and unconventional superconductors induced by weak, moderate and strong electron interactions.

1 Authors acknowledge the computing facilities provided by the CFN at BNL, supported by the U.S. DOE (Contract DE-AC02-98CH10886), user facility at LANL (Contract DE-AC52-06NA25396) and Sandia National Laboratories (Contract DE-AC04-94AL85000).

4:54PM W1.00011 ABSTRACT WITHDRAWN –

5:06PM W1.00012 Bound states in single and bilayer graphenes by a one-dimensional potential well: continuum model versus lattice model, AKIHIRO OKAMOTO, TAKEHITO YOKOYAMA, Department of Physics, Tokyo Institute of Technology, SHUICHI MURAKAMI, TIES, Tokyo Institute of Technology — Edges of a graphene show characteristic edge states depending on its edge shapes such as zigzag or armchair. Instead of these edge states, we consider bound states on a graphene with a one-dimensional potential well. We set the potential well which has a finite width in one direction and is infinitely extended in the other direction. We consider both the single layer and bilayer graphenes. In the continuum model of Dirac cones, we can analytically calculate the bound states, and discuss their properties. Then we also calculate analytically the bound states, also for the tight-binding model for single-layer graphene. It reproduces the results for the continuum model, such as a linear dispersion of bound states near K and K’ points. We discuss how the bound states dispersion change for various potential profiles.

5:18PM W1.00013 Graphene nanopatterning with 2.5 nm precision: combining bottom-up and top-down techniques, JOSE M. GOMEZ-RODRIGUEZ, ANTONIO J. MARTINEZ-GALERA, IVAN BIHRUEGA, Dept. Fisica de la Materia Condensada, Universidad Autonoma de Madrid, Spain, ANGEL GUTIERREZ-RUBIO, TOBIAS STAUBER, Instituto de Ciencia de Materiales de Madrid, CSIC, Spain — The selective modification of pristine graphene represents an essential step to fully exploit its potential. Here we merge bottom-up and top-down strategies to tailor graphene with nanometer accuracy. In a first step, graphene electronic properties are macroscopically modified using the periodic potential generated by the self assembly of metal cluster superlattices on a graphene/Ir(111) surface. Then, we show that individual metal clusters can be selectively removed at room temperature by a STM tip with perfect reproducibility, which enables one to nanopattern the system down to the 2.5 nm limit given by the distance between neighbouring clusters, i.e., the periodicity of the moire-pattern. The method can be carried out on micrometer sized regions, with clusters of different materials which allows tuning the strength of the periodic potential and the structures so created are stable even at room temperature. As a result, we can strategically combine graphene regions that should present large differences in their electronic structure to design graphene nanostructures with specific functionalities.

Thursday, March 5, 2015 2:30PM - 5:30PM – Session W2 DMP: Focus Session: Beyond Graphene - Devices I 001B - Xia Hong, University of Nebraska-Lincoln

2:30PM W2.00001 Optically Induced PN Junction Diode and Photovoltaic Response on Ambipolar MoSe2 Field-effect Transistor, NIHAR PRADHAN, ZHENGGUANG LU, DANIEL RHODES, National High Magnetic Field Laboratory, Tallahassee, Florida, USA, MAURICIO TERRONES, Department of Physics, Pennsylvania State University, University Park, PA, USA, DMITRY SMIRNOV, LUIS BALICAS, National High Magnetic Field Laboratory, Tallahassee, Florida, USA — Transition metal dichalcogenides (TMDs) have emerged as an attractive material for electronic and optoelectronic devices due to their sizable band gap, flexibility and reduced dimensionality, which makes them promising candidates for applications in transparent optoelectronics components, such as solar cells and light emitting diodes. Here, we present an optically induced diode like response and concomitant photovoltaic effect in few-atomic layers molybdenum diselenide (MoSe2) field-effect transistors. Compared to recently reported PN junctions based on TMDs, ambipolar MoSe2 shows nearly ideal diode rectification under illumination, with a sizable photovoltaic efficiency. The observed light induced diode response under fixed gate voltage, yields a maximum open circuit voltage 0.28V and short circuit current 230mA at 30uW incident laser power. The sense of current rectification can be altered by changing the polarity of the applied gate voltage (Vbg). We show that the method can produce devices with external quantum efficiency ~ 30%.

2:42PM W2.00002 Electrical energy harvesting from single-atomic-layer MoS2, LEI WANG, Columbia University, WENZHUO WU, Georgia Institute of Technology, YILEI LI, TONY HEINZ, Columbia University, ZHONG LIN WANG, Georgia Institute of Technology, JAMES HONE, Columbia University — Monolayer MoS2 is predicted to be strongly piezoelectric, an effect that disappears in the bulk due to the opposite orientations of adjacent atomic layers. We observe the first experimental study of the piezoelectric properties of two-dimensional (2D) MoS2. We find that cyclic stretching and releasing of thin MoS2 flakes with an odd number of atomic layers produces oscillating piezoelectric voltage and current outputs, while no output is observed for flakes with an even number of layers. In agreement with theoretical predictions, the output increases with decreasing thickness and reverses sign when the strain direction is rotated by 90 degrees. Transport measurements show a strong piezoelectric effect in single layer MoS2, but not in bilayer and bulk MoS2. The coupling between piezoelectricity and semiconducting properties in 2D nanomaterials may enable applications in powering nanodevices, adaptive bio-probes and tunable/stretchable electronics/optoelectronics.

2:54PM W2.00003 Dimensionality effects on electronic properties of lateral two-dimensional junctions, HENRY YU, ALEX KUTANA, BORIS I. YAKOBSON, Materials Science and NanoEngineering, Rice University — We study lateral junctions of two-dimensional materials, including graphene, 2D BN, and transition metal dichalcogenides. A common feature of low-dimensional contacts is that unlike bulk devices, local charge transfer near the contact cannot equilibrate Fermi levels throughout the material, necessitating nonlocal charge redistribution. These nonlocal charges will affect the physical properties of the junction. We obtain the solution for carrier and potential distributions in symmetric and asymmetric 2D junctions with different densities of states and doping levels, using a macroscopic model and DFT calculations. The scaling of the depletion length with doping level and built-in voltage is determined by the dimensionality of the junction. The implications for operation of low-dimensional devices are discussed.
Control and characterization of the metallic surface state of bulk insulating Bi$_2$Se$_3$.

Michael Fuhrer, School of Physics, Monash University, 3800 Victoria, Australia and CNAM, University of Maryland, College Park, MD 20472-4111 USA — Bi$_2$Se$_3$ is a three dimensional strong topological insulator with a conducting two-dimensional surface state whose existence is guaranteed by topology. The bulk Bi$_2$Se$_3$ has a 300 meV bandgap, but is often a degenerately n-doped metal in as-grown material. I will discuss our efforts to remove this doping in thin crystals and films to achieve surface-dominated conduction. Electrochemical gating (using PEO+LiClO$_4$ electrolyte) or molecular doping (using F4-TCNQ) is shown to effectively bring the Fermi energy of thin (3-20 nm) exfoliated Bi$_2$Se$_3$ crystals to the conduction band edge, where it can be further modulated at low temperature using field-effect gating. These techniques allowed us to reveal the gapless ambipolar transport in the topological surface, and measure the minimum conductivity, electron-phonon phonon scattering, thermopower, and inter-surface coupling of the topological surface. Recently we have developed techniques to measure the transport properties of Bi$_2$Se$_3$ in situ during growth in ultra-high vacuum, enabling better understanding of the doping mechanisms.[6] We have also studied vacuum-deposited MoO$_3$ as a highly effective acceptor dopant which remains stable on air exposure for time scales of days.[1]

This work is supported by NSF Grants DMR-1105224, DMR-0520471, and DMR-0952716, and an ARC Laureate Fellowship.

D. Kim et al., Nature Physics 8, 460 (2012)


J. Hellerstedt et al., APL 105, 173506 (2014)

M.T. Edmonds et al., ACS Nano 8, 6400 (2014)

3:42PM W2.00005 Charge Transport of MoS$_2$ Supported by Thiol-Decorated Self-Assembled Monolayer

Doron Naveh, Vlad Artel, Moshe Kirshner, Dept. of Electrical Engineering, Bar-Ilan University, Ramat-Gan, Israel 52900 — Intrinsic charge transport in MoS$_2$ supported by thiols was recently reported[1] and was attributed to passivation of sulfur vacancies and suppression of charged impurities from the dielectric substrate. In this talk, we will present the transport characteristics of single layer and few-layer MoS$_2$ on thiol-decorated self-assembled alkyli-siloxane monolayer.


3:54PM W2.00006 Generation and electric control of spin–valley-coupled circular photogalvanic current in WSe$_2$.

Hongtao Yuan, Harold Y. Hwang, Yi Cui, Stanford University and SIMES SLAC — Compared to the weak spin-orbit-interaction (SOI) in graphene, layered transitionmetal chalcogenides MX$_2$ have heavy 4d/5d elements with strong atomic SOI, providing a unique way to extend functionalities of novel spintronics and valleytronics devices. Such a valley polarization achieved via valley-selective circular dichroism has been predicted theoretically and demonstrated with optical experiments in MX$_2$ systems. Despite the exciting progress, the generation of a valley/spin current by valley polarization in MX$_2$ remains elusive and a great challenge. A spin/valley current in MX$_2$ compounds caused by such a valley polarization has never been observed, nor its electric-field control. In this talk, we demonstrated, within an electric-double-layer transistor based on WSe$_2$, the manipulation of a spin-coupled valley photocurrent whose direction and magnitude depend on the degree of circular polarization of the incident radiation and can be further greatly modulated with an external electric field. Such room temperature generation and electric control of valley/spin photocurrent provides a new property of electrons in MX$_2$ systems, thereby enabling new degrees of control for quantum-confined spintronics devices. (In collaboration with S.C. Zhang, Y.L. Chen, Z.X. Shen, B. Tian, H.J. Zhang, G. Xu, Y. Xu, B. Zhou, X-Q. Wang, B. Shen X-F. Fang) Acknowledge the support from DoE, BES, Division of MSE under contract DE-AC02-76SF00515.

1 Acknowledge the support from DoE, BES, Division of MSE under contract DE-AC02-76SF00515


Ming-Wei Lin, Xufan Li, Kai Wang, Alexander Puretzky, Christopher Rouleau, David Geohegan, Kai Xiao, Oak Ridge National Laboratory, CNMS, ORNL TEAM — By changing the layer numbers, the electrical transport of field effect transistors based on CVD grown two-dimensional (2D) layered materials of transition metal dichalcogenides (TMDCs) such as MoS$_2$, WSe$_2$ and WS$_2$ shown the different characteristics will be demonstrated. The transport measurements show that the altered semiconductor characteristics of these 2D materials can be possibly attributed to the shift of Fermi level when changing the number of layers. Besides, the transport characteristics can be tuned by adjusting the W/Mo doping level and mobility is also increased with increasing the layer numbers. In addition, the annealing effect on these CVD grown 2D layered materials will be discussed.

This work is conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

1 This work is supported by NSF Grants DMR-1105224, DMR-0520471, and DMR-0952716, and an ARC Laureate Fellowship.

D. Kim et al., Nature Physics 8, 460 (2012)


J. Hellerstedt et al., APL 105, 173506 (2014)

M.T. Edmonds et al., ACS Nano 8, 6400 (2014)

4:18PM W2.00008 Coulomb blockade in few-layer MoS2 based single electron transistor.

Kyunghoon Lee, Zhaohui Zhong, Department of Electrical and Computer Science, University of Michigan — Transition metal dichalcogenides (TMDCs) based two dimensional materials are attracting much attention for their interesting electronic and optical properties, including high on/off current ratio, indirect to direct band gap transition, and valley polarized carrier transport. Nevertheless, study of the low temperature electron transport in atomic thin layered TMDCs is still in its infancy. One of the major hurdles for electron transport study lies in the large metal/semiconductor junction barrier for carrier injection, which leads to the contact resistance dominated charge transport in short channel nanoscale devices. Here, we report on the fabrication of few-layer MoS$_2$ single electron transistor using low work function metal for the contact electrodes. We observed Coulomb blockade phenomena attributed to single electron charging on a fairly clean quantum dot. The details of the bias, gate and temperature dependence will be discussed.

4:30PM W2.00009 Annealing and ionic liquid gating on suspended molybdenum disulfide devices.

Fenglin Wang, Petr Stepanov, Mason Gray, Mikhail Itkis, Robert Haddon, Chun Ning Lau, University of California Riverside — We fabricate suspended molybdenum disulfide (MoS$_2$) field effect transistors (FET) devices and develop an effective gas annealing technique that significantly improves device quality and increases conductance by 3-4 orders of magnitude. Temperature dependence measurements reveal two transport mechanisms: electron-phonon scattering at high temperatures and thermal activation over a gate-tunable barrier height at low temperatures. Our results suggest that transport in these devices is not limited by the substrates. Moreover, this suspended MoS$_2$ device structure provides double surface access for ionic liquid gating. We are able to extract the dielectric constant of the ionic liquid, and the latest experimental results will be presented.
4:42PM W2.00010 Influence of the Metal-MoS\(_2\) interface on MoS\(_2\) Transistor Performance

HUI YUAN, Dept of Electrical and Computer Eng, George Mason University, Fairfax, VA, GUANGJUN CHENG, ANGELA HIGHT WALKER, LIN YOU, JOSEPH J. KOPANSKI, Semiconductor and Dimensional Metrology Div, NIST, Gaithersburg, MD, QILIANG LI, Dept of Electrical and Computer Eng, George Mason University, Fairfax, VA, CURT A. RICHTER, Semiconductor and Dimensional Metrology Div, NIST, Gaithersburg, MD — We compare the electrical characteristics of MoS\(_2\) field-effect transistors (FETS) with Ag source/drain contacts with transistors with Ti contacts, and we demonstrate that the metal-MoS\(_2\) interface is crucial to the final device performance. The topography of Snm Au/Snm Ag (contact layer) and Snm Au/Snm Ti metal films deposited onto monofew-layer MoS\(_2\) was characterized by using scanning electron microscopy and atomic force microscopy. The surface morphology of the Au/Ti films on MoS\(_2\) shows a rough, dewetting pattern while Au/Ag forms smooth, dense films. These smoother and denser Au/Ag contacts lead to improved carrier transport efficiency. FETS with Ag contacts show more than 60 times higher on-current and a steeper subthreshold slope. Raman spectroscopy of MoS\(_2\) covered with Au/Ag or Au/Ti films revealed that the contact layer is Ag or Ti, respectively. In addition, there is a dramatic difference in the heat transfer between the MoS\(_2\) and the two metals: while laser heating is observed in Au/Ti covered MoS\(_2\), no heating effects are seen in Au/Ag covered MoS\(_2\). It is reasonable to conclude that the smoother and denser Ag contact leads to higher carrier transport efficiency and contributes to the improved thermal properties.

4:54PM W2.00011 Negative Differential Transconductance in a MoS\(_2\)/WSe\(_2\) Heterojunction Field Effect Transistor

AHMAD ZAUBIR, Massachusetts Institute of Technology, AMIRHASAN NOURBAKSH, Massachusetts Institute of Technology, IMEC, MILDRED DRESSELHAUS, Massachusetts Institute of Technology, STEFAN DE GENDT, IMEC, TOMAS PALACIOS, Massachusetts Institute of Technology — In this work, we demonstrate the negative transconductance in heterojunction transistors made of two-dimensional materials for the first time. Negative transconductance plays a key role in multi-valued logic/memory and frequency multiplication circuits. The simpler fabrication method of stacked van der Waals heterostructures compared to the conventional bulk semiconductors and large CVD growth of the layered 2D materials systems makes it a prime candidate for scalable novel applications of their heterostructures. Vertically stacked MoS\(_2\)/WSe\(_2\) heterostructures are fabricated by mechanical exfoliation and an in-house dry transfer process. A two-step process of e-beam lithography and metal deposition (Au on MoS\(_2\), and Pd on WSe\(_2\)) were performed to fabricate heterojunction field-effect transistors (HJFETs). The transfer characteristics of overlapping regions shows the expected characteristics of the n-type, MoS\(_2\) FET and ambipolar WSe\(_2\) FET. At the same time, the transfer characteristics of the overlapping region between MoS\(_2\) and WSe\(_2\) show negative differential conductance with proper scaling and careful optimization this negative differential transconductance will lead to novel applications.

5:06PM W2.00012 Quantum transport measurement of few-layer WTe\(_2\) field effect devices

JIANGHAO CHEN, XIN LIU, SHIBING TIAN, CHENGLONG ZHANG, SHUANG JIA, International Center for Quantum Materials, School of Physics, Peking University; Collaborative Innovation Center of Quantum Matter, Beijing, China — We have performed systematic quantum transport measurement on field effect devices fabricated from few-layer WTe\(_2\) single crystals. We found that the magnetoresistance of few-layer WTe\(_2\) could be very different from that of bulk samples, which may arise from the imbalance of electron and hole carriers in the samples. We shall discuss our findings in more details in light of recent progress in our experiment.

5:18PM W2.00013 Electronic Transport of Encapsulated WSe\(_2\) Fabricated by Pick-up of Pre-patterned hBN

YAFANG YANG, HUGH CHURCHILL, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — We report high quality WSe\(_2\) devices encapsulated between two hexagonal boron nitride (hBN) flakes using a pick-up method with etched hBN flakes. Previous work on graphene has shown that sample disorder can be greatly reduced via isolation from charge impurities in the substrate by means of encapsulation. However, the effect of encapsulation still remains unknown for dichalcogenides devices. Besides, the quality of contact to TMDs is also a critical factor limiting the transport performance of such devices. To measure the transport properties of dichalcogenide devices as a function of temperature, low resistance electrical contacts must be made to the material. To achieve this, we encapsulate few-layer WSe\(_2\) in hexagonal boron nitride that has been patterned to allow ionic liquid doping of the contact region. This technique simultaneously protects the WSe\(_2\) surface above and below, resulting in the highest mobility few-layer WSe\(_2\) devices reported to date.

Thursday, March 5, 2015 2:30PM - 5:30PM – Session W3 FEd: Invited Session: Growing the Physics Major 002AB - Duncan McBride, National Science Foundation

2:30PM W3.00001 Physics Majors in the US: Trends and Implications

THEODORE HODAPP, American Physical Society — The number of undergraduate physics majors has doubled over the last 15 years, with more growth in sight. In that same time period the total number of PhDs awarded as well as those earned by domestic students has seen a similar rise. The picture is not so rosy when we look at underrepresented groups including women, and minority students. Nevertheless, we are now educating record numbers of physics students. This talk will explore some of the underlying issues, and present evidence for why some of these trends are present. Part of the discussion will include implications for physics programs. How big can programs become? What changes might be needed? What do we sacrifice, and what do we gain as a discipline? Will our new graduates get jobs? Bring your questions and thoughts to the discussion.

3:06PM W3.00002 Strengthening the Physics Program at Brigham Young University – What Have We Learned?

SCOTT SOMMERFELDT, Brigham Young University — During the decade of the 1990s, the Department of Physics and Astronomy at Brigham Young University (BYU) experienced remarkable growth, growing from approximately 200 majors in the first half of the decade to over 300 majors by the end of the decade. Since that time, the number of majors has held fairly steady, fluctuating between 300-350 majors. One can naturally ask, what led to this significant growth? This is a difficult question to answer, as a number of variables are potentially involved, all of which may have had some impact on the outcome. This paper will explore a number of items that have been implemented in the program over this time that may have contributed to establishing a strong physics program that provides an excellent education for our undergraduate majors. Many of these possible contributors can be viewed as an outgrowth of perhaps one major characteristic of the department – a strong and unified commitment to providing excellent undergraduate training in physics. This commitment to undergraduate education has informed many of the decisions that have been made over the past several decades. Several examples that will be discussed include the implementation of the requirement that each student complete a mentored learning experience before graduation, the introduction of several different degrees to better accommodate the range of student interests, and moving the experimental and computational lab courses to earlier in the student’s program to allow later courses and research to build upon these skills. As a result of the greatly enhanced program of program assessment that has been put in place at BYU, these various elements are reviewed regularly, which provides feedback and allows us to make modifications as warranted to try and further strengthen the program.
3:42PM W3.00003 Losing and Saving and Losing Physics in Texas. MICHAEL MARDER. Univ of Texas, Austin — Texas has the second-largest population of the states, and played even a larger role in education reform movements of the past 15 years than its size would indicate. In the Fall of 2011, physicists across the country were surprised to learn that six university physics programs in Texas were threatened with closure because of small graduation numbers. Five of them ultimately closed. Many of the faculty at the institutions losing programs came together and formed a consortium that eventually made it possible to continue offering physics, by unconventional means, to their undergraduates. In the Spring of 2013 came an even larger change. PHS1, the state funded high school graduation plan in Texas. As part of a bill making sweeping changes to high school graduation requirements and accountability, the physics requirement was removed. Physics may partly be failing student to the national focus on STEM, which suggests that the various disciplines of science are interchangeable and not individually important. None of the changes in Texas are hard to imagine coming to other states as well.

4:18PM W3.00004 Morehouse Physics & Dual Degree Engineering Program: We C.A.R.E. Approach. WILLIE S. ROCKWARD, Morehouse College — Growing the physics major at any undergraduate institution, especially Morehouse College – a private, all-black, liberal arts HBCU, can be very challenging. To address this challenge at Morehouse, the faculty and staff in the Department of Physics and Dual Degree Engineering Program (Physics & DDEP) are applying a methodology and pedagogical approach called “We C.A.R.E.” which stands for Curriculum, Advisement, Recruitment/Retention/Research, and Extras. This approach utilizes an integrated strategy of cultural (family-oriented), collaborative (shared-governance), and career (personalized-pathways) modalities to provide the momentum of growing the physics major at Morehouse from 10-12 students to over 100 students in less than 5 years. Physics & DDEP at Morehouse, creatively, altered faculty course assignments, curriculum offerings, and departmental policies while expanding research projects, student organizations, and external collaborations. This method supplies a variety of meaningful, academic and research experiences for undergraduates at Morehouse and thoroughly prepares students for graduate studies or professional careers in STEM disciplines. Thus, a detailed overview of the “We C.A.R.E.” approach will be presented along with the Physics & DDEP vision, alterations and expansions in growing the physics major at Morehouse College.

4:54PM W3.00005 How to double the number of undergraduate physics majors. SACHA KOPP, SUNY Stony Brook — Many colleges and universities around the country have a solid physics program that prepares students bound for graduate physics study. For a variety of reasons, the number of students choosing to major in physics may be small, typically <1% of the student body. When compared to other majors, this population is experiencing negligible growth. I will describe a campaign launched while at the University of Texas at Austin aimed at recruiting and retaining of majors. This campaign includes actual programmatic changes in the curriculum and instruction of majors. Additionally, it includes a direct marketing campaign that attempted to change student attitudes about physics and its relation to their current major. Finally, it includes a program to reach out to high schools and engage students in a discussion about their career choices before they apply for college. I will share some numerical and attitudinal data that suggest positive changes in the student population.

Thursday, March 5, 2015 2:30PM - 5:18PM — Session W5 DMP DCOMP: Focus Session: Magnetism and Transport in Fe-Based Superconductors

3:30PM W5.00001 Intrinsic band pictures of (122) and (11) iron pnictides from magnetotransport measurements. K. HUYNH, WPI-AIMR, Tohoku University, Japan. Y. TANABE, T. URATA, Dep. Phys., Graduate School of Science, Tohoku University, S. HEGURI, K. TANIGAKI, WPI-AIMR, Tohoku University, Japan. M. HAGIWARA, T. KIDA, Center for advanced high magnetic field science, Osaka University. H. OGURO, K. WATANABE, High field laboratory for superconducting materials, Tohoku University — In this report, the band picture of the typical (122) BaFe$_2$As$_2$ and (11) FeSe single crystals will be discussed from the view point of transport properties under high magnetic fields. By applying the technique of mobility spectrum analysis, we are able to describe the numbers of electrons and holes in terms of distribution functions of mobility; the partial contribution of each Fermi pocket to the overall transport properties is thus can be clarified. The analyses show that in both (122) and (11) materials the conduction of mobility spectrum analysis, we are able to describe the numbers of electrons and holes in terms of distribution functions of mobility; the partial contribution of each Fermi pocket to the overall transport properties is thus can be clarified. The analyses show that in both (122) and (11) materials the conduction of electron is much more complex than that of hole. The mobility spectra of holes always indicates isotropic pockets. On the other hand, in the electron side the spectra are broad and associated with a long tail extended to very high mobility region, highlighting the existence of Dirac cones [1, 2]. The unusual features of the mobility spectra will be discussed in comparison with various models and observations of band structures.

1Department of Physics and Dual Degree Engineering Program, Atlanta, Georgia 30314

1Morehouse College.

2Approach will be presented along with the Physics & DDEP vision, alterations and expansions in growing the physics major at Morehouse College.

2Work in collaboration with: A. Dusza, L. Degiorgi (ETH Zurich) and J.H. Chu, H.H. Kuo, I.R. Fisher (Stanford University)

2:42PM W5.00002 Sharp enhancement of spin fluctuations by nematic order in iron pnictides. QIANG ZHANG, Ames Laboratory and Iowa state university, JIAQIANG YAN, SONGXUE CHI, Oak Ridge National Laboratory, GREGORY, S. TUCKER, Ames Laboratory and Iowa state university, DANIEL. K. PRATT, JEFFREY. W. LYNN, NIST Center for Neutron Research, National Institute of Standards and Technology, R. W. MCCALLUM, PAUL. C. CANFIELD, THOMAS A. LOGRASSO, ALAN I. GOLDMAN, DAVID VAKNIN, ROBERT J. MCQUEENNEY, Ames Laboratory and Iowa state university — Inelastic neutron scattering was employed to investigate the impact of electronic nematic order on the magnetic spectra of LaFeAsO and Ba(Fe$_{0.5}$Co$_{0.5}$)$_2$As$_2$. These materials are ideal to study the paramagnetic-nematic state, since the nematic order, signaled by the tetragonal-to-orthorhombic transition at $T_N$, sets in well above the stripe antiferromagnetic ordering at $T_{NC}$. We find that the temperature-dependent dynamic susceptibility displays an anomaly at $T_N$ followed by a sharp enhancement in the spin-spin correlation length, revealing a strong feedback effect of nematic order on the low-energy magnetic spectrum. Our findings can be consistently described by a model that attributes the structural/nematic transition to magnetic fluctuations, and unveils the key role played by nematic order in promoting the long-range stripe antiferromagnetic order in iron pnictides.

1US DOE, Office of Basic Energy Sciences, DMSE, under Contract No. DE-AC02-07CH11358; DOE, under Award Number DE-SC0012336; DOE, Scientific User Facilities Division; US Department of Commerce

2:54PM W5.00003 Electrododynamic response in the electronic nematic phase of BaFe$_2$As$_2$. C. MIRRI, ETH Zurich — We measure the in-plane optical reflectivity of BaFe$_2$As$_2$ beyond the MIR interval, studied so far, covering the spectral range from the far infrared (FIR) to the ultraviolet (UV) at several combinations of pressure, used to detwin the specimen, and temperature. Our goal is to probe the anisotropic response in the real part of the optical conductivity $\sigma_1(\omega)$, extracted from the reflectivity data via Kramers-Kronig transformations. We thus elucidate how the anisotropic optical metallic response evolves as a function of pressure, considered as an external symmetry breaking field, and across the ferro-elastic structural transition. At the center of our attention we then place the analysis of the spectral weight reshuffling over a large energy interval. We provide evidence of how the anisotropic charge carriers, which allows a direct link to the yet astonishing dc transport properties.

1Work in collaboration with: A. Dusza, L. Degiorgi (ETH Zurich) and J.H. Chu, H.H. Kuo, I.R. Fisher (Stanford University)
Emergent Defect States as a Source of Resistivity Anisotropy in the Ne- 
matic Phase of Iron pnictides


4:30PM W5.00009 Critical Charge Fluctuations and Ingap Collective Modes in the Superconducting State of the NaFe$_{1-x}$Co$_x$As Iron Pnictide Superconductor$^1$. VERNER THORSMOLLE, University of California at San Diego, MAXIM KHODAS, Racah Institute of Physics, The Hebrew University, ZHIPING YIN, Rutgers, The State University of New Jersey, CHEGLIN ZHANG, The University of Tennessee, SCOTT CARR, PENGCHENG DAI, Rice University, GIRSH BLUMBERG, Rutgers, The State University of New Jersey — We use polarization-resolved Raman spectroscopy to study the Raman susceptibility ($\chi(\omega,T,x)$) of the x-T phase diagram of NaFe$_{1-x}$Co$_x$As [1]. Above the structural $T_S(x)$ and the superconducting $T_c(x)$ transition, $\chi(\omega,T,x)$ is dominated by a low-frequency quasielastic peak in B$_{2g}$ symmetry displaying critical behavior across the entire phase diagram. Below $T_c(x)$, sharp ingap modes emerge for $x>0.0165$ in A$_{1g}$ ($\approx 65$ cm$^{-1}$) and B$_{2g}$ ($\approx 25$ and $\approx 55$ cm$^{-1}$) symmetry. The critical charge fluctuations are interpreted in terms of plasma waves of quadruple excitations which below $T_c(x)$ undergo a metamorphosis into the ingap modes. The A$_{1g}$ mode is a particle-hole (p-h) charge exciton consistent with a non-conventional s$^\pm$ superconducting groundstate. The minor B$_{2g}$ mode is a Bardasis-Schrieffer Cooper pair exciton of d-wave symmetry which exists only in a narrow doping window of density wave and superconductivity coexistence. The major B$_{2g}$ mode is a bound state of d+-p-h plasma oscillations.

$^1$VKT and GB acknowledge support from NSF DMR-1104884 and from U.S. DOE, BES, Award DE-SC0005463. CZ, SVC and PD acknowledge support from U.S. DOE, BES, Contract DE-FG02-05ER46202.

4:42PM W5.00010 Magnetic fluctuations under the superconducting dome of Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ from flux-flow resistivity$^1$. XINYI HUANG, DEREK HANEY, YOGESH SINGH, SHUAI ZHANG, Kent State University, HAI-HU WEN, Nanjing University, TAO HU, Shanghai Institute of Microsystem and Information Technology, CAS, MAXIM DZERO, CARMEN ALMASAN, Kent State University — We investigate the magnetism inside the superconducting phase of Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ crystals (on both sides of the optimal doping) by inducing superconducting vortices via applied field and performing current-voltage measurements. This allows us to measure the quasiparticle scattering within the normal cores, despite being inside the superconducting dome. Analysis of the free-flux-flow resistivity within the superconducting phase shows a sharp increase in the quasiparticle scattering with decreasing temperature and applied field, which we attribute to the presence of critical spin fluctuations inside the vortex core. The fluctuations are strongest in the doping with the highest critical temperature, and the behavior is suppressed as the material is more underdoped. For each doping measured, at different temperatures and applied fields, the vortex dissipation curves scale and show an exponential relationship. We will discuss the physics behind the exponential relationship for each doping range.

$^1$This work was supported by the National Science Foundation (Grant No. NSF DMR-1006606) and the Ohio Board of Regents (Grant No. OBR-RIP-220573) at KSU.

4:54PM W5.00011 Correlation, doping, and interband effects on the optical conductivity of iron superconductors$^1$. LUCA DE’ MEDICI, European Synchrotron Radiation Facility, Laboratoire de Physique et Etude des Matériaux, CNRS/ESPCI/UPMC, France, MARIA J. CALDERON, BELEN VALENZUELA, ELENA BASCONES, ICMM-CSIC, Spain — Optical conductivity is one of the tools traditionally used to study strongly correlated systems. For single band systems, the interpretation of these data is rather straightforward and very well known. This is not the case for multiorbital systems, where electronic interactions lead to nontrivial features in the optical spectrum. We have studied the case of iron superconductors by means of a model that introduces the orbital dependent interactions. We find that interband transitions make a non-negligible contribution to the low-energy plateau found in the optical spectrum of undoped compounds and account for a large fraction of the spectral weight at the cutoff frequencies currently used to determine the Drude weight. This fraction is strongly enhanced in hole-doped samples as the larger effect of interactions towards half-filling strongly suppresses the Drude weight. We analyze the relationship between the Drude weight and the kinetic energy and their renormalizations. We show that with orbital differentiation, the renormalization of both the Drude weight and the kinetic energy are not equal, not even within a Fermi liquid picture. Phys. Rev B 90, 115128 (2014).

$^1$MINECO, Spain FIS2011-29689 and No. FIS2012-33521

5:06PM W5.00012 Direct characterization of photo-induced multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multferoelectric, B. 2001, 8, 1357, 1515; 2002, 41, 758., MATTHEW WANG, SYLVIA R. WANG, RANJITH D. R. KANTAM, KUN YANG, JAMES CLARKSON, JIN-ARL LEW, KENNETH BECK, GREAT NEDO CAO, SUNG HYUN LEE, HUI YUN LEE, SANG YOUNG CHOI, JAE-MIN BONG, KI-JOON LEE, SANG JUN LEE, MINSEONG KIM, DONG HYUN KIM, RAHUL C. SCHLUMPF, SLAC National Accelerator Laboratory, 536, 144600 Sect. 6.04. 1:1. 1:1./2, 2:30PM W5.00013 Collective exhibition of photo-induced excitation in the multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multferoelectric. 5:00PM W5.00014 Direct characterization of photo-induced multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multiferroic multferoelectric, B. 2001, 8, 1357, 1515; 2002, 41, 758., MATTHEW WANG, SYLVIA R. WANG, RANJITH D. R. KANTAM, KUN YANG, JAMES CLARKSON, JIN-ARL LEW, KENNETH BECK, GREAT NEDO CAO, SUNG HYUN LEE, HUI YUN LEE, SANG YOUNG CHOI, JAE-MIN BONG, KI-JOON LEE, SANG JUN LEE, MINSEONG KIM, DONG HYUN KIM, RAHUL C. SCHLUMPF, SLAC National Accelerator Laboratory, 536, 144600 Sect. 6.04. 1:1.

Thursday, March 5, 2015 2:30PM - 5:30PM — Session W6 DMP DCMP: Focus Session: Nanostructures and Metamaterials IV 006A - Oded Rabin, University of Maryland

2:30PM W6.00001 ABSTRACT WITHDRAWN —
over an interval of wavelength centered on the wavelength of the Dirac points. In our initial CL measurement, silver pillars in honeycomb lattices, we have observed strong radiation patterns near the Brillouin zone edge, integrated we have utilized cathodoluminescence (CL) spectroscopy to study angular emission patterns and construct band structures of the silver pillars in honeycomb.

91125, United States — Surface plasmons in honeycomb lattices of Ag nanoparticles exhibit Dirac-like band structures, similar to the electronic band structure of graphene. Full wave simulations for an infinite honeycomb lattice of silver nano-pillars reveal hybridization of localized plasmonic modes between two neighboring pillars.

ALBERT POLMAN, AMOLF, HARRY ATWATER, Thomas J. Watson Laboratory of Applied Physics, California Institute of Technology, Pasadena, California 91125, United States, BENJAMIN BRENNY, AMOLF, SONDRA =

2:42PM W6.00007 Dirac-like plasmons in Ag nanopillar honeycomb lattices , SIYING PENG, Thomas J. Watson Laboratory of Applied Physics, California Institute of Technology, Pasadena, California 91125, United States, BENJAMIN BRENNY, AMOLF, SONDRA HELLSTROM, Thomas J. Watson Laboratory of Applied Physics, California Institute of Technology, Pasadena, California 91125, United States, TOON COENEN, ALBERT POLMAN, AMOLF, HARRY ATWATER, Thomas J. Watson Laboratory of Applied Physics, California Institute of Technology, Pasadena, California 91125, United States — Surface plasmons in honeycomb lattices of Ag nanoparticles exhibit Dirac-like band structures, similar to the electronic band structure of graphene. Full wave simulations for an infinite honeycomb lattice of silver nano-pillars reveal hybridization of localized plasmonic modes between two neighboring pillars and the consequent formation of bonding and anti-bonding modes that are energetically degenerate at Dirac points. Electromagnetic simulations reveal the existence of plasmonic edge states in finite width nanoribbons of the honeycomb nanoparticle lattice. Nanoscale architecture of the honeycomb lattice may provide a new way to control plasmon propagation by selective excitation of directional surface plasmon edge states without backscattering. Experimentally, we have utilized cathodoluminescence (CL) spectroscopy to study angular emission patterns and construct band structures of the silver pillars in honeycomb lattices. In our initial CL measurement, silver pillars in honeycomb lattices, we have observed strong radiation patterns near the Brillouin zone edge, integrated over an interval of wavelength centered on the wavelength of the Dirac points.

2:54PM W6.00003 Super Resolution Measurements of the Near-Field Coupling of the Polarized Modes of Gold Nanorods to Fluorescent Emitters , BENJAMIN ISAACOFF, JESSICA DONEHUE, JULIE BITEEN, Univ of Michigan - Ann Arbor — The localized surface plasmon resonances of metal nanoparticles result in complex light-matter interactions that depend strongly on the nanoparticle geometry. In this work, we use single-molecule super-resolution imaging and single-particle spectroscopy to study the polarization dependent response of gold nanorods (GNRs), which support two orthogonal plasmon modes. Furthermore, we measure the emission intensity and polarization of single fluorescent molecules coupled to the GNR as a function of excitation polarization and spectral overlap with the GNR modes. Based on such differential excitation, we demonstrate polarization control of plasmon-enhanced fluorescence from single molecules coupled to single nanoparticles. These experiments are compared with broadband finite difference time domain (FDTD) simulations studying the role of fluoroaphore position and orientation, revealing the underlying mechanisms of this coupling. These super-resolution measurements and the associated simulations demonstrate how polarization can be used to actively control nanoparticle plasmonics and opens the door to a new framework for controlling and optimizing nanoparticle-fluorophore interactions.

3:06PM W6.00004 Influence of Surfactant Bilayers and Substrate Immobilization on the Refractive Index Sensitivity of Anisotropic Gold Nanoparticles , MOHAMAD SHAHJAMALI, NICOLAS LARGE, Northwestern University, ERIK MARTINSSON, Linkoping University, NEGIN ZARAAE, GEORGE SCHATZ, Northwestern University, DANIEL ALLI, Linkoping University, CHAD MIRKIN, Northwestern University — Shape-controlled synthesis of gold nanoparticles (AuNPs) generally involves the use of surfactants to regulate the nucleation growth process and to obtain colloidal stable AuNPs. The surfactants adsorb on the NP surface making further functionalization difficult and therefore limit their practical use in many applications such as bio- and molecular sensing, surface-enhanced spectroscopies, and NP assembly. Herein, we report on how cetyltrimethylammonium (CTAX, X=Cl−, Br−), a common surfactant used in anisotropic AuNPs synthesis, affects the nanoparticle sensitivity to local dielectric environment changes and limits refractometric plasmonic sensing. We experimentally and theoretically show that the CTAX bilayer significantly reduces the refractive index (RI) sensitivity of anisotropic AuNPs such as flat and concave nanocubes, nanorods, and nanoprism. We show that the RI sensitivity can be improved by up to 40% by removing the CTAX from immobilized AuNPs using oxygen plasma treatment. The substrate effect on the RI sensitivity caused by NP immobilization is also investigated. The strategy presented herein is a simple and effective method to improve the RI sensitivity of CTAX-stabilized AuNPs, thus increasing their potential in nanoplasmic sensing and in biomedical applications.

3:18PM W6.00005 Surface plasmons excitation and manipulation by low-energy electrons , MICHAEL J. BURNS, JUAN M. MERLO, YITZI M. CALM, MICHAEL J. NAUGHTON, Boston College — Surface plasmons coupled by optical fields have been widely used to control the propagation of electromagnetic fields in the nanoscale range. We propose numerically the use of low-energy electrons to excite and manipulate surface plasmons in metallic surfaces by using different configurations of tunneling junctions. Modeling the inelastic electron scattering at tunneling junctions as an electric dipole, it is possible to use an electromagnetic model to reproduce experimental results already reported [1]. Following this methodology, we demonstrate that is it possible to mimic novel plasmonic elements that can be excited only by optical fields, i.e. focused beams. Our results open a wide range of applications because it avoids the noise produced by direct light excitation in the detection of surface plasmons. Finally, as an application of our proposed scheme, we study the unidirectional surface plasmon coupler, getting similar results to those recently reported [2].


3:30PM W6.00006 Optical Properties of Scalable Nano-Mesh Films , KYLE ALVINE, BRUCE BERNACKI, WENDY BENNETT, ALAN SCHEMER-KOHRN, Pacific Northwest Natl Lab — We describe here the optical properties of a scalable nano-mesh film both experimentally measured and calculated by FDTD numerical modeling. Typically, applications for optically responsive nano-plasmonic or photonic films are limited by virtue of tractable fabrication techniques to several hundred microns or a few millimeters in size. The films described here have been demonstrated over an extent of several inches and could be readily scaled to larger sizes. The films are comprised of a quasi-regular periodic array of nanoscale holes in metallic film. The nanostructure is fabricated in a scalable fashion in a multi-step fashion via sputtering on a nanoscale template created by nanoparticle self-assembly. Both the numerical modeling and experimentally measured scattering demonstrate that these films are highly resonant with the resonance location in the visible or near infrared and set by the hole size and pattern geometry. Such films can also be readily made on flexible substrates if desired. Potential applications include new proposed photonic thermal management coatings or plasmoelectric devices.

3:42PM W6.00007 Optical Properties of Scalable Nano-Mesh Films , KYLE ALVINE, BRUCE BERNACKI, WENDY BENNETT, ALAN SCHEMER-KOHRN, Pacific Northwest Natl Lab — We describe here the optical properties of a scalable nano-mesh film both experimentally measured and calculated by FDTD numerical modeling. Typically, applications for optically responsive nano-plasmonic or photonic films are limited by virtue of tractable fabrication techniques to several hundred microns or a few millimeters in size. The films described here have been demonstrated over an extent of several inches and could be readily scaled to larger sizes. The films are comprised of a quasi-regular periodic array of nanoscale holes in metallic film. The nanostructure is fabricated in a scalable fashion in a multi-step fashion via sputtering on a nanoscale template created by nanoparticle self-assembly. Both the numerical modeling and experimentally measured scattering demonstrate that these films are highly resonant with the resonance location in the visible or near infrared and set by the hole size and pattern geometry. Such films can also be readily made on flexible substrates if desired. Potential applications include new proposed photonic thermal management coatings or plasmoelectric devices.
3:54PM W6.00008 MEMS for Tunable Plasmonic Coupling, TOM STARK, MATTHIAS IMBODEN, SABRI KAYA, ALKET MERTIRI, SHYAMSUNDER EMMONILLI, DAVID BISHOP, Boston Univ. — The localized surface plasmon resonance (LSPR) of sub-wavelength holes in metals depends upon the geometry, composition, refractive index, and near field coupling to neighboring particles. Sub-wavelength holes in metals can exhibit extraordinary optical transmission (EOT) at the resonance frequency and, for certain geometries, polarization-dependent transmission. We present a microelectromechanical system, tunable Fabry-Perot etalon. One interface is a suspended gold metatmaterial and the other is a gold reflector. The reflectance, measured with a Fourier transform infrared spectrometer, exhibits the convolution of the EOT through the holes and Fabry-Perot resonances. Using MEMS, we translate the etalon from the far to the near field by tuning the free spectral range from about 5000 to 250 cm\(^{-1}\) and shifting the reflection minima and maxima across the infrared. When the separation between the metatmaterial and gold reflector approaches the decay length of the LSP electric fields, interactions with image currents generated in the gold reflector become significant. By tuning the separation in this regime, we will tune the near field coupling between the LSPR and image currents and tune the LSPR of the system, effectively creating a sensing substrate with a tunable LSPR frequency.

4:06PM W6.00009 Digitally Programmable Micro Evaporation Source for Nanofabrication, HAN HAN, MATTHIAS IMBODEN, Boston University, PABLO DEL CORRO, Instituto Balseiro, THOMAS STARK, RICHARD LALLY, Boston University, FLAVIO PARDO, CRIS BOLLE, Bell Labs, Alcatel-Lucent, DAVID BISHOP, Boston University — There is a significant world-wide effort to develop nanomanufacturing methods that can extend into the deep nanoscale region, below 20 nm. Techniques include photolithography, nano-imprint and direct write methods such as dip-pen lithography and atomic calligraphy. A central component of any fabrication setup is the deposition control of the materials to be used. Here we present a MEMS based, multi-material evaporation source array with each source element consisting of a polysilicon plate suspended by two electrical constrictions. When resistively heating the plate, the pre-loaded material is thermally evaporated off of the plate. By arranging many of these devices into an array, one has a multi-material, digitally programmable evaporation source. Pulsing the source with precisely controlled peak voltage and timing can emit atom fluxes with an unprecedented level of control in terms of what, when and how many atoms get deposited. By varying their dimensions and arrangement, the source array can provide controllable atom fluxes ranging over ten orders of magnitude. Such a material source can provide precise control and flexibility when conducting nanopatterning and nanolithography.

4:18PM W6.00010 Soft Nanoimprint Lithography for Direct Printing of Crystalline Metal Oxide Nanostructures, ROHIT KOTHARI, MICHAEL BEAULIEU, JAMES WATKINS, Univ. of Massachusetts Amherst — We demonstrate a solution-based soft nanoimprint lithography technique to directly print dimensionally-stable crystalline metal oxide nanostructures. A patterned PDMS stamp is used in combination with a UV/thermal cure step to imprint a resist containing high concentrations of crystalline nanoparticles in an inorganic/organic binder phase. The as-imprinted nanostructures are highly crystalline and therefore undergo little shrinkage (less than 5% in some cases) upon thermal annealing. High aspect ratio nanostructures and sub-100 nm features are easily realized. Residual layer direct imprinting (no etching) was achieved by choosing the resist with the appropriate surface energy to ensure dewetting at stamp-substrate interface. The technique was further extended to stack the nanostructures by deploying a layer-by-layer imprint strategy. The method is scalable and can produce large area device quality nanostructures in a rapid fashion at a low cost. CeO\(_2\), ITO and TiO\(_2\) nanostructures are illustrated for their potential use in fuel cell electrodes, solar cell electrodes and photonic devices, respectively.

4:30PM W6.00011 Resolving the two-dimensional self-assembly of iron oxide nanoparticles on a liquid surface, JIAYANG HU, DATONG ZHANG, Columbia University, CHENGUANG LU, National Center for Nanoscience and Technology, SEUNG WHAN LEE, FAN YE, IRVING P. HERMAN, Columbia University — In situ small-angle X-ray scattering (SAXS) is used to monitor the self-assembly of iron oxide nanoparticles (NPs) dispersed in alkanes that are drop-cast on a diethylene glycol liquid surface. We found that the surface separations of NP cores in 2D superlattices (SLs) are generally farther apart than in 3D SLs with corresponding NPs. At these separations, the van der Waals (vdW) energy is smaller than the Brownian motion energy and so the previous 3D vdw force driven self-assembly models fail to explain the stable closed-packed structure. Strong ligand-ligand interactions likely bind the structure after the upper solvent dries. Entropy effects are found not to be the likely driving force for the observed close packing structures.

4:42PM W6.00012 Imaging of Bottom-up Graphene Nanoribbons Synthesized Using Combined Solution and Surface Reactions, DANNY HABERER, CHEN CHEN, ZAHRA PEDRAMRAZI, RYAN CLOKE, TOMAS MARANGONI, WON-WOO CHOI, FELIX FISCHER, CROMMIE MICHAEL, UC Berkeley, CROMMIE GROUP TEAM, FISCHER GROUP TEAM — Bottom-up graphene nanoribbons (GNRs) are a new class of material that has promising applications in next-generation electronic, spintronic, and optical devices. Bottom-up synthesis using molecular precursors provides precise control over GNR width and edge geometry, which determine GNR electronic structure. However, previously used on-surface polymerization techniques can be hindered by molecular diffusion barriers and by undesired side products. Alternative in-solution polymerization techniques potentially have better yield and higher selectivity. Using combined in-solution polymerization and on-surface cyclodehydrogenation reactions, we have successfully synthesized N\(_2\)-armchair GNRs. Scanning tunneling microscopy was used to reveal the precise width and edges of the resulting nanoribbons. This method may be generalized to synthesize graphene nanoribbons that are difficult to fabricate through exclusive on-surface reactions.

4:54PM W6.00013 Dynamically tunable graphene/dielectric photonic crystal transmission lines, IAN WILLIAMSON, S. HOSSEIN MOUSAVI, ZHENG WANG, Univ of Texas, Austin — It is well known that graphene supports plasmonic modes with high field confinement and lower losses when compared to conventional metals. Additionally, graphene features a highly tunable conductivity through which the plasmon dispersion can be modulated. Over the years these qualities have inspired a wide range of applications for graphene in the THz and infrared regimes. In this presentation we theoretically demonstrate a graphene parallel plate waveguide (PPWG) that sandwiches a 2D photonic crystal slab. The marriage of these two geometries allows a large two dimensional band gap that can be dynamically tuned over a very broad bandwidth. Our device operates in the low-THz band where the graphene PPWG supports a quasi-TEM mode with a relatively flat attenuation. Unlike conventional photonic crystal slabs, the quasi-TEM nature of the graphene PPWG mode allows the slab thickness to be less than 1/10 of the photonic crystal lattice constant. These features offer up a wealth of opportunities, including tunable metamaterials with a possible platform for large band gaps in 3D structures through tiling and stacking. Additionally, the geometry provides a platform for tunable defect cavities without needing three dimensional periodicity.

5:06PM W6.00014 Toward Controlled In-Solution Stacking of Solvent Exfoliated 2-Dimensional Nanoflakes and Heterostructures, DALE BROWN, A. NICOLE CHANG, RICHARD LIVINGSTON, DAVID ESTRADA, Boise State University — As a result of quantum confinement, materials with one dimension confined to a few atomic diameters, including single- and few-layer graphene and transition metal dichalcogenides (TMDs), often have properties unique from those of their bulk counterparts. Included in these emergent properties is photoluminescence in thin flakes of some semiconducting TMDs. Additionally, the creation of heterostructures via the stacking of 2D materials allows for the synthesis of new materials with properties unique from those of the starting materials. While much of the research published to date in this area relies on labor intensive methods, including stacking each subsequent layer by hand to synthesize these heterostructures, some researchers have demonstrated random stacking of suspended 2D flakes in solution, with limited control over the thickness of the resulting heterostructures. By modifying the surface energy mismatch between the solvent and the suspended, exfoliated 2D materials therein, we aim to demonstrate the ability to actively control the propensity for and duration of stacking in liquid suspensions of 2D materials.
5:18PM W6.00015 Bottom-up synthesis of N=11 armchair graphene nanoribbons via new sp3 to sp2 cyclization route. ZAHRA PEDRAMRAZI, CHEN CHEN, DANNY HABERER, WADE PERKINS, FELIX FICHERER, MICHAEL CROMMIE, UC Berkeley, CROMMIE GROUP TEAM. FISCHER GROUP TEAM. — Bottom-up synthesis is a powerful fabrication tool for controlling the atomic scale structures of graphene nanoribbons (GNRs). The electronic properties of GNRs, 1D strips of graphene that exhibit energy gaps in their electronic structure due to quantum confinement, is highly dependent on precise width and atomic edge structure. The molecular precursors used to date for bottom-up synthesis are based on conjugated systems of sp2-bonded carbon atoms. Here we demonstrate a new molecular precursor for synthesis of bottom-up N=11 armchair GNRs that exhibits cyclohydrogenation of ‘out-of-plane‘, sp3-bonded elements. Scanning tunneling microscopy imaging was used to characterize the GNR growth reaction at different annealing temperatures, allowing observation of the sp3 to sp2 cyclization process. This demonstrates a new chemical route for achieving armchair GNRs, as well as new insight into surface-based covalent self-assembly of organic molecules.

Thursday, March 5, 2015 2:30PM - 5:30PM – Session W7 DMP DCMP: Focus Session: Novel Topological Phases: Theory II 006B - Jens Bardarson, Max Plank Institute, Dresden

2:30PM W7.00001 disorder effect on quantum transport properties of ultra thin Fe film. XIAOTIAN ZHANG, Peking Univ, KOHJI NAKAMURA, Mie University, RYUICHI SHINDOU, ICOM, School of Physics, Peking University — Ferromagnetic ultrathin films are experimentally known to often exhibit perpendicular magnetic anisotropy, when being placed on certain substrates. Based on reported ab-initio band calculations of free-standing Fe-monolayer and that on MgO substrate, we will introduce an effective tight-binding model, which capture a part of an electronic structure near Fermi level for both cases. We will show that the model supports electronic bands with non-zero Chern number and chiral edge modes which cross a direct band gap on the order of 50meV. Unluckily, however, the direct band gap is also masked by another dispersive bands which has zero Berry’s curvature in the k-space. To demonstrate how disorder kills conducting characters of the latter bulk bands while leave intact those of the chiral edge modes, we will clarify behaviors of localization length and conductance in the effective model with on-site disorders.

2:42PM W7.00002 Complex Band Structure of the Topological Insulator Bi$_2$Se$_3$. SHIJIE LI, Univ of Nebraska - Lincoln, JESUAN BETANCOURT, University of Puerto Rico, J.D. BURTON, Univ of Nebraska - Lincoln, JULIAN P. VELEV, University of Puerto Rico, EVGENY Y. TSYMBAL, Univ of Nebraska - Lincoln — Recently there is a surge of interest in using topological insulators for electronic and spintronic applications. For applications it is important to understand the complex band structure (CBS) of the topological insulator, which determines the decay rate of the protected surface states into the bulk of the material. The Bi$_2$Se$_3$ family of three-dimensional topological insulators is the most studied and best understood. In this work we investigate the CBS of Bi$_2$Se$_3$ using first-principles density-functional calculations. We determine the decay rates and the symmetry of the evanescent states and we follow their evolution from those of the band insulator. We complement these results with Bi$_2$Se$_3$ (0001) slab calculations to explore the penetration depth, oscillatory behavior and spin texture of the surface states. The CBS provides a new insight into the topologically protected states and could be used for the search of new topological insulators and device concepts.

2:54PM W7.00003 Prediction of Large-Gap Two-Dimensional Topological Insulators Consisting of Hydrogenated Bilayers of Group III Elements with Bi. CHRISTIAN P. CRISOSTOMO, LIANG-ZI YAO, ZHI-QUAN HUANG, CHIA-HSIU HSU, FENG-CHUAN CHUANG, Natl. Sun Yat-sen U., HSIN LIN, Natl. U. of Singapore, MARVIN A. ALBAO, U. of the Philippines Los Banos, ARUN BANSIL, Northeastern U. — We use first-principles electronic structure calculations to predict a new class of two-dimensional (2D) topological insulators (TIs) in hydrogenated binary compositions of group III elements (B, Al, Ga, In, and TI) and bismuth (Bi). We identify band inversions in unhydrogenated pristine GaBi, InBi, and TIBi bilayers, with gaps as large as 556 meV for the TIBi case, making these materials suitable for room-temperature applications. Double-sided hydrogenation in which hydrogen was added on opposite sides also exhibited band inversions in the case of GaBi, InBi, and TIBi just as in the unhydrogenated pristine ones. Furthermore, we report the gap to be 885 meV for the hydrogenated TIBi case. Hydrogenation enhance the band gap without changing the band topology. Moreover, our study also aim to demonstrate the possibility of strain engineering in that the topological phase transition in systems whose phase was nontrivial could be driven by suitable strain. Finally, the effect of placing hydrogen to topological edges was also demonstrated. Our findings suggest that the buckled honeycomb structure is a versatile platform for hosting nontrivial topological states and spin-polarized Dirac fermions with the flexibility of chemical and mechanical tunability. The robustness of III-Bi upon hydrogenation shows that these materials are possible to synthesize by growing on substrates.

3:06PM W7.00004 Topological Crystalline Insulators. TIMOTHY HSIEH, Massachusetts Inst of Tech-MIT — Topological crystalline insulators (TCIs) are new phases of matter in which nontrivial band topology and crystal symmetry unite to protect metallic states on the boundary. Remarkably, TCIs have been predicted and observed in the conveniently simple rocksalt SnTe class of IV-VI semiconductors. Despite the simple crystal structure, the interplay between topology and crystal symmetry in these materials have led to a rich variety of new phenomena, including the coexistence of massless and massive Dirac fermions arising from ferroelectric distortion and strain-induced flat band superconductivity. These new physical mechanisms are not only of intrinsic interest but may also find application in new transistor devices. After discussing the topological nature and potential uses of IV-VI family TCIs, I will present recent predictions of TCIs in several anti-perovskite materials. The origin of TCI in this new class of materials is strikingly different and involves the band inversion of two J states, which cross a direct band gap on the order of 50meV. Unluckily, however, the direct band gap is also masked by another dispersive bands which has zero Berry’s curvature in the k-space. To demonstrate how disorder kills conducting characters of the latter bulk bands while leave intact those of the chiral edge modes, we will clarify behaviors of localization length and conductance in the effective model with on-site disorders.

3:42PM W7.00005 The nontrivial electronic structure of Bi/Sb honeycombs on SiC(0001). FENG-CHUAN CHUANG, CHIA-HSIU HSU, ZHI-QUAN HUANG, CHIEN-CHENG KUO, Natl. Sun Yat-sen U., YU-TZU LIU, HSIN LIN, Natl. U. of Singapore, ARUN BANSIL, Northeastern U. — We discuss two-dimensional (2D) topological insulators (TIs) based on planar Bi/Sb honeycombs on a SiC(0001) substrate using first-principles computations. The Bi/Sb planar honeycombs on SiC(0001) are shown to support a nontrivial band gap as large as 0.56 eV, which harbors a Dirac cone lying within the band gap. Effects of hydrogen atoms placed on either just one side or on both sides of the planar honeycombs are examined. The hydrogenated honeycombs are found to exhibit topologically protected edge states for zigzag as well as armchair edges, with a wide band gap of 1.03 eV and 0.14 eV in bismuth and antimony films, respectively. Our findings pave the way for using planar bismuth and antimony honeycombs as potential new 2D-TI platforms for room-temperature applications.
3:54PM W7.00006 Hydrogenated ultra-thin tin films predicted as two-dimensional topological insulators. ZHI-QUAN HUANG, BO-HUNG CHOU, CHIA-HSIU HSU, FENG-CHUAN CHUANG, Natl. Sun Yat-sen U., YU-TZU LIU, HSIN LIN, Natl. U. of Singapore, ARUN BANSIL, Northeastern U. — Using thickness-dependent first-principles electronic structure calculations, we predict that hydrogenated ultra-thin films of tin harbor a new class of two-dimensional (2D) topological insulators (TIs). A single bilayer (BL) tin film assumes a 2D-TI phase, but it transforms into a trivial insulator after hydrogenation. In contrast, tin films with 2 and 3 BLs are found to be trivial insulators, but hydrogenation of 2 to 4 BL films results in a non-trivial Tl phase. For 1 to 3 BLs, H-passivation converts the films from being metallic to insulating. Moreover, we examined iodine-terminated tin films up to 3 BLs, and found these to be non-trivial, with the films becoming semi-metallic beyond 1 BL. In particular, the large band gap of 340 meV in an iodine-terminated tin bilayer is not sustained in the iodine-terminated 2BL and 3BL tin films.

4:06PM W7.00007 Real-structure influence on topological states of HgTe quantum wells: Ab initio studies. SEBASTIAN KUEFNER, FRIEDHELM BECHSTEDT, Friedrich-Schiller Universitaet Jena — The electronic properties of HgTe quantum well structures are studied by means of ab-initio calculations including spin-orbit interaction and quasiparticle effects. In agreement with earlier kp calculations and experiments we find a topological transition from the trivial insulator into the quantum-spin Hall (QSH) state with increasing QW thickness. The QSH state is characterized by the existence of spin-polarized helical edge states bridging the fundamental gap giving rise to intrinsic spin currents. The occurrence and localization of the edge states are independent of the interface orientation and barrier material. Together with their spin polarization this indicates that they are topologically protected. The nonexistence of inversion symmetry, the atomic geometry, and the real QW barriers do not completely destroy the predictions within toy models but cause significant deviations. The deviations concern the critical thickness, the number and localization of edge states, and the possibility to find QW subbands between edge states.

1We gratefully acknowledge financial support of the Austrian Fond zur Foerderung der Wissenschaftlichen Forschung in the framework of SFB 25 Infrared Optical Nanostructures.

4:18PM W7.00008 Edge state transport in 2D topological insulators without inversion symmetry. YANG-ZHI CHOU, MATTHEW FOSTER, Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA — We investigate finite temperature transport within one and between two edges of a 2D Z_2 topological insulator. For experimentally relevant systems (e.g., HgTe and GaSb/InAs quantum wells), inelastic spin flip backscattering can occur in the absence of inversion symmetry. We use bosonization and the effective action formalism to compute the dc conductivity of helical Luttinger liquid edge states in the absence of inversion symmetry, due to interactions and disorder. These perturbations manifest as irrelevant operators that control the temperature dependence of the conductivity in a single edge. With respect to two edges, the importance of the inelastic mechanism and applications to Coulomb drag will be discussed.

4:30PM W7.00009 Twisting a topological phase on a lattice. MENG CHENG, Microsoft Research Station Q, YI-ZHUANG YOU, University of California, Santa Barbara — When a two-dimensional topological phase inhabits a torus, it possesses a ground state degeneracy robust to any local perturbations. These degenerate ground states can transform nontrivially under modular transformations of the torus, generated by Dehn twists. Representation of Dehn twists on the ground states characterizes the topological order. We propose that the Dehn twists can be obtained as a non-Abelian Berry phase of an adiabatic deformation of the lattice model. We apply this method to the example of a p_x + i p_y superconductor and provide a TQFT interpretation of the numerical results.

4:42PM W7.00010 Quantum criticality of 1D topological Anderson insulators. ALEX KAMENEV, University of Minnesota, DMITRY BAGRETS, ALEX ALTLAND, University of Koln — We present an analytic theory, based on exact transfer-matrix solutions of super-symmetric nonlinear sigma-models, of quantum criticality in quasi one-dimensional topological Anderson insulators. We describe these systems in terms of two parameters (g, χ) representing localization and topological properties, respectively. Certain critical values of χ (half-integer for Z classes, or zero for Z2 classes) define phase boundaries between distinct topological sectors. Upon increasing system size, the two parameters exhibit flow similar to the celebrated two parameter flow of the integer quantum Hall insulator. However, unlike the quantum Hall system, an exact analytical description of the entire phase diagram can be given. We check the quantitative validity of our theory by comparison to numerical transfer matrix computations.

1Support of NSF grant DMR1306734 is acknowledged.

4:54PM W7.00011 Berry Curvature and Chiral Plasmons in Massive Dirac Materials. JUSTIN SONG, Caltech, MARK RUDNER, University of Copenhagen — In the semiclassical model of carrier dynamics, quasiparticles are described as nearly free electrons with modified characteristics modified characteristics such as effective masses which may differ significantly from those of an electron in vacuum. In addition to being influenced by external electric and magnetic fields, the trajectories of electrons in topological materials are also affected by the presence of an interesting quantum mechanical field - the Berry curvature - which is responsible for a number of anomalous transport phenomena recently observed in Dirac materials including G/3hBN, and MoS2. Here we discuss how Berry curvature can affect the collective behavior of electrons in these systems. In particular, we show that the collective electronic excitations in metallic massive Dirac materials can feature a chirality even in the absence of an applied magnetic field. The chirality of these plasmons arises from the Berry curvature of the massive Dirac bands. The corresponding dispersion is split between left- and right-handed modes. We also discuss experimental manifestations.

5:06PM W7.00012 First-Principles Study on Dirac Cones in a Single-Component Molecular Crystal Under High Pressure. TAKAO TSUMURAYA, RIKEN/NIMS, HENG-BO CUI, RIKEN, HIORI KINO, NIMS-MANA, TSUYOSHI MIYAZAKI, NIMS, REIZO KATO, RIKEN — Most single-component molecular crystals show insulating or semiconducting properties at ambient pressure. Recently, metal dithiolene complexes have attracted much attention ever since a metallic state was realized in Ni(bdt)2 at ambient pressure. Even if the system is insulating at ambient pressure, it possibly turns into a metallic or superconducting state by application of pressure. In this study, we have found anisotropic linear (tilted Dirac cone) dispersions near the Fermi level in a single-component molecular crystal, Pd(ddt)2, at 8 GPa by first-principles density functional theory calculations. Recent electrical resistivity at 12.6 GPa shows temperature independent behavior as is observed in the massless Dirac fermion system, ϵ=-(BEDT-TTF)2I3. Our analysis of the electronic structure indicates that the band structure at ambient pressure has quasi-one-dimensional character, which corresponds to the stacking of Pd(ddt)2 molecules along the b-axis, and the dimensionality of the band structure near the Fermi level is changed under the pressure of 8 GPa, where intermolecular hybridization increases due to the reduced intermolecular distances. We also discuss anisotropy of the Dirac cones and their possible origin in the multi-orbital system.
the symmetry of the band edge states; in addition, the band crossing occurs at the band center with notice that all IFS’s appear in the plasmonic band gap of the 1DHMM, and the dielectric- or metallic-like properties of the 1DHMMs are strongly related to can occur in the dielectric/1DHMM interface. Furthermore, we show the existence of the IFS between the dielectric-like 1DHMM and metallic-like 1DHMM. 

\[ \text{light, we theoretically demonstrate an HCG focusing lens with transmissivity of 83.0\% and numerical aperture of 0.77, and a VLM with beam deflection angle} \]

2:30PM W8.00001 Broadband Tunable Transparency in rf SQUID Metamaterial. DAIMENG ZHANG, MELISSA TREPANIER, Univ of Maryland-College Park, OLEG MUKHANOV, Hyuples Inc, PHILIPP JUNG, SUSANNE BUTZ, ALEXEY USTINOV, KIT, STEVEN ANLAGE, Univ of Maryland-College Park — We demonstrate a metamaterial with broadband tunable transparency in microwave electromagnetic fields. This metamaterial is made of Radio Frequency Superconducting Quantum Interference Devices (rf SQUIDs) [1]. We show both experimentally and theoretically that the resonance of this metamaterial totally disappears when illuminated with electromagnetic waves of certain power ranges, so that waves can propagate through the metamaterial with little dissipation in a wide frequency spectrum. Unlike traditional electromagnetically induced transparency, high transmission through this metamaterial is due to the intrinsic nonlinearity of the rf SQUID. Transparency occurs when the metamaterial enters its bistability regime. We can control the metamaterial to be transparent or opaque by switching between the two states depending on the initial conditions and signal scanning directions. We also show that the degree of transparency can be tuned by temperature, power of the incident wave, and dc magnetic field and discuss analytical and numerical models that reveal how to systematically control the transparency regime. The metamaterial has potential application in fast tunable digital filter, power limiter and auto-cloaking.


2:42PM W8.00002 Plasmonic metastructures exhibiting a narrow transparency window within a broad extinction spectrum. LUCAS V. BESTEIRO, Department of Physics and Astronomy, Ohio University, HUI ZHANG, Department of Physics and Astronomy, Rice University, KIVANC GUNGOR, Institute of Materials Science and Nanotechnology, Bilkent University, HILM VOKLANKOY, Institute of Materials Science and Nanotechnology, Bilkent University; School of Physical and Mathematical Sciences, Nanyang Technological University, ALEXANDER GOVOROV, Department of Physics and Astronomy, Ohio University — Metallic nanostructures have proven to be a valuable resource in accessing new ways of manipulating light, allowing the creation of novel metamaterials with a number of different applications. By controlling the size and geometry of these structures they can be tailored to strongly interact with specific wavelengths of incident light. We propose an approach to the design of composite systems that takes advantage of that property. Using finite elements calculations, we have studied several structure geometries suitable to be deployed using lithographic or colloidal synthesis techniques, such as discs, nanorods and nanocrosses. We discuss specific layouts of these structures, arranged in a modular fashion, to construct plasmonic metamaterials with a wide extinction profile that also present a transparency window for a narrow range of frequencies. This kind of metamaterials, made in the form of plasmonic metasolutions or as a stacked solid-state metastructure, may be used to create frequency filters for electromagnetic radiation. To realize this objective, it is instrumental to choose the right ensemble of nanostructures and to control the interaction between them.

2:54PM W8.00003 Metasurfaces based on Gallium Nitride High Contrast gratings at Visible Range. ZHENHAI WANG, SHUMIN HE, QIFA LIU, WEI WANG, YONGJIN WANG, HONGBO ZHU, Grünberg Research Centre, Nanjing University of Posts and Telecommunications, Nanjing 210003, China, GRÜNBERG RESEARCH CENTRE TEAM — Metasurfaces are currently attracting global attention due to their ability to achieve full control of light propagation. However, these metasurfaces have thus far been constructed mostly from metallic materials, which greatly limit the diffraction efficiencies because of the ohmic losses. Semiconducting metasurfaces offer one potential solution to the issue of losses. Besides, the use of semiconductor materials can broaden the applicability of metasurfaces, as they enable facile integration with electronics and mechanical systems and can benefit from mature semiconductor fabrication technologies. We have proposed visible-light metasurfaces (VLMs) capable of serving as lenses and beam deflecting elements based on gallium nitride (GaN) high contrast gratings (HCGs). By precisely manipulating the wave-fronts of the transmitted light, we theoretically demonstrate an HCG focusing lens with transmissivity of 83.0\% and numerical aperture of 0.77, and a VLM with beam deflection angle of 6.03\° and transmissivity as high as 93.3\%. The proposed metasurfaces are promising for GaN-based visible light-emitting diodes (LEDs), which would be robust and versatile for controlling the output light propagation and polarization, as well as enhancing the extraction efficiency of the LEDs.

3:06PM W8.00004 Interface States between two one-dimensional Hyperbolic Metamaterials. IENG-WAI UN, TA-JEN YEN, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan, R.O.C — In this work, we investigate the interface state(IFS) between two 1D hyperbolic metamaterials(1DHMM). At first, we scrutinize the existence of IFS in three kinds of interface-dielectric/1DHMM, metal/1DHMM, and 1DHMM/1DHMM, respectively. We find that these interface states depend on three factors of thicknesses (d_a, d_m), dielectric constants (\varepsilon_a, \varepsilon_m), and the transverse momentum k_T in the 1DHMM. For the case of d_a > d_m, the 1DHMM behaves like metal(dieletric) as k_T > k_T^{(\text{max})} because IFS exists in the dielectric/1DHMM interface. For the case of d_a < d_m, there is no band crossing and IFS can occur in the dielectric/1DHMM interface. Furthermore, we show the existence of the IFS between the dielectric-like 1DHMM and metallic-like 1DHMM. Notice that all IFS’s appear in the plasmonic band gap of the 1DHMM, and the dielectric- or metallic-like properties of the 1DHMMs are strongly related to the symmetry of the band edge states; in addition, the band crossing occurs at the band center with k_T = k_T^{(\text{max})} and is contributed from the material dispersion. In conclusion, we present a simple method to determine the existence of the IFS in three kinds of interfaces and the surface properties of 1DHMM from its bulk properties.
3:30PM W8.00006 Metasurface-Enabled Anisotropic Quantum Vacuum over Macroscopic Distances, PANKAJ JHA, XINGJIE NI, CHIHUI Wu, YUAN WANG, XIANG ZHANG, University of California, Berkeley — Quantum vacuum (QV) of an electromagnetic field has a profound effect on the optical response of a quantum emitter. QV in the vicinity (few tens of nm) of a metallic interface is strongly anisotropic and can be harnessed to induce quantum interference among the spontaneous emission channels from nearly degenerate excited states in a multi-level atom. Unfortunately, trapping an atom within this range is extremely challenging in experiments. Here, utilizing the exceptional light manipulation properties, both phase dependent and polarization selective response, of a metasurface we engineer the reflected field, from the spontaneous emission, back to the atom itself. A strong anisotropy in the decay rate of the atom is induced even when the atom is located at some macroscopic distance from the metasurface. Quantum vacuum engineering with metasurfaces will create unprecedented opportunities for long-range interaction between quantum emitters, new regime of cavity-free QED, solid-state quantum optics, spintronics etc.

3:42PM W8.00007 Strategy for designing broadband vibration isolation systems through exactly solvable models of graded elastic networks, KA KI NG, WAI SOEN CHAN, KIN WAH YU, Department of Physics, The Chinese University of Hong Kong — Motivated by the need of seismic base isolation, we have proposed a strategy to design vibration isolation systems to achieve near-zero amplitude vibration under external excitations over a broad frequency band. The strategy combines two ideas from previous works: (i) zeros assignment for broadband epsilon-near-zero metamaterials [Sun, and Yu (2012)]; and (ii) the localization of vibrational modes in graded elastic networks [Xiao, Yakubo, and Yu (2006)]. Firstly, we aim to assign zeros (anti-resonance frequencies) over an operating frequency band. Starting from an exactly solvable model of zigzag diatomic chains, we demonstrate a one-to-one correspondence between the zeros and one type of the masses after solving the models. Hence, the zeros can be assigned at will by tuning the masses. Second, in order to achieve further vibrational suppression by gradon localization, a band overlapping picture is applied to tune the rest of the masses to an optimal value. The results can be generalized to 2D and 3D structures for more realistic applications.

3:54PM W8.00008 Ultra-broadband sound absorption by acoustic metamaterials, XUE JIANG, BIN LIANG, JIAN-CHUN CHENG, Nanjing University — Metamaterials with extraordinary properties unavailable in nature have opened up new design possibilities. Acoustic absorbers are of particular significances for acoustics-based devices and find applications in various scenarios, but subject to the inherent restriction of the natural acoustical parameters and limited operating bandwidth. We report the theoretical design, numerical calculation and experimental study on the realization of a metamaterial-based acoustic absorber with a simple yet efficient structure. The proposed acoustic absorber works in an ultra-broad band without restricted by the material type or requiring extra absorbing material. Such distinct effects stem from the localization and dissipation of different spectrum components at predesigned spatial positions. Theoretical predictions developed based on classical acoustic theory agree well with numerical and experimental results. The realization of ultra-broadband acoustic absorber with unique properties of stiffness and environmental-friendliness has paved the way for designing conceptual acoustical devices, and has potential applications in situations with special requirements on acoustic absorption characteristics.

4:06PM W8.00009 Strong Coupling of Terahertz Cyclotron Resonance with a One-Dimensional Photonic Crystal Cavity, MINHAN LOU, QI ZHANG, Department of Electrical and Computer Engineering, Rice University, Houston, Texas, USA, RODION KONONCHUK, ANDREY CHABANOV, Department of Physics and Astronomy, University of Texas at San Antonio, San Antonio, Texas, USA, JUNICHIRO KONO, Department of Electrical and Computer Engineering, Rice University, Houston, Texas, USA — Achieving strong light-matter interaction is essential for the study of cavity quantum electrodynamics. In the ultrastrong coupling regime, where the ratio of the vacuum Rabi splitting to the transition frequency is close to or larger than one, intriguing quantum effects, e.g., the Bloch-Siegert Shift and interaction-dependent ground states, are expected to appear, due to the breakdown of the rotating wave approximation. Since this ratio increases with the transition wavelength, going to the terahertz (THz) range is promising for exploring new strong-coupling phenomena. Here, we experimentally demonstrate strong coupling between the cyclotron resonance of a high-mobility two-dimensional electron gas and a photonic defect mode in a one-dimensional (1D) THz photonic crystal (PC) cavity. Compared to THz cavities based on split-ring metamaterials, the 1D PC cavity exhibits a higher quality $(\mathcal{Q})$ factor and lower loss, in spite of a larger mode volume. Our 1D PC cavities consist of quarter-wave intrinsic silicon / sapphire slabs and air gaps. The $\mathcal{Q}$ factor can be tuned in a wide range by changing the materials and the number of layers. An ultrathin modulation-doped GaAs quantum well is placed at the electric field maximum of the defect mode in the 1D THz PC cavity.

4:18PM W8.00010 Unidirectional Spectral Singularities, HAMIDREZA RAMEZANI, HAO-KUN LI, YUAN WANG, XIANG ZHANG, University of California, Berkeley — We introduce a new class of spectral singularities with directional response emerging from the interplay of parity-time (PT) symmetry and Fano resonances. We show that, without breaking the reciprocity, one is able to obtain a simultaneous unidirectional lasing and unidirectional reflectionless mode. For such a mode one side reflection tends to infinity, the other side reflection becomes zero, and the transmission coefficient remains finite. These singularities emerge from the resonance trapping and delay time associated with the reflected signal residing in the gain or loss part of the parity-time symmetric cavity. In addition, we show that in the absent of loss (gain) and at threshold gain (loss), the structure still acts as a unidirectional laser (reflectionless system). In the passive-loss case our structure acts as a unidirectional perfect absorber. When the system possesses pure balanced gain, transmission and reflection from the left and right side of the system tends to infinity and we recover the conventional lasing modes.
4:30PM W8.00011 Light propagation in synthetic pseudo-passive media with balanced gain and loss\textsuperscript{1}, ALLI BASIRI, TSAMPIKOS KOTTOS, Wesleyan Univ, ILYA VITEBSKIY, The Air Force Research Laboratory, Sensors Directorate — Optical materials exhibiting exotic values of permittivity \( \varepsilon \) and/or permeability \( \mu \) are often prohibitively lossy. This is especially true for composite optical metamaterials. A natural solution to the problem is to add a gain component and, thereby, to offset the losses. There are two different ways to do so. The first one involves a photonic structure composed of judiciously arranged loss and gain components. A well-known example of such balanced loss-gain structures is the so-called PT symmetric photonic crystals. An alternative approach is to compensate the losses with gain while preserving uniformity of the medium. Here we consider this second case where both constituents are complex such that \( \varepsilon = \varepsilon' + i\varepsilon'' \), \( \mu = \mu' + i\mu'' \) with \( p \) being real. In this case the material would have a uniform real refractive index \( n = \sqrt{\varepsilon \mu} = \text{constant} \).

We demonstrate that this type of pseudo-passive synthetic structures show novel transport characteristics uncommon to regular lossless structures.

\textsuperscript{1}AFOSR MURI grant FA9550-14-1-0037 and NSF DMR-1306984

4:42PM W8.00012 Localized Guided-Mode and Cavity-Mode Double Resonance in Photonic Crystal Nanocavities\textsuperscript{1} , XUQING LIU, TAKASHI SHIMADA, RYOHEI MIURA, SATOSHI IWAMOTO, YASUHIKO ARAKAWA, YUICHIRO K. KATO, The University of Tokyo — We investigate the use of guided modes bound to defects in photonic crystals for achieving double resonances. Photoluminescence enhancement by more than three orders of magnitude has been observed when the excitation and emission wavelengths are simultaneously in resonance with the localized guided mode and cavity mode, respectively. We find that the localized guided modes are relatively insensitive to the size of the defect for one of the polarizations, allowing for flexible control over the wavelength combinations. This double resonance technique is expected to enable enhancement of photoluminescence and nonlinear wavelength conversion efficiencies in a wide variety of systems. For example, such tuning of double resonance would be particularly effective for carbon nanotubes that show sharp absorption peaks [1].


\textsuperscript{1}Work supported by KAKENHI, SCOPE, Canon Foundation, Asahi Glass Foundation, and KDDI Foundation as well as the Project for Developing Innovation Systems, Nanotechnology Platform, and Photon Frontier Network Program of MEXT, Japan.

4:54PM W8.00013 Self-assembled tunable photonic hyper-crystals\textsuperscript{1} , IGOR SMOLYANINOV, University of Maryland, VERA SMOLYANINOVA, BRADLEY YOST, DAVID LAHNEMAN, THOMAS GRESOCK, Towson University, EVGENII NARIMANOV, Purdue University — We demonstrate a novel artificial optical material, the photonic hyper-crystal, which combines the most interesting features of hyperbolic metamaterials and photonic crystals. Similar to hyperbolic metamaterials, photonic hyper-crystals exhibit broadband divergence in their photonic density of states due to the lack of usual diffraction limit on the photon wave vector. On the other hand, similar to photonic crystals, hyperbolic dispersion law of extraordinary photons is modulated by forbidden gaps near the boundaries of photonic Brillouin zones. Three dimensional self-assembly of photonic hyper-crystals has been achieved by application of external magnetic field to a cobalt nanoparticle-based ferrofluid. Unique spectral properties of photonic hyper-crystals lead to extreme sensitivity of the material to monolayer coatings of cobalt nanoparticles, which should find numerous applications in biological and chemical sensing.

\textsuperscript{1}This work was supported in part by NSF grant DMR-1104676, NSF Center for Photonic and Multiscale Nanomaterials, ARO MURI and Gordon and Berry Moore Foundation.

5:06PM W8.00014 Optical properties of self-induced plasma structures , ROTEM KUPFER, Department of Physics, The University of Texas at Austin, BORIS BARMASHENKO, ILANA BAR, Department of Physics, Ben Gurion University of the Negev — We show, using detailed particle-in-cell simulations and a simplified theoretical model, how to manipulate femtosecond laser produced plasma to form functional structures by using the interference pattern of two or more beams. Two examples will be presented: The use of Moiré pattern of two intersecting beams to create a waveguide array and plasma-made photonic crystal generated by two pairs of counter propagating beam. We will discuss the implications of this phenomenon to the prospect of plasma based lasers.

5:18PM W8.00015 Optical instabilities and spontaneous light emission in moving media\textsuperscript{1}, MARIO SILVERINHA, Univ de Coimbra - Instituto de Telecomunicacoes — We show that when an uncharged plasmatic material is set in relative motion with respect to another uncharged polarizable body the system may be electromagnetically unstable. Particularly, when the relative velocity of the two bodies is enforced to remain constant the system may support natural oscillations that grow exponentially with time, even in presence of realistic material loss and dispersion. It is proven that a friction-type force acts on the moving bodies to oppose their relative motion. Hence, the optical instabilities result from the conversion of kinetic energy into electromagnetic energy. This new purely classical phenomenon is analogous to the Cherenkov and Smith-Purcell effects but for uncharged polarizable matter. We link the optical instabilities to a spontaneous parity-time symmetry breaking of the system, and demonstrate the possibility of optical amplification of a light pulse in the broken parity-time symmetry regime.

\textsuperscript{1}This work is supported in part by Fundação para a Ciência e a Tecnologia grant number PTDC/EEI-TEL/2764/2012.

Thursday, March 5, 2015 2:30PM - 5:18PM – Session W10 DCMP: Topological Insulators: Optical and Other Properties (Theory) 007A - Bitan Roy, University of Maryland

2:30PM W10.00001 Skyrmion spin texture in ferromagnetic semiconductor-superconductor heterostructures , KRISTOFER BJÖRNSON, ANNICA BLACK-SCHAFFER, Uppsala Univ — Topological superconductors are of interest because they are predicted to host Majorana fermions. One example are two-dimensional ferromagnetic semiconductor-superconductor heterostructures, where Majorana fermions are predicted to appear in vortices. The system has previously been classified using a Chern number, but we show that the Chern number is related to a Skyrmion spin texture in the band structure. The Skyrmion spin texture has the advantage of enabling direct experimental measurements of the topological invariant through for example spin-polarized ARPES. The Skyrmion spin texture is also of interest from a conceptual point of view, as it provides a more intuitively accessible topological invariant than the otherwise rather abstract Chern number.
2:42PM W10.00002 Compressibility as a probe of topological quantum phase transitions in 1D systems\(^1\). DAVID NOZADZE, NANDINI TRIVEDI, Department of Physics, The Ohio State University, Columbus, OH 43210, USA — We investigate the behavior of the compressibility \(\kappa\) in the Kitaev chain using the Bogoliubov-de Gennes approach. For a closed chain, we show that the topological phase transition is signaled by the divergence of \(\kappa\) at the quantum critical point tuned by the chemical potential. We also explore the effect of disorder on the local compressibility \(\kappa(x)\). In the presence of disorder the compressibility across the transition becomes finite and the height of the peak becomes smaller with increasing disorder strength. Our results provide a direct method, the local compressibility, for detecting the quantum phase transition in a Kitaev chain that can be realized in superconductor-semiconducting nanowire hybrid structures with strong spin-orbit coupling.

\(^1\)This work has been supported by NSF-DMR1309461

2:54PM W10.00003 Quantized Electromagnetic Response of Three Dimensional Chiral Topological Insulators\(^1\). SHENG-TAO WANG, DONG-LING DENG, Univ of Michigan - Ann Arbor, JOEL MOORE, University of California, Berkeley, KAI SUN, LUMING DUAN, Univ of Michigan - Ann Arbor — Protected by the chiral symmetry, three dimensional chiral topological insulators are characterized by an integer-valued topological invariant. How this invariant could be realized in practice is an important question. Here, we quantized response with ultracold atoms in optical lattices.

\(^1\)NBRPC (973 Program) 2011CBA00300 (2011CBA00302), the IARPA MUSIQC program, the ARO, the AFOSR MURI program, NSF DMR-1206515, the Simons Foundation, NSF under Grant No. PHY1402971 and the MCubed program at University of Michigan

3:06PM W10.00004 Charged skyrmions on the surface of a 3D topological insulator. HILARY HURST, DMITRY EFIMKIN, VICTOR GALITSKI, Condensed Matter Theory Center, University of Maryland College Park — We consider the interplay between magnetic skyrmions in an insulating thin film and the Dirac surface states of a 3D topological insulator (TI), coupled by proximity effect. The nontrivial magnetic texture of skyrmions can lead to confinement of Dirac states at the skyrmion radius, where out of plane magnetization vanishes. This confinement results in charging of the skyrmion. We find that the bound states are robust in an external magnetic field, which is needed to stabilize skyrmions. It is expected that for reasonable experimental parameters skyrmions will have a small number of bound states that can be tuned using an external magnetic field. We argue that these charged skyrmions can be manipulated directly by an electric field, with skyrmion mobility proportional to the number of bound states at the skyrmion radius. Coupling skyrmionic thin films to a TI surface can provide a more direct and efficient way of controlling skyrmion motion in insulating materials.

3:18PM W10.00005 Braiding statistics of loop excitations in three dimensions\(^1\). CHENJIE WANG, MICHAEL LEVIN, University of Chicago — While it is well known that three dimensional quantum many-body systems can support non-trivial braiding statistics between particle-like and loop-like excitations, or between two loop-like excitations, we argue that a more fundamental quantity is the statistical phase associated with braiding two loops. The physical picture leads to a “natural” bulk dynamic topological quantum field theory (TQFT) description for the braiding of two loops, which is based on the loop statistics. The braiding phase is a universal quantity which can be measured in experiments. We also study the three-loop braiding statistics in the context of a topological field theory.

\(^1\)This work is supported by the Alfred P. Sloan foundation and NSF under grant No. DMR-1254721.

3:30PM W10.00006 Vortex-line condensation in three dimensions: A physical mechanism of bosonic topological insulators\(^1\). PENG YE, ZHENG-CHENG GU, Perimeter Inst for Theo Phys — 3d bosonic topological insulators (BTI) are symmetry protected topological(SPT) phases with U(1) and \(Z_N^2\) (time-reversal symmetry with \(T^2=1\)). BTI were first proposed based on the group cohomology theory which suggests two distinct root states. Soon after, surface anomalous topological orders were proposed to identify different root phases and also leads to a new root state beyond group cohomology. Nevertheless, it is still unclear what is the universal physical mechanism for BTI phases. In this work, we answer the question by proposing an universal physical mechanism via vortex-line condensation in a superfluid, e.g., helium-4 or cold atoms in optical lattices. Using such a simple physical picture, we find three root phases, of which two of them are classified by group cohomology theory while the other is beyond group cohomology classification. The physical picture also leads to a “natural” bulk dynamic topological quantum field theory (TQFT) description for BTI and gives rise to a physical pathway of practical realization. Finally, we generalize the vortex-line condensation picture to other symmetries and find that in three dimensions, even for a unitary \(Z_2\) symmetry, there is a nontrivial \(Z_2\) SPT phase beyond the group cohomology classification.

\(^1\)Research at Perimeter Institute is supported by the Government of Canada through Industry Canada and by the Province of Ontario through the Ministry of Economic Development and Innovation.

3:42PM W10.00007 Topological BF theory of the quantum hydrodynamics of incompressible polar fluids. APOORV TIWARI, XIAO CHEN, University of Illinois, Urbana Champaign, TITUS NEUPERT, Princeton Center for Theoretical Science, Princeton University, LUIZ SANTOS, Perimeter Institute for Theoretical Physics, Waterloo, Canada, SHINSEI RYU, University of Illinois at Urbana-Champaign, CLAUDIO CHAMON, Physics Department, Boston University, Boston, CHRISTOPHER MUDRY, Condensed Matter Theory Group, Paul Scherrer Institute, Villigen, Switzerland — We analyze a hydrodynamical model of a fluid in (3+1)-dimensional spacetime. We explore a spacetime symmetry — volume preserving diffeomorphisms — to construct an effective description of this fluid in terms of a topological BF theory. The two degrees of freedom of the BF theory are associated to the mass (charge) flows of the fluid and its polarization vorticities. We discuss the quantization of this hydrodynamic theory, which generically allows for fractionalized excitations. We propose an extension of the Girvin-MacDonald-Platzman algebra to (3+1)-dimensional spacetime by the inclusion of the vortex-density operator in addition to the usual charge density operator and show that the same algebra is obeyed by massive Dirac fermions that represent the bulk of \(Z_2\) topological insulators in three-dimensional space.
3:54PM W10.00008 Berry phase and Rashba fields in realistic semiconductor quantum rings under tilted magnetic field1. VIVALDO LOPES-OLIVEIRA, VICTOR LOPEZ-RICHARD, Univ Fed de Sao Carlos, SERGIO EDUARDO ULOA, Ohio University, OPTICAL, VIBRATIONAL, SPIN AND TRANSPORT PROPERTIES IN SEMICONDUCTOR NANOSTRUCTURES COLLABORATION, DEPARTMENT OF PHYSICS AND ASTRONOMY COLLABORATION — The geometric Berry phase has been experimentally measured and manipulated in InGaAs-based mesoscopic rings, as seen from magnetotransport data [1]. Motivated by these experiments, we present here an analysis of the influence of the magnetic field orientation and intensity on the Berry phase experienced by electrons in a realistic quantum ring structure (similar model has been used in ref. [2]). We use the $k\cdot p$ formalism and fully incorporate the effects of confinement asymmetry, as well as the resulting Rashba spin-orbit-coupling (SOC) fields within the same framework. We obtain spin maps for angle and magnetic field intensities for different levels. At the anticrossing regions, with strong level mixing produced by varying flux dependence, we observe pronounced asymmetry effects in the shape and character of excited states. The asymmetry plays an important role in determining the Berry phase of the different states. We also find that effects of varying magnetic field tilt and intensity, as well as SOC, are more pronounced in the ground state. The substantial phase modulation observed in the lower energy level manifold can be monitored and exploited in transport experiments. [1] F. Nagasawa et al. Nat. Comm. 4, 2526 (2013); [2] V. Lopes-Oliveira et al. PRB 90, 125315 (2014).

1Supported by CAPES-Brazil and MWN/CIAM-NSF

4:06PM W10.00009 Uhlmann Measure in Topological Insulators and Superconductors at Finite Temperature, OSCAR VIYUELA, ANGEL RIVAS, MIGUEL ANGEL MARTIN-DELGADO, Univ Complutense — I will introduce the Uhlmann geometric phase as a tool to characterise density matrices of 1D and 2D topological insulators and superconductors. We achieve this goal by constructing new topological invariants called Topological Uhlmann numbers. Since this phase is formulated for general mixed quantum states, it provides a way to extend topological properties to finite temperature situations. New effects appear such as the existence of critical temperatures, novel thermal-topological transitions in models with high Chern numbers, breakdown of the usual bulk-edge correspondence, etc. Moreover, as the Uhlmann phase is an observable itself, we analyse potential measurement schemes that could be applicable to current experimental setups like cold atoms in optical lattices.


4:18PM W10.00010 Equilibrium currents in chiral systems with nonzero Chern number, OLEG STARYKH, EUGENE MISHCHENKO, University of Utah — We describe a simple quantum-mechanical approach to calculating equilibrium particle current along the edge of a system with nontrivial band spectrum topology. The approach does not require any a priori knowledge of the band topology and, as a matter of fact, treats topological and nontopological contributions to the edge currents on the same footing. We illustrate its usefulness by demonstrating the existence of “topologically nontrivial” particle currents along the edges of three different physical systems: two-dimensional electron gas with spin-orbit coupling and Zeeman magnetic field, surface state of a topological insulator, and kagome antiferromagnet with Dzyaloshinskii-Moriya interaction.

4:30PM W10.00011 Surface plasmon polaritons in topological insulators, JUNJIE QI, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, HAIWEN LIU, X.C. XIE, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China — We study surface plasmon polaritons on a topological insulator-vacuum interface. When the time-reversal symmetry is broken due to ferromagnetic coupling, the surface states exhibit a magneto-optical Kerr effect. This effect gives rise to a novel transverse-type surface plasmon polariton, within the same framework. We obtain spin maps for angle and magnetic field intensities for different levels. At the anticrossing regions, with strong level mixing produced by varying flux dependence, we observe pronounced asymmetry effects in the shape and character of excited states. The asymmetry plays an important role in determining the Berry phase of the different states. We also find that effects of varying magnetic field tilt and intensity, as well as SOC, are more pronounced in the ground state. The substantial phase modulation observed in the lower energy level manifold can be monitored and exploited in transport experiments. [1] F. Nagasawa et al. Nat. Comm. 4, 2526 (2013); [2] V. Lopes-Oliveira et al. PRB 90, 125315 (2014).

4:42PM W10.00012 Giant Faraday effect due to Pauli exclusion principle in 3D topological insulators, HARI PAUDEL, MICHAEL LEUENBERGER, Univ of Central Florida — Experiments using ARPES, which is based on the photoelectric effect, have shown that the surface states in 3D topological insulators (TI) are gapless. Here we consider Weyl interface fermions due to band inversion in narrow-bandgap semiconductors, such as Pb$_{1-x}$Sn$_x$Te. We determine the optical selection rules of electron-hole pair excitation by means of the solutions of the 3D Dirac equation. We calculate explicitly the electric dipole matrix elements by means of bandstructure calculations for Pb$_{1-x}$Sn$_x$Te. Using the 3D Dirac equation and bandstructure calculations, we show that the transitions between positive and negative energy solutions, giving rise to electron–hole pairs, obey strict optical selection rules. We apply our results to calculate the Faraday effect due to the Pauli exclusion principle in a pump–probe setup using a 3D TI double interface of a PbTe/Pb$_{0.31}$Sn$_{0.69}$Te/PbTe heterostructure. The Faraday rotation angle exhibits oscillations as a function of probe wavelength and thickness of the heterostructure. The maxima in the Faraday rotation angle are of the order of mrad.

4:54PM W10.00013 Effect of electron-phonon interaction on the finite frequency conductivity of 3D Dirac materials, BORIS PAULOVIC, ELISABETH J. NICOL, University of Guelph, Canada — Recently, interest has been directed toward identifying and characterizing materials with 3D Dirac energy dispersions. We present our theoretical results for the finite frequency optical conductivity of 3D Dirac materials with the inclusion of an electron-phonon (e-p) interaction. Using a Holstein e-p interaction and allowing for varying chemical potential, we show how the e-p self energy modifies the electronic density of states and the optical conductivity. The results for 3D are contrasted with their 2D analogs, as previously discussed for graphene.[1][1] J.P. Carbotte, E.J. Nicol and S.G. Sharapov, PRB 81, 045419 (2010).

5:06PM W10.00014 Thermoelectric Effect in Topological Insulators, YONG XU, SHOU-CHENG ZHANG, Stanford University — Improving the thermoelectric figure of merit $zT$ is one of the greatest challenges in material science. The recent discovery of topological insulators (TIs) offers new promise in this prospect. In this talk, we demonstrate theoretically that $zT$ is strongly size dependent in TIs, and the size parameter can be tuned to enhance $zT$ to be significantly greater than 1. Furthermore, we show that the lifetime of the edge states in TIs is strongly energy dependent, leading to large and anomalous Seebeck effects with an opposite sign to the Hall effect. Some recent experimental progress will also be introduced.

Thursday, March 5, 2015 2:30PM - 5:06PM –
Session W11 DMP: Cuprates: Josephson Junctions 0078 - Mike Osofsky, Naval Research Laboratory
We find that for hole doping level $T\in$ cuprates and Fe-base compounds using scanning tunneling spectroscopy (STS) will discuss the extension of these techniques to study atomic scale variations in Josephson current. Present superconducting Pb tip measurements performed at temperatures below 250mK in a dilution refrigerator STM. By controlling the junction resistance, scanning Josephson spectroscopy measurements have the potential to characterize of a wide variety of superconducting materials on the atomic scale. I will present superconducting Pb tip measurements performed at temperatures below 250mK in a dilution refrigerator STM. By controlling the junction resistance, we are able to explore a wide range of tunneling regimes. Josephson measurements on Pb samples exhibit features multiple Andreev reflections, and I will discuss the extension of these techniques to study atomic scale variations in Josephson current.

2:42PM W11.00002 High-resolution Josephson spectroscopy with a scanning tunneling microscope, MALLIKA T. RANDERIA, BENJAMIN E. FELDMAN, ILYA K. DROZDOV, ALI YAZDANI; Princeton University — Conventional scanning tunneling microscopy (STM) measurements use a normal metal tip to probe local quasi-particle density of states with atomic resolution. Using a superconducting tip to conduct spectroscopy significantly boosts the energy resolution of the measurements, thus expanding the STM capabilities. Moreover, superconducting tips make it possible to probe superconductivity via the Josephson effect, which provides a direct measure of the local superconducting order parameter. Therefore, scanning Josephson spectroscopy measurements have the potential to characterize of a wide variety of superconducting materials on the atomic scale. I will present superconducting Pb tip measurements performed at temperatures below 250mK in a dilution refrigerator STM. By controlling the junction resistance, we are able to explore a wide range of tunneling regimes. Josephson measurements on Pb samples exhibit features multiple Andreev reflections, and I will discuss the extension of these techniques to study atomic scale variations in Josephson current.

2:54PM W11.00003 Studies of superconductivity (SC) and competing-order (CO) interplay in cuprates and Fe-base compounds using scanning tunneling spectroscopy (STS), M.L. TEAGUE, C.-C. CHEN, N.C. YEH, Dept. of Physics, Caltech, Pasadena, CA 91125, USA, Z.J. FENG, Dept. of Physics, Shanghai University, Shanghai, China — STS studies of $\text{YBa}_2\text{Cu}_4\text{O}_{7-\delta}$ ($\text{Y}-123$) and Ca-doped $\text{Y}-123$ from under- to over-doped regimes demonstrate that the origin of the pseudogap (PG) is due to competing orders (COs), and that the presence (absence) of PG above the SC transition $T_c$ is associated with a CO energy $\Delta_{\text{CO}}$ larger (smaller) than the SC gap $\Delta_{\text{SC}}$. We find that for hole doping level $p \leq 0.16$, $\Delta_{\text{CO}} > \Delta_{\text{SC}}$, whereas both $\Delta_{\text{SC}}$ and $\Delta_{\text{CO}}$ decrease with $p$ for $p > 0.16$, and $\Delta_{\text{CO}}$ ($\sim 10$ meV) $< \Delta_{\text{SC}}$ ($\sim 13$ meV) at $p \approx 0.23$. The CO wave-vectors $Q_{\text{SC}}$ and $Q_{\text{PDW}}$ along the Cu-O bond are determined from Fourier transformation of the STS as a function of $p$, and are found to occur at 1/3 and 2/3 of the reciprocal lattice constant (2$\pi/a$) for $p = 0.16$. The pairing symmetry also evolves from pure $d_{x^2-y^2}$ to $(d_{x^2-y^2} + s)$ for $p > 0.16$, where the $s$-wave component increases with $p$. Moreover, under a finite magnetic field the ratio of the vortex “halo” radius ($\xi_{\text{halo}}$) relative to the SC coherence length $\xi_{\text{SC}}$ decreases with $p$, from $\sim 8$ for $p = 0.16$ to $\sim 3$ for $p = 0.216$, suggesting PG contributions to the vortex halo. Magnetic resonance mode at $\Omega_0 \sim 2\Delta_{\text{SC}}$ is also observed as a function of $p$. Finally, we present comparative STS studies of Fe-based superconductors, including $\text{Fe}_1-x\text{Co}_x\text{Se}_2$ and $\text{Rb}_{0.8}\text{Fe}_1\text{Se}_2$. This work was supported by NSF.

3:06PM W11.00004 Interpretation of scanning tunneling quasiparticle interference and impurity states, ANDREAS KREISEL, Niels Bohr Institute, Denmark, P. CHOUBEY, University of Florida, USA, T. BERLIJN, Oak Ridge National Laboratory, USA, B.M. ANDERSEN, Niels Bohr Institute, Denmark, P.J. HIRSCHFELD, University of Florida, USA — We use a simple method of calculating inhomogeneous, atomic-scale phenomena in superconductors to obtain real-space conductance maps as measured in scanning tunneling spectroscopy (STM). Our approach makes use of first principles Wannier functions in conjunction with self-consistent solutions of the Bogoliubov-de Gennes equations on a lattice to image superconducting phenomena. This method is a powerful tool since it captures correctly local symmetries on the surface that can be lower than the global lattice symmetry; it improves the spatial resolution from one pixel per lattice point to the sub-atomic scale; and simplifies the interpretation of STM data. As an example, we show how the pattern observed around a Zn impurity in Bi-2201 can be understood by accounting for the tails of the Cu Wannier functions, and thus compare perfectly to experimental findings. Further applications of this method include the investigation of impurity states in multiorbital systems as well as the study of quasi particle interference phenomena to enable a better understanding of novel phenomena in high temperature superconductors.

3:18PM W11.00005 Relaxation Oscillations in Josephson STM Junctions at mK Temperatures, MICHAEL DREYER, ANITA ROYCHOWDHURY, RAMI DANA, WANTING LI, SHU-CHU LIAO, University of Maryland — Small Josephson junctions can exhibit relaxation oscillations between the superconducting and normal state. The switching time depends on the charging time of the junction capacitance and the R-L time constant of the electrical connections, usually in the $\mu$s range. We observed similar oscillations in the tunnel current between a Nb sample and a Nb tip in our STM operated at 30 mK. The oscillations occur in two forms, either of which is triggered by lowering the gap resistance. The first type occurs in voltage ranges where the I(V) curves show negative differential conductance, which in turn is caused by coupling to the electrical environment. The oscillations span only a fraction of the superconducting gap and run at maximum frequencies below 10 kHz. The possible existence of “minor” loops was already mentioned in the original article, though thought to be a result of an applied in plane magnetic field. The second type appears at lower gap resistances and affects the whole bias range. The frequency was too high to be determined by our current setup, and thus could be due to a conventional relaxation oscillation. Our results will be discussed in detail.

1P.C., A.K., and P.I.H. were supported by DOE DE-FG02-05ER46236, T.B. as a Wigner Fellow at the Oak Ridge National Laboratory, and B.M.A. and A.K. by Lundbeckfond fellowship (grant 9318).

2Splitly funded by NSF.
3:30PM W11.00006 Improved heat exhaust and the characteristics of the high $T_c$ superconducting terahertz emitter$^1$, T. KASHIWAGI, University of Tsukuba, T. YAMAMOTO, National Institute for Materials Science, T. KITAMURA, K. ASANUMA, T. YASUI, Y. SHIBANO, C. WATANABE, K. NAKADE, Y. SAIWAI, H. KUBO, K. SAKAMOTO, T. KATSURAGAWA, University of Tsukuba, M. TSUJIMOTO, Kyoto University, R. YOSHIZAKI, University of Tsukuba, H. MINAMI, Kyoto University, R.A. KLEMM, University of Central Florida, K. KADOWAKI, University of Tsukuba — In our previous study it is known that THz emitting efficiency improves greatly when the stand-alone type of mesa structure is used for the THz emitting device.$^2$ The principle reason for that lies in the heat removal from the mesa, in which a gigantic amount of heat is generated while the mesa is in the resistive state. Recently, we developed a new device structure based on the stand-alone type of mesa structure of Bi$_2$212 single crystal in order to make high exhaust of Joule heating. The results show that although the power is comparable and is not significantly increased, very wide the radiation frequencies ranging from 0.3 to 1.6 THz were obtained. We will discuss the details of the radiation characteristics of this one.$^3$

$^1$This study has been supported by CREST-JST. TK is also supported by the Matsuda grant and JST A-STEP. This work is in part performed in collaboration with Dr. Wai Kwok and his group in Argonne National Lab.

$^2$K. Kadowaki et al., Physica C 491, (2013) 2

3:42PM W11.00007 Comparison of luminescent and scanning laser thermal micro-imaging of self-heating in Bi$_2$Sr$_2$CaCu$_2$O$_8$ mesa THz sources$^1$, TIMOTHY BENSEMAN, ALEXEI KOSHELEV, VITALII VLASKO-VLASOV, YANG HAO, WAI-KWONG KWOK, ULRICH WELP, Argonne Natl Lab, COURTNEY KEISER, Northern Iowa University, BORIS GROSS, MATTHIAS LANGE, DIETER KOELLE, REINHOLD KLEINER, University of Tuebingen, KAZUO KADOWAKI, University of Tsukuba — Scanning laser thermal microscopy of stacked Bi$_2$Sr$_2$CaCu$_2$O$_8$ Josephson junction terahertz sources has revealed both electromagnetic cavity resonance modes and strongly non-uniform self-heating in these devices. However, this technique — in which a modulated laser beam is rastered across the surface of a device — excites a number of physical phenomena, and thus the resulting images can be difficult to interpret. Here we compare scanning laser images taken on Bi$_2$Sr$_2$CaCu$_2$O$_8$ mesa THz sources with micro-images collected via a thermoluminescent technique under identical conditions. The latter technique directly measures the device surface temperature, and we find excellent agreement with the scanning laser results, confirming that scanning laser thermal microscopy is indeed primarily probing device temperature.

$^1$This research was supported by the Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

3:54PM W11.00008 The stability of current filaments in Bi$_2$Sr$_2$CaCu$_2$O$_8$ observed via luminescent thermal microscopy$^1$, YANG HAO, TIMOTHY BENSEMAN, ALEXEI KOSHELEV, VITALII VLASKO-VLASOV, WAI-KWONG KWOK, ULRICH WELP, Argonne Natl Lab, COURTNEY KEISER, Northern Iowa University, BORIS GROSS, MATTHIAS LANGE, DIETER KOELLE, REINHOLD KLEINER, University of Tuebingen, KAZUO KADOWAKI, University of Tsukuba — Stacks of Intrinsic Josephson Junctions (IJJs) in Bi$_2$Sr$_2$CaCu$_2$O$_8$ (Bi-2212) designed as emitters of THz-radiation are prone to strong self-heating and thermal instability due to the poor thermal conductivity and semiconducting resistivity along the c-axis. Recent theory and experimental evidence indicate a possible correlation between strong self-heating and THz power emission. Here we study the temperature distribution in stacks of IJJs using current-voltage (I-V) characteristics and direct thermal imaging. At low bias currents and at low temperature, we observe the nucleation of small hot-spots near the corners or edges of the sample. These hot-spots carry 20-30% of the entire bias current thus forming current filaments. With increasing current and at elevated temperatures the size of the hot-spot increases and it moves to the center of the sample. These observations are in excellent agreement with theoretical analysis regarding the stability of current filaments.

$^1$This research was supported by the Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

4:06PM W11.00009 A role of temperature inhomogeneity and hot-spot formation on the THz emission from high-$T_c$ superconducting intrinsic Josephson junction mesa devices, CHIHARU WATANABE, HIDETOSHI MINAMI, TAKEO KITAMURA, KENTARO ASANUMA, KURAMA NAKADE, TAKAKI YASUI, YOSHIHIKO SAIWAI, YUKI SHIBANO, University of Tsukuba, TAKASHI YAMAMOTO, National Institute for Materials Science, TAKANARI KASHIWAGI, University of Tsukuba, RICHARD KLEMM, University of Central Florida, KAZUO KADOWAKI, University of Tsukuba — It is well known that the mesa device fabricated from single crystalline Bi$_2$Sr$_2$CaCu$_2$O$_8$ (Bi-2212) gets heated enormously and forms very inhomogeneous temperature distribution along the c-axis. Recent studies have revealed both electromagnetic cavity resonance modes and strongly non-uniform self-heating in these devices. However, this technique — in which a modulated laser beam is rastered across the surface of a device — excites a number of physical phenomena, and thus the resulting images can be difficult to interpret. Here we compare scanning laser images taken on Bi$_2$Sr$_2$CaCu$_2$O$_8$ mesa THz sources with micro-images collected via a thermoluminescent technique under identical conditions. The latter technique directly measures the device surface temperature, and we find excellent agreement with the scanning laser results, confirming that scanning laser thermal microscopy is indeed primarily probing device temperature.

4:18PM W11.00010 Nano-(Bi$_{0.7}$Pb$_{0.3}$)Sr$_2$Ca$_2$Cu$_3$O$_{10}$ crystals synthesis by sol-gel improved with acrylamide and microwaves, E. CHAVIRA, F. FLORES, UNAM, A. CONDE, CINVESTAV, H. MONTIEL, D. CABRERO, C. FLORES, O. NOVELO, A. TEJEDA, G. ZAVALA, UNAM, L. ALMEIDA, G.E. TORRES, FQUJAT — We obtain (Bi$_{1-y}$Pb$_y$)$_3$Sr$_2$Ca$_2$Cu$_3$O$_{10}$ nano-crystals by sol-gel improved with acrylamide and microwaves, not reported in the literature. TGA gives an idea of the reaction temperatures (200-550 °C) for the formation of binary, ternary and unknown materials. SEM and TEM shows morphology and crystal size 30-33 nm. We studied the thermodynamic and kinetic stability of the gel quenching, by varying the temperature and time according to a previous thermal analysis. Starting compounds (bismuth oxide, strontium carbonate, copper acetate, lead nitrate and calcium sulfate) were analyzed by XRD. By AFM we observed the dehydrated gel surface absorbed water from the environment. From the micrographs we measured the size of the fibers, grains and nano-crystals. We found at 560 °C Bi$_{1.4}$Pb$_{0.6}$Sr$_2$Ca$_2$Cu$_3$O$_{10}$ compound with tetragonal crystal structure, corresponding to the 2:2:2:3 compound, with $T_c$ 110 K. At 860 °C seen a shift of some reflections corresponding to two phases. Xerogel magnetic measurement shows antiferromagnetic behavior at 63 K.

4:30PM W11.00011 A Study on Nucleation, Crystallization Kinetics, Microstructure and Mechanical Properties of Ru-Bi Partial Substituted BSCCO Glass Ceramics, AHMET TOLGA TASCI, OZGUR OZTURK, TUGBA GOKCEN, Kastamonu University, SUKRU CAVDAR, HALUK KORALAY, Gazi University, ABDULKADIIR SENOL, Kastamonu University — This study deals with the effects of Ru-Bi partial substitutions on the thermal, structural and mechanical properties of Bi$_{0.8}$-xRu$_x$Pb$_{0.2}$Sr$_2$CaCu$_2$O$_{8+4}$ ($x$=0.0, 0.025, 0.050, 0.075), produced with glass-ceramics method have been investigated. The effects of Ru-Bi Partial substitutions on glass transition, nucleation and crystallization temperature are analyzed by differential thermal analyzer (DTA). Furthermore, micro-structure and micro-mechanical properties of Ru-Bi partial substituted BSCCO glass ceramics have been investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM) and Vickers micro-hardness measurements. From the DTA results, nucleation kinetics have been obtained by using Ozawa, Augis-Bennett, Takher and Kissinger equations. Also activation energies and Avrami parameters have been found. Oxidation amount is seen to be increased with increasing Ru concentration in consequence of thermogravimetric analyses results. Moreover, Lattice parameters, volume fractions and surface morphologies of the samples are obtained from XRD and SEM measurements, respectively.
4:42PM W11.00012 Oxygen Annealing in the Synthesis of the Electron-Doped Cuprates1, J. S. HIGGINS, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, Maryland, P. L. BACH, University of Santiago de Compostela, Spain, W. YU, Department of Physics, Renmin University of China, Beijing, China, B. D. WEAVER, Naval Research Laboratory, Washington, DC, R. L. GREENE, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, Maryland — Post-synthesis oxygen reduction (annealing) in the electron-doped, high-temperature superconducting cuprates is necessary for the establishment of superconductivity. It is not established what effect this reduction has microscopically on the lattice structure. Several mechanisms have been put forth as explanations; they range from disorder minimization1, antiferromagnetic suppression2, and copper migration3. Here we present an electronic transport study on electron-doped cuprate Pr2Cu3-xCxCuO4±δ (PCCO) thin films in an attempt to better understand the need for this post-synthesis process. Several different cerium doping concentrations of PCCO were grown. Within each doping, a series of films were grown with varying levels of oxygen concentration. As a measure of disorder on the properties of PCCO, several films were irradiated with various doses of 2 MeV protons. Analysis within each series, and among the different dopings, favors disorder minimization through the removal of apical oxygen as the explanation for the necessary post-synthesis annealing process. 1P. K. Kang, et al., Physical Review Letters, 93 (2):027002, 2004. 2P. Richard, et al., Physical Review B, 70 (6), 064513, 2004. 3Hy Jung Kang, et al., Nature Materials, 2007.

1Supported by NSF DMR 1104256

4:54PM W11.00013 Fabrication of Small Edge Josephson Junctions Between Sr2RuO4 and Al, BRIAN ZAKRZEWSKI, XINXIN CAI, YIQUN YING, Pennsylvania State Univ, DAVID FOBES, TIJIANG LIU, ZHIQIANG MAO, Tulane University, YING LIU, Pennsylvania State Univ — Sr2RuO4 is predicted to have a chiral p-wave orbital pairing. However, attempts to measure the chiral edge currents have yielded results inconsistent with theoretical predictions. Josephson junctions between Sr2RuO4 and an s-wave superconductor such as Al may provide an avenue for directly measuring the edge currents. We report progress on fabricating these junctions, using Al electrodes with no oxide barrier. The Josephson junctions are placed on the naturally formed edges of cleaved Sr2RuO4 thin crystal, which is expected to feature a surface less disordered than ramped junctions prepared by focused ion beam and ion mills. Transmission electron microscope studies provide a powerful tool to characterize the interface. We have systematically investigated the effects of nanofabrication processes on the quality of the junction interface. In particular, several post-lithography processes appear to cause irreversible damage to the surface layer of Sr2RuO4, which highlights potential issues for general small scale device fabrication. We also report preliminary measurements of Josephson tunneling from these devices.

Thursday, March 5, 2015 2:30PM - 5:18PM – Session W12 DCMP: Insulators: Synthesis and Experiment 007C - Ben White, University of California, San Diego

2:30PM W12.00001 ABSTRACT WITHDRAWN –

2:42PM W12.00002 Growth Mechanism of Pumpkin-Shaped Vaterite Hierarchical Structures1, GUOBIN MA, YIFEI XU, MU WANG, National Laboratory of Solid State Microstructures, and School of Physics, Nanjing University, Nanjing 210093 — CaCO3-based biominerals possess sophisticated hierarchical structures and promising mechanical properties. Recent researches imply that vaterite may play an important role in formation of CaCO3-based biominerals. However, as a less common polymorph of CaCO3, the growth mechanism of vaterite remains not very clear. Here we report the growth of a pumpkin-shaped vaterite hierarchical structure with a six-fold symmetrical axis and lamellar microstructure. We demonstrate that the growth is controlled by supersaturation and the intrinsic crystallographic anisotropy of vaterite. For the scenario of high supersaturation, the nucleation rate is higher than the lateral extension rate, favoring the “double-leaf” spherulitic growth. Meanwhile, nucleation occurs preferentially in <1120> as determined by the crystalline structure of vaterite, modulating the grown products with a hexagonal symmetry. The results are beneficial for an in-depth understanding of the biomineralization of CaCO3. The growth mechanism may also be applicable to interpret the formation of similar hierarchical structures of other materials.

1The authors gratefully acknowledge the financial support from National Science Foundation of China (Grant Nos. 51172104 and 50972057) and National Basic Research Program of China (Grant No. 2010CB630705).

2:54PM W12.00003 ABSTRACT WITHDRAWN –

3:06PM W12.00004 Athermal fading of luminescence in Al2O3 ceramic substrates, IAN TERRY, ETFYCHIA KOUROUKLA, IAN K. BAILIFF, University of Durham — Retrospective dosimetry aims to reconstruct ionising radiation dose to populations following a radiological incident using materials not designed for that purpose. Sintered alumina ceramic can function as a dosimeter with its luminescence properties and related trapped charge storage mechanism. Its widespread use as a substrate in surface mount devices and incorporation in devices such as mobile phones make it a ubiquitous potential dosimeter. We investigated the optically (OSL) and thermally (TL) stimulated luminescence properties of sintered alumina substrates. In contrast to their single crystal analogue developed for personal dosimetry, Al2O3:Cr, the substrates exhibit a significant loss of trapped charge (fading) within hours following irradiation at RT that seriously limits their utility for dosimetry over an extended timescale. The fading rates of OSL and TL signals of 0402 resistors were analysed under various storage conditions (time and temperature), complemented by a study of their microstructure. The results support a model of athermal loss of trapped charge due to electron tunnelling from trapping states; this contrasting behaviour is attributed to a physical modification of the trap environment arising from the manufacturing process.

3:18PM W12.00005 Ion Channeling study of Jahn-Teller lattice distortions and the phonon properties in magnetic transition element implanted SrTiO3 Crystals, KALYAN SASMAL, D. WIJESUNDERA, Y. HE, B. TILAKARATNE, Q. CHEN, J.H. MILLER, WEI-KAN CHU, Texas Center for Superconductivity & Physics at Univ of Houston — SrTiO3 is perovskite functional material. STO doped with magnetic transition element (Cr, Fe etc.) is important for electro- and magneto-optical applications. Cr4+ (d3), Cr5+ (d2) and Fe3+ (high-spin d5) substituting host Ti4+ exhibits Jahn-Teller distortion. Rutherford backscattering spectrometry (RBS) in ion channeling orientation is sensitive method for determining structure, position of impurity atom to study defects of crystals and provides direct evidence for JT effect at Cr4+, Cr5+ and Fe3+ centers in STO lattice. Different masses of STO elements helps to investigate such impurities using ICh method by determining distortions of sub lattices without taking into account of small ICh effect from impurities. Axial ion channeling of 2.0 MeV He ions was applied to study JT lattice distortions of ion implanted STO crystals. Angular ICh spectra of Sr and Ti sub lattices (crystal axes [110] & [100]) were obtained for pure and ion implanted STO crystals. The ratio of minima of ICh yield for Sr and Ti sub lattices was used for quantitative determination of lattice distortions observed in STO: Cr/Fe crystals due to presence of impurities. JT Cr4+ and Fe3+ impurity could induce Raman-active localized oxygen vibrational mode, which does not involve motion of nearest Fe or Ti ions.
3:30PM W12.00006 Rapid Microwave Synthesis of Perovskite Oxide Nanostructures with Enhanced Functionality

GREGORY SALAZAR, ANUJA DATTA, Florida Cluster for Advanced Smart Sensor Technologies and Department of Physics, University of South Florida, BRITTISH MUKHERJEE, Center for Integrated Functional Materials and Department of Physics, University of South Florida — Perovskite oxides are an important class of materials having high dielectric and piezoelectric coefficients, switchable ferroelectric (FE) polarization and interesting optical and electrical properties. Realization of functional devices based on classic perovskite oxides such as Pb(Zr0.52Ti0.48)O3 (PZT), and emerging Pb-free noncentrosymmetric (NCS) oxides, such as, ZnSnO3, ZnTiO3 and CaTiO3 have reinforced the investigation of these materials in multiple dimensions and length scales. However, large-scale synthesis and integration of ordered low-dimensional structures is a challenge, due to their complicated methodologies, high-cost and difficulties with phase stability. We discuss a generalized, cost-effective, rapid microwave synthesis route for size and shape selective nanostructure growth of these functional perovskite oxides on industrially viable flexible and hard substrates, stabilized by an enhanced ionic covalence. The rational synthesis approach allowed improved tunability of the size, shape, and orientation of the structures with improved electrical and FE properties. The facile fabrication route of these nanostructures may expand the outreach of probes for understanding the structure-property relationships in these hitherto unexplored and technologically important materials.

3:42PM W12.00007 Possible Phase Transition in H2O Ice Ih near 110 K

DAVID T. W. BUCKINGHAM, SUELI H. MASUNAGA, FORREST C. GILE, JOHN J. NEUMEIER, Montana State University — The thermal expansion of single-crystalline H2O ice Ih was measured with ~10^4 times greater relative resolution than has previously been done. Plots of the thermal expansion coefficient, µ, along the a- and c-axes reveal features which have never before been observed in thermal expansion measurements of H2O ice:

- A jump in µ of magnitude Δµ ≈ 10^{-5} K^{-1} in the temperature range 98–117 K along the c-axis, which appears to be a phase transition. No such transition is observed along the a-axis.

- Hysteresis of the transition temperature, Tc, of as much as 5 K for cooling rates from -5.0 to -0.1 K/min.

There is reason to believe this transition is the ferroelectric transition reported by Dengel et al. if so, the shift in Tc would result from the freezing-in of the H2O molecular configurations. We will discuss our own measurements of the dielectric constant in the vicinity of Tc.

This work is supported by NSF Award DMR-1204146.

3:54PM W12.00008 Raman and Luminescence Investigation of Rare Earth Doped Laser-Induced Crystals-in-Glass

BRIAN KNORR, Fairleigh Dickinson University, ADAM STONE, CEA Marcoule, HIMANSHU JAIN, VOLKMAR DIEROLF, Lehigh University — Laser induced crystallization of glasses is a highly spatially selective process which has the potential to produce compact, integrated optics within a glass matrix. In LaB6O7 low temperature Combined Excitation Emission Spectroscopy (CEES) revealed that erbium incorporates into both glass-ceramics and laser-induced crystals-in-glass in predominantly one type of environment (site). The energy levels of this site were quantified. The fluorescence characteristics of the erbium ions in any site in the laser-induced crystals were found to be only weakly influenced by the irradiation conditions during growth. On the other hand, a hidden parameter, potentially boron deficiency-related defects, resulted in a significant change in the incorporation behavior of the erbium ions. Scanning confocal Raman and fluorescence spectroscopy showed that the energies of the Raman modes are shifted and the erbium fluorescence intensity is inhomogeneously distributed, despite the host glass being homogeneously doped, across the cross-sections of laser-induced crystals in glass. These fluctuations within the Raman and fluorescence are spatially correlated, implying that different erbium sites form preferentially at different locations in the crystal cross-section.

This work is supported by NSF Award DMR-1204146.

4:06PM W12.00009 Brillouin light scattering as a probe for low frequency quasiparticles in solids

NIKITA KLIMOVICH, KEVIN OLSSON, KYONGMO AN, SEAN SULLIVAN, ANNIE WEATHERS, LI SHI, XIAOQIN LI, Univ of Texas, Austin — In increasingly small electronic and spintronic devices, electrons, optical phonons, acoustic phonons, and magnons are often driven out of local thermal equilibrium. Thermal transport based on equilibrium dynamics does not adequately describe these systems necessitating a better understanding of non-equilibrium transport processes. Measuring the specific temperatures of the different energy carriers is therefore crucial in understanding the thermal transport. Brillouin light scattering (BLS) has recently been explored as a temperature sensor for low frequency acoustic phonons in glass, and also magnons in metallic and insulating ferromagnetic materials. We report the measured BLS spectra of acoustic phonons in Silicon at different temperatures. The temperature dependence of the BLS peak frequency, linewidth, and integrated intensity are examined to evaluate their potential uses as temperature sensors of acoustic phonons. We also observe a large nonequilibrium in phonon-magnon temperature in YIG under the effects of laser heating and thereby extract a value for the phonon-magnon coupling coefficient.

This work is funded by the National Science Foundation and the Army Research Office.

4:18PM W12.00010 Model for Charge Injection with Electron Beams into Highly Disordered Insulating Materials

JOHN DENNISON, Utah State University, ALEC SIM, Irvine Valley College, GREG WILSON, Montana State University — The Walden-Wintle model for charge injection and transport through highly disordered insulating materials has been extended to include charge injection with a charged particle beam. The original model is applicable to charge injection in a dielectric material from a pair of electrodes in a parallel-plate geometry. It provides a versatile approach to predict the time-dependent current at a rear grounded electrode and the incident surface voltage, as the injection current density evolves over time with the development of a space charge barrier near the injection electrode. The Walden-Wintle model has been applied to many standard cases including Fowler-Nordheim injection, Schottky injection, space charge limited injection, and various tunneling mechanisms. The present model modifies the approach to include electrode-less charge injection via a charged particle beam, along with concomitant effects for the injection current, surface voltage, and electron emission as a charge is built up in the insulator. The approach is equally valid for near-surface injection and for bulk injection of both non-penetrating and penetrating radiation. The results are based on our dynamic emission model for electron emission yields dependent on accumulating charge in both the positive and negative charging regimes.

Supported through funds from NASA GSFC and a Senior Fellowship from the National Research Council and AFRL.
4:30PM W12.00011 Plasmon Polariton Modes in High Index Dielectric Structures, KODIAK MURPHY, KYLE HOKE, BRAD JOHNSON, JANELLE Leger, Western Washington University — The need to interface optical signals with high density electronic devices has led to an interest in subwavelength waveguides. Surface plasmon polaritons (SPPs) are surface charge density oscillations localized to a metal/dielectric interface, and as such are capable of confining energy in a structure which is not diffraction limited. Waveguides based on the excitation of SPPs are promising for short-range application, but in these structures Ohmic damping limits propagation length due to the bulk of the electric field propagating along a metal interface. Here we show that by selecting a core dielectric with a higher refractive index than the substrate, high index dielectric plasmon polariton modes (HP-PPMs) can be supported. Modes in the core dielectric exhibit electric fields with the bulk of their electric field confined in the dielectric layer. Therefore, damping may be reduced in such structures. Here we report the demonstration of HP-PPM in Au/TiO2/Au MIM devices using attenuated total reflectance. Characterization of these modes was performed for devices of differing core dielectric thickness. Results are in good agreement with theory. We will discuss the application of these waveguides to several technologies related to solar energy conversion.

4:42PM W12.00012 Optical and vibrational properties of YBO$_3$:Eu$^{3+}$, Ce$^{3+}$, Tb$^{3+}$ microstructures for light emitting diodes, SANDEEP SOHAL, Texas Tech University, MOHAMMAD NAZARI, Texas State University, X. ZHANG, E. HASSAN-ZADEH, V.V. KURYATKOV, J. CHAUDHURI, L. HOPE-WEEKS, JUYANG HUANG, Texas Tech University, MARK HOLTZ, Texas State University — Structural and optical properties of yttrium orthoborate YBO$_3$:Eu$^{3+}$, Ce$^{3+}$, Tb$^{3+}$ microstructures, focusing on the role of terbium concentration, are investigated by x-ray diffraction (XRD), photoluminescence (PL) ~ 363.8 nm excitation wavelength, photoluminescence excitation (PLE) and Raman spectroscopies. For constant cerium and europium concentrations, the PL bands belong to Ce$^{3+}$ and Tb$^{3+}$ color centers are diminished with increasing concentration of Tb$^{3+}$. Simultaneously, the intensities of PLE bands related to both Ce$^{3+}$ and Tb$^{3+}$ for red emission from the Eu$^{3+}$ are increased. The results are consistent with a Ce$^{3+}$$\rightarrow$ Tb$^{3+}$$\rightarrow$ Eu$^{3+}$ energy transfer scheme, where $n$ denotes a chain of terbium ions. Raman spectroscopy shows a systematic change, with Tb$^{3+}$ concentration, in the terminal oxygen bending mode of B$_2$O$_3$ ring structure related to the host lattice. The terminal oxygen atoms of the ring structure are coordinated to yttrium sites where dopant ions substitute. The structural changes are interpreted as variations in the local neighborhood of these sites in the YBO$_3$:Ce$^{3+}$, Tb$^{3+}$, Eu$^{3+}$ crystal structure.

4:54PM W12.00013 Scintillation properties of polycrystalline La$_x$Y$_{1-x}$O$_3$ ceramic, SUNIL SAHI, WEI CHEN, RASOOL KENARANGUI, Univ of Texas, Arlington — Scintillators are the material that absorbs the high-energy photons and emits visible photons. Scintillators are commonly used in radiation detector for security, medical imaging, industrial applications and high energy physics research. Two main types of scintillators are inorganic single crystals and organic (plastic or liquid) scintillators. Inorganic single crystals are expensive and difficult to grow in desirable shape and size. Also, some efficient inorganic scintillator such as NaI and CsI are not environmentally friendly. But on the other hand, organic scintillators have low density and hence poor resolution which limits their use in gamma spectroscopy. Polycrystalline ceramics can be an effective alternative to expensive inorganic single crystal scintillators. Here we have fabricated La$_{0.2}$Y$_{0.8}$O$_3$ ceramic scintillator and studied their luminescence and scintillation properties. Ceramic scintillators were fabricated by vacuum sintering of La$_{0.2}$Y$_{0.8}$O$_3$ nanoparticles at temperature below the melting point. La$_{0.2}$Y$_{0.8}$O$_3$ ceramic were characterized structurally using XRD and TEM. Photoluminescence and radioluminescence studies were done using UV and X-ray as an excitation source. We have used gamma isotopes with different energy to study the scintillation properties of La$_{0.2}$Y$_{0.8}$O$_3$ scintillator. Preliminary studies of La$_{0.2}$Y$_{0.8}$O$_3$ scintillator shows promising result with energy resolution comparable to that of NaI and CsI.

5:06PM W12.00014 Prediction of Silicon-Based Layered Structures for Optoelectronic Applications, WEI LUO, Fudan Univ, YANNING MA, JiJin Univ, XINGAO GONG, HONGJUN XIANG, Fudan Univ, CCMG TEAM — A method based on the particle swarm optimization (PSO) algorithm is presented to design quasi-two-dimensional (Q2D) materials. With this development, various single-layer and bilayer materials in C, Si, Ge, Sn, and Pb were predicted. A new Si bi-layer structure is found to have a much-favored energy than the previously widely accepted Si monolayer. The Si monolayer has an insulating gap of 5.25 eV and the Si nanolayer has an insulating gap of 4.75 eV, limiting their usages in optoelectronic applications. Hydrogenation has therefore been used to tune the electronic and optical properties of Si layers. We discover two hydrogenated materials of layered Si materials, WEI LUO, Fudan Univ, YANMING MA, Jilin Univ, XINGAO GONG, HONGJUN XIANG, Fudan Univ, CCMG TEAM — A method based on the particle swarm optimization (PSO) algorithm is presented to design quasi-two-dimensional (Q2D) materials. With this development, various single-layer and bilayer materials in C, Si, Ge, Sn, and Pb were predicted. A new Si bi-layer structure is found to have a much-favored energy than the previously widely accepted Si monolayer. The Si monolayer has an insulating gap of 5.25 eV and the Si nanolayer has an insulating gap of 4.75 eV, limiting their usages in optoelectronic applications. Hydrogenation has therefore been used to tune the electronic and optical properties of Si layers. We discover two hydrogenated materials of layered Si materials.

Thursday, March 5, 2015 2:30PM - 5:30PM — Session W13 Focus Session: Manganite Thin Films and Interfaces 007D - Ganesh Panchapakesan, Oak Ridge National Laboratory

2:30PM W13.00001 Emergent Magnetic Phenomena at Manganite Interfaces, YURI SUZUKI, Stanford University — Emergent phenomena at transition metal oxide interfaces have been the focus of recent intense study since the discovery of metallic at the interface of LaAlO$_3$ and SrTiO$_3$ a decade ago. Emergent magnetic phenomena at transition metal oxide interfaces had been studied even earlier. However there have been surprisingly few systems demonstrating interfacial ferromagnetism especially combined with metallicity. Recently, we have developed a general picture describing the origin of interfacial ferromagnetism in CaMnO$_3$ based systems. Density functional theory attributed the interfacial ferromagnetism to a double exchange interaction among interfacial Mn ions (just in the single unit cell of CaMnO$_3$) mediated by conduction electrons from the neighboring itinerant layer. We have demonstrated interfacial ferromagnetism in superlattices composed of the antiferromagnetic insulator CaMnO$_3$ and an itinerant metal (CaRuO$_3$ or LaNiO$_3$). Through polarized neutron spectrometry, x-ray magnetic circular dichroism and bulk magnetometry, we have shown that the ferromagnetism originates from Mn ions in a single unit cell of the CaMnO$_3$:t at the interfaces as theoretically predicted. The modulation of interfacial ferromagnetic moment as a function of constituent layer thicknesses as well as long-range antiferromagnetic correlations in the CaMnO$_3$, observed by neutron diffraction, are indicative of the competing magnetic interactions at play.

3:06PM W13.00002 Thickness effect on magnetic and electronic response in phase separated manganese thin films, HYOUNG JEEN JEEN$^1$, Department of Physics, Pusan National University, S. Korea, AMLAN BISWAS, Department of Physics, University of Florida — Thickness variation can be used to observe confinement effects and to control the strain state of thin films. Such confinement and strain state variation often creates unconventional physical properties in thin films of complex oxides such as phase separated (La$_x$(Sr$_{1-x}$)Sr$_y$Ca$_{y-1}$)$_3$MnO$_7$. Because of the observed magnetic and electronic properties, a thin film of LPCMO shows different from bulk samples such as, in-plane magnetic anisotropy and strain-driven anisotropic dynamic percolation. In this presentation, we will show the relation between lattice strain and the formation of an antiferromagnetic charge ordered insulating phase and the effect of strain relaxation on the magnetic anisotropy and single domain to multi-domain transition in electronically phase separated LPCMO thin films. We observed an increase in residual resistivity, a reduction of in-plane magnetic anisotropy, and an increase of the domain transition temperature as the thickness of the thin films is increased.

$^1$NSF DMR 1410237
$^2$Department of Physics, University of Florida
**3:18PM W13.00003 First-principles study of magnetic electronic and optical properties of double perovskite Bi$_2$FeMnO$_6$**

TOWFIQ AHMED, DZMITRY YAROTSKI, QUANXI JIA, JIAN-XIN ZHU, Los Alamos Natl Lab — We study magnetic, electronic and optical properties of double perovskite Bi$_2$FeMnO$_6$ (BFMO) using density functional theory. In these systems, the exchange interaction between Fe and Mn sites gives rise to a ferromagnetic ordering, which is captured in our ab initio calculations. Thin film Bi$_2$FeMnO$_6$ (BFMO) are generally grown on substrates such as SrTiO$_3$ and Si. Significant strain has been experimentally observed in BFMO unit cells due to slight lattice mismatch between the thin film and substrate unit cells. In this work, we find that the net magnetic moment in BFMO depends on the “c”/“a” ratio of the unit cell, suggesting the strain dependence of magnetization in such system. We further calculate x-ray magnetic dichroism (XMCD) signals of Fe and Mn ions in BFMO for L2 and L3 edges. By applying the XMCD sum rules, we adopted an alternative approach to estimate the spin and orbital magnetic moment from our DFT calculations.

**3:30PM W13.00004 Pressure-induced modification of colossal magnetoresistive magnanites**

PETRO MAKSYMOWYCH, S. KELLY, R. VASUDEVAN, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, E. ELISEEV, Institute for Problems of Materials Sciences, National Academy of Science of Ukraine, A. MOROZOVSKA, Institute of Physics, National Academy of Science of Ukraine, M.D. BIEGALSKI, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, J.F. MITCHELL, H. ZHENG, Materials Science Division, Argonne National Laboratory, J. AARTS, Leiden Institute of Physics, Leiden University, Netherlands, S.V. KALININ, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — Nanoscale chemical control of oxides using confined fields, conceptually similar to electrical switching of ferroelectrics, is not obvious. We investigated CMR manganites using UHV force microscopy and tunneling microscopy. Scanning the surface with a metal tip was found to create a strongly insulating state, at least a few nm deep, even at zero applied bias. The state could be due to charge order, polaron disorder, chemical disorder or a combination thereof. Based on concomitant changes of surface potential we propose that contact-pressure modifies electrochemical potential of oxygen vacancies via the Vegard effect, causing vacancy motion and changes of electronic properties. Given broad similarities in defect chemistry, mechanical control of oxides may be universal. (MD) supported by Center for Nanophase Materials Sciences, a DOE Office of Science User Facility. (PM, SVK, RV, JFM, HZ) supported by U.S. DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering. [1] Nanotechnology 25 (2014) 475302.

**3:42PM W13.00005 Ferroelectric control of spin injection in La0.7Sr0.3MnO3/BaTiO3/La0.5Ca0.5MnO3 multiferroic tunnel junctions with a bilayer barrier**

YUEWEI YIN, L.D. MIAO, R.Z. DU, Q. LI, Pennsylvania State Univ — Using a ferroelectric (FE) barrier with ferromagnetic electrodes has become a promising method for controlling spin injection by purely electrical means, which is an important challenge in spintronics. Recently, we have designed a La0.7Sr0.3MnO3/LSMO /BaTiO3/BTO /La0.5Ca0.5MnO3/LCMO /LSMO tunnel junctions in which the reversal of FE polarization of BTO will magnetoelectrically lead to a FM metallic - antiferromagnetic insulating phase transition in LCMO and result in an enhanced tunneling electromagnetoresistance (TER). [1] Using the bilayer barrier, we observed that the spin injection can be controlled by barrier polarization reversal as shown in the change of tunneling magnetoresistance (TMR). The temperature evolution of tunnel electromagnetoresistance (TEMR) (percentage ratio between the TMR values for the two polarization states), which is directly proportional to the change of tunnel-current spin polarization, was studied and larger TEMR was obtained with increasing temperature. Meanwhile, TEMR increases with TER effect for samples with different LCMO insertion thicknesses, suggesting a controllable strong electric control of tunnel-current spin polarization using a designed structure with proper interfaces. [1] Y. W. Yin et al, Nat. Mater. 12, 397 (2013)

**3:54PM W13.00006 Oxygen Pressure during Deposition on Atomic-Scale Surface Features of La$_{0.75}$Ca$_{0.25}$MnO$_3$ Films**

A. TSELEV, R.K. VASUDEVAN, ORNL, Oak Ridge, TN, USA, A. GIANFRANCESCO, ORNL/University of Tennessee Knoxville, TN, USA, L. QIAO, P. GANESH, T.L. MEYER, H.-N. LEE, M.D. BIEGALSKI, A.P. BADDORF, S.V. KALININ, ORNL, Oak Ridge, TN, USA — We have used in situ scanning tunneling microscopy to visualize atomic-scale surface structure of a mixed-valence manganite La$_{0.75}$Ca$_{0.25}$MnO$_3$ films grown by pulsed laser deposition. Surface termination and chemical composition were identified in situ with angle-resolved x-ray photoelectron spectroscopy. We find a strong effect of the background oxygen pressure during deposition on structural and chemical features of the film surface. Deposition at 50 mTorr leads to mixed-terminated films with atomic-scale structurally imperfect B-site (MnO$_6$)$_2$ termination. A small reduction of the pressure from 50 mTorr to 20 mTorr results in a dramatic change of the atomic-scale surface structure. The surface is dominated by nearly perfectly ordered B-site (MnO$_6$)$_2$ states. However, this was accompanied by surface roughening at a mesoscopic length scale with formation of mound-like structures. These results can be interpreted as a strong influence of oxygen on the adatom mobility during growth. The effect of the oxygen pressure on dopant surface segregation is also noticeable: Ca surface segregation is reduced with decrease of the oxygen pressure.

**4:06PM W13.00007 Trends in (LaMnO$_{3n}$/SrTiO$_3$)$_m$ superlattices with varying layer thicknesses**

JILI LIU, JIUER FABRIZIO COSSIL, UDO SCHWINGENSCHLOGL, KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia — We investigate the thickness dependence of the structural, electronic, and magnetic properties of (LaMnO$_{3n}$/SrTiO$_3$)$_m$ (n = 2, 4, 6, 8) superlattices using density functional theory. The structure relaxation turns out to be highly sensitive to the onsite Coulomb interactions. In contrast to bulk SrTiO$_3$, strongly distorted O octahedra are observed in the SrTiO$_3$ layers with a systematic off centering of the Ti atoms. The systems favour ferromagnetic spin ordering rather than the antiferromagnetic spin ordering of bulk LaMnO$_3$, and all show half-metallicity, while a systematic reduction of the minority spin band gaps as a function of the LaMnO$_3$ and SrTiO$_3$ layer thicknesses originates from modifications of the Ti d$_{xy}$ states.

**4:18PM W13.00008 Variational calculations for spin canting at ferromagnetic/antiferromagnetic interfaces**

G. RICHARD, Department of Physics and Astronomy, James Madison University, J.-X. ZHU, Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, A.V. BALATSKY, Institute for Materials Science, Los Alamos National Laboratory, J.T. HARALDSEN, Department of Physics and Astronomy, James Madison University — Understanding the complex interaction between materials is critical for the development of spintronic and electronic devices in the technology industry. In this report, we examine the canting of local moments throughout a ferromagnetic/antiferromagnetic heterostructure, where a combination of interlayer mixing and orbital reconstruction can be described as a local exchange field at the interface. Using a variational method and semi-classical approach, we examine the canting of spins throughout the full multilayer heterostructure. We approximate the interlayer interactions as an effective field throughout the interface and apply a standard spin Hamiltonian with spin anisotropy for the intralayer interactions of the ferromagnetic and antiferromagnetic layers. Overall, we show that observed finite magnetization and rotation of the local moment observed in LSMO/BFO is due to the interface interactions. Furthermore, we predict a size limit for this effect in the antiferromagnetic (BFO) layer.
4:30PM W13.00009 Phase separation in strained ultrathin La$_{0.67}$Sr$_{0.33}$MnO$_3$/SrTiO$_3(100)$ films

IN HAE KWAK, SARAH TOTH, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, FL 32611 — Atomically smooth and ultrathin La$_{0.67}$Sr$_{0.33}$MnO$_3$ (LSMO) films were grown on TiO$_2$ terminated SrTiO$_3$(100) (STO) substrates using pulsed laser deposition. The lattice mismatch between LSMO and STO generated uniform tensile strain on the LSMO film, and it significantly changed the electrical and magnetic properties of LSMO/STO thin films. Compared to the fully spin polarized ferromagnetic metallic state of bulk LSMO below a Curie temperature near 350 K, we observed a decrease in Curie temperature and the insulator to metal transition temperature as the thickness of LSMO was reduced down to 5 unit cells. Furthermore, the reduction of the saturation magnetization as the film thickness is reduced indicates phase separation in ultrathin LSMO/STO films. Therefore, it is possible to obtain a phase separated state close to room temperature in uniformly strained LSMO thin films.

1 NSF DMR-1410237

4:42PM W13.00010 Magnetic coercive field changes in microstructured (La$_{1-x}$Pr$_x$)$_{1-x}$Ca$_x$MnO$_3$ thin films

DANIEL GRANT, MICHAEL RYAN, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, FL 32611 — The hole-doped manganite (La$_{1-x}$Pr$_x$)$_{1-x}$Ca$_x$MnO$_3$ (LPCMO) shows effects such as phase coexistence and colossal magnetoresistance. Since the phase coexistence occurs at length scales of up to 10 micrometers, it is relatively straightforward to reduce the sample size to the scale of phase separation. We present magnetization data that show a change in the magnetic coercive fields of LPCMO thin films by a factor of about 2 when the sample size is reduced to 100 micrometers using a photolithography process. The amount of the increase of the coercive field increases with film thickness. We will discuss the increased coercive field in the context of the competition between shape and stress magnetic anisotropies. We will also describe the role of dimensionality in determining the coercive field behavior. This process can be used to control the phase separation and the magnetic hardness of manganites.

1 NSF DMR-1410237

4:54PM W13.00011 Effect of A-site ordering on the magnetoelectric properties in (111)-oriented LaMnO$_3$/SrMnO$_3$ superlattices

MINHUI HU, RUINAN SONG, JIANDONG GUO, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — It is expected that the chemical order that occurs over the crystallographic A-sites might strongly influence the distribution of the charges, magnetic and transport properties of the perovskite magnets. In this work, we focus on growing LaMnO$_3$/SrMnO$_3$ superlattices on (111)-oriented by PLD. The superlattices were characterized by magnetic as well as electronic transport measurements, and compared with the La$_2$/Sr$_1$/MnO$_3$ thin film having the same components in which the A-site dopants are randomly distributed. The superlattices had different properties from the thin film: higher Curie temperature of FM and metal-insulator transitions, larger magnetization, and lower resistivity. This will allow for an understanding of the dependence of the intrinsic properties with respect to the long-range ordering of dopants. These differences can be explained by Mn$^{3+}$/Mn$^{4+}$ double exchange separation arising from the artificially induced order of the A-site cations in the superlattices. Our proposed superlattices will allow for understanding of the fundamental magnetic and electronic interactions arising from dopant ordering in transition metal oxides.

5:06PM W13.00012 Large Relaxation (Polar distortion) of SrTiO$_3$ interfaced with La$_{2/3}$Sr$_{1/3}$MnO$_3$

ZHEN WANG, HANGWEN GUO, LINA CHEN, MOHAMMAD SAGHAYEZHIAN, E.W. PLUMMER, JIANDI ZHANG, Louisiana State Univ - Baton Rouge, JING TAO, LIJUN WU, HUOLIN XIN, YIMEI ZHU, Brookhaven National Laboratory — The physics of thickness-induced metal-insulator transition in metallic oxide thin films is very interesting. The question is the behavior intrinsic or extrinsic. We explore the origin of such transition by manipulating the thickness of La$_{2/3}$Sr$_{1/3}$MnO$_3$ (LSMO) thin film grown on SrTiO$_3$ (STO) substrate and detailed property measurements and structural characterization. We observed an unexpected structural relaxation in STO when interfaced with La$_{2/3}$Sr$_{1/3}$MnO$_3$ (LSMO) by using scanning transmission electron microscopy (STEM). A large out-of-plane polar distortion of STO extends up to 8 — 10 unit cell (u.c.) across the interface with the 4 u.c. insulating LSMO film, while only very moderate relaxation were found with thicker and metallic LSMO films. The energy loss electron spectrum (ELS) studies reveal that the charge transfer across the interface is similar in both films. The nature of such an overlayer-dependent structural relaxation will be discussed: Is this thickness dependent relaxation of the STO an inherent property of metallic/insulating properties of the ultrathin film?

Supported by U.S. DOE under Grant No. DOE DE-SC0002136.

5:18PM W13.00013 Interfacial intermixing in δ-doped oxide superlattices

VALENTINO R. COOPER, MSTD, Oak Ridge National Laboratory, HOULONG L. ZHUANG, P. GANESH, CNMS, Oak Ridge National Laboratory, HAIXUAN XU, Department of Materials Science and Engineering, The University of Tennessee, P. R. C. KENT, CNMS and CSMD, Oak Ridge National Laboratory — First principles studies of the interfaces between dissimilar insulating oxides have been fundamental in understanding both the origin of emergent interfacial phenomena and ways to control conduction pathways and charge carrier densities. However, these calculations often assume sharp interfaces; neglecting the effects of interfacial cation intermixing. Using density functional theory, we examine the effect of A-site interfacial intermixing on the stability and electronic structure of oxide δ-doped heterointerfaces. We find that the dominant effect of interfacial intermixing is the reduction in carrier densities of the 2DEG states at the interface. Our previous work suggest that this reduction in carrier density (i.e. fractional δ-doping) may lead to enhancements in electron mobilities. These results offer a plausible explanation for the deviations in carrier mobilities and densities measured in different experimental samples. Furthermore, our calculations show that intermixing above 1/4 concentration is unstable relative to a clean interface; thus having implications for large scale production, where experimental growth techniques, such as chemical vapor deposition, may be a viable alternative.

1 Support from LDRD of ORNL (VRC, HZ, PG, PRCK) and (HX) JDRD of UT and UT/ORNL JIAM. This research used resources of NERSC.

Thursday, March 5, 2015 2:30PM - 5:18PM
Session W15 DCMP: Glasses and Quasicrystals 008B - Erdal C. Oguz, Princeton University

2:30PM W15.00001 Correlation of Local Structure and Electronic Properties of Glass Materials

VINCENTO LORDI, NICOLE ADELSTEIN, Lawrence Livermore National Lab — Wide band gap glasses such as silica and its derivatives are typically considered insulators. However, electronic transport in glasses can be important for certain applications, such as when used as the host material for a scintillator radiation detector. Here we explore the relationship between local structure in glass materials and the corresponding electronic properties of carrier transport and charge trapping. We present a novel analysis that decomposes the distribution of localized band tail states in terms of specific local structural features in the glass. Comparison of the structure-related transport properties of different glass compositions is given, using silica and sodium silicate as prototypes.

1 Prepared by LLNL under Contract DE-AC52-07NA27344.
2:42PM W15.00002 Structural manifestations of aging in Se-rich glasses1. S. DASH, S. RAVINDREN, P. CHEN, P. BOOLCHAND, Univ of Cincinnati — We examine weakly cross-linked Ge-Se100-x (0%<x<7%) binary glasses in modulated DSC and Raman scattering experiments. Homogeneity of melts was carefully verified using FT-Raman line profiling. Upon aging at RT for 4 months, we find the width of the glass transition W(x) steadily decreasing from 10°C at 7% Ge to 2°C for pure Se. The 5-fold reduction of W(x) with a decrease of Ge content is accompanied by a 2-fold increase in the non-reversing enthalpy. Rejuvenation of the aged glasses changes W(x) from 15°C at 7% Ge to 7°C for pure Se. Tg is found to decrease upon rejuvenation with the difference (Tg(aged)-Tg(rejuv)) showing a maximum near 3% Ge and vanishing for pure Se and 6% of Ge, which are topological thresholds. These results in Se-rich glasses are consistent with aging induced decoupling of Se6 crowns and growth of extended range structural correlations between polymeric Sen chains due to lone pair interactions. At higher x, near 8-10% of Ge, eustetic effects are manifested.

1Work supported by NSF grant DMR 08-53957

2:54PM W15.00003 The effect of semiconducting CdSe and ZnSe nanoparticles on the fluorescence of Sm3+ in lead borate glasses. SAISUDHA MALLUR, STEPHEN FATOKUN, P.K. BABU, Western Illinois Univ — We studied the fluorescence spectra of Sm3+ doped lead borate glasses containing zinc selenide (ZnSe) and cadmium selenide (CdSe) nanoparticles with the following compositions (x PbO: 96.5-x B2O3:0.5 Sm2O3:3ZnSe/CdSe, x = 36.5 and 56.5 mol%). These glass samples are prepared using the melt-quenching technique. Each sample is annealed just below the glass transition temperature at 400°C for 3 hrs and 6 hrs. We have chosen PbO-B2O3 glasses to incorporate Sm3+ ions because they have large glass forming region, high refraction index, and good physical and thermal stability. Fluorescence spectra of these samples are obtained with the excitation wavelength at 477 nm. Four fluorescence transitions are observed at 563 nm, 598 nm, 646 nm and 708 nm. The transition at 646 nm is found to be a hypersensitive transition that strongly depends on the covalency of the Sm-O bond and the asymmetry of the crystal field at Sm site. The 646 nm/598 nm fluorescence intensity ratio has been studied for different annealing times and PbO concentration for both ZnSe and CdSe samples. The presence of CdSe nanoparticles is seen to produce the greatest influence on the fluorescence intensity ratio. This could be due to the size of the CdSe nanoparticles and covalency of the Sm-O bond.

3:06PM W15.00004 Topological phases in Ba-Borate glasses1. CHAD HOLBROOK, ANDREW CZAJA, PUNIT BOOLCHAND, University of Cincinnati — Twelve compositions in the (BaO)x(B2O3)100-x pseudo binary, in the 15%<x<40% range, were synthesized by induction melting Boric acid and anhydrous BaCO3, taking care to handle the materials in a dry ambient environment. Modulated-DSC and Raman scattering experiments were undertaken systematically as function of BaO content (x). Calorimetric measurements reveal Tg(x) to show a broad maximum and the non-reversing enthalpy to show a Gaussian-like reversibility window2, both centered near x = 28%. Raman scattering displays rich lineshapes with modes similar to those observed in Na-Borates3. Modes near 808 cm−1, 770 cm−1, 740 cm−1 and 705 cm−1 are observed, and identified with breathing modes of pure and mixed rings from characteristic structural groupings4. These preliminary results suggest that glasses at x<24% are in the stressed-rigid phase, in the 24%<x<30% in the Intermediate Phase and at x>30% in the flexible phase.

1 Supported by NSF grant DMR 08-53957

3:18PM W15.00005 Revealing Structural Details of SiCO Ceramics with GIPAW Calculations of Model Structures and Analysis of Experimental 29Si Nuclear Magnetic Resonance Spectroscopy. JOHN NIMMO, PETER KROLL, The University of Texas at Arlington — The occurrence of the various SiC04-x (1≤x≤4) mixed tetrahedra in silicon oxy carbide (SICO) is often quantified by means of experimental 29Si nuclear magnetic resonance. The structural centers are assigned to individual peaks in the spectrum, which can be integrated to give the relative populations. Using a recently-developed method, we show that this is also possible to recover information on the connectivity of these tetrahedra. By combining a huge library of model structures an GIPAW calculations, we show that simple relations exist between the Si-O-Si linking angles and the 29Si NMR chemical shift. In this work, we perform detailed analyses of SICO 29Si NMR spectra available in literature. We extract angular distributions in agreement with the experimental X-ray and neutron diffraction data. Furthermore, in glasses with large amounts of so-called “free” carbon, we observe a significant portion of the {Si}4O4 tetrahedra which have disproportionally large angles. These angles indicate the presence of internal SiO2 surfaces or cages-like voids, similar to those found in zeolites or clathrates. This analysis suggests that in SiCO, the “free” carbon is incorporated into these voids, which produces strain on the bonding angles of the surrounding host glass.

3:30PM W15.00006 Correlations between dynamics and atomic structures in Cu64.5Zr35.5 metallic glass1. C.Z. WANG, Y. ZHANG, F. ZHANG, M.I. MENDELEV, M.J. KRAMER, K.M. HO, Ames Laboratory-USDOE, Iowa State University, Ames, Iowa 50011, USA — The atomic structure of Cu-Zr metallic glasses (MGs) has been widely accepted to be heterogeneous and dominated byicosahedral short range order (ISRO). However, the correlations between dynamics and atomic structures in Cu-Zr MGs remain an enigma. Using molecular dynamics (MD) simulations, we investigated the correlations between dynamics and atomic structures in Cu64.5Zr35.5 MG. The atomic structures are characterized using ISRO and the Bergman-type medium range order (BMRO). The simulation and analysis results show that the majority of the mobile atoms are not involved in ISRO or BMRO, indicating that the dynamical heterogeneity has a strong correlation to structural heterogeneity. Moreover, we found that the localized soft vibration modes below 1.0 THz are mostly concentrated on the mobile atoms. The diffusion was studied using the atomic trajectory collected in an extended time interval of 1.2 μs at 700 K in MD simulations. It was found that the long range diffusion in MGs is highly heterogeneous, which is confined to the liquid-like regions and strongly avoids the ISRO and the Bergman-type MO. All these results clearly demonstrate strong correlations between dynamics (in terms of dynamical heterogeneity and diffusion) and atomic structures in Cu64.5Zr35.5 MGs.

1This work was supported by the U.S. Department of Energy, Basic Energy Sciences, Division of Materials Science and Engineering under the Contract No. DE-AC02-07CH11358.

3:42PM W15.00007 Onset of plasticity and its relation to structure in CuZr metallic glasses: a molecular dynamics study1. GONZALO GUTIERREZ, MATIAS SEPULEDA, NICOLAS AMIGO, Departamento de Física, Facultad de Ciencias, Universidad de Chile — The plastic behavior of crystalline metals is well understood. It is known that this regime is mainly mediated by the nucleation and propagation of dislocations as well as by grain boundary sliding. In metallic glasses (MGs), the plastic behavior is quite different from their crystalline counterparts. It is well known that bulk metallic glasses, in addition to the high yield strength and a elastic deformation to a strain limit about 2% (i.e., more than an order of magnitude greater than conventional crystalline metals), are brittle at room temperature. Interestingly, MG nanowires present an important degree of ductility, and is an ideal system to study the onset of plasticity in MG. Here we present a computational tensile test which shows the evolution of the atomic structure of a Cu64.5Zr35.5 metallic glass nanowire at 300 K according to the applied strain increased. The system consists of a million atoms CuZr nanowire metallic glass. Local structure of atoms is analyzed by means of the Voronoi polyhedral technique and the nucleation and propagation of SBS by monitoring the atomic strain.

1Supported by grant Fondecyt-Chile 1120603
3:54PM W15.00008 Study the formation of metastable crystalline phases from amorphous metallic systems with an integrated approach, ZHUO YE, FENG ZHANG, Ames Laboratory, YANG SUN, University of Science and Technology of China, MIKHAIL MENDELEV, RYAN OTT, EUN-SOO PARK, MATT BESSLER, MATT KRAMER, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory — An efficient genetic algorithm (GA) is integrated with experimental diffraction data to solve a metastable Al_{20}Sm_{5} phase that evolves during rapid solidification of an amorphous Al-10%Sm alloy produced by magnetron sputtering. The excellent match between calculated and experimental X-ray diffraction patterns confirms that this new phase appeared in the crystallization of the alloy. We discover the strong similarity of the underlying atomic structure between the amorphous alloy and this phase. Both phases share the same Sm-centered motif, providing a low-barrier pathway to form this Al_{20}Sm_{5} phase in the glass matrix at low temperatures. Molecular dynamic simulations of crystal growth from the liquid phase predict the formation of disordered anti-site defects in the devitrified crystal.

4:06PM W15.00009 Ab Initio Simulation of Nickel-Palladium-Phosphorus Bulk Metallic Glasses, RAYMOND ATTA-FYNN, Department of Physics, University of Texas at Arlington, PARTHAPRATIM BISWAS, Department of Physics and Astronomy, The University of Southern Mississippi — Using first principles molecular dynamics simulations, we model the structural and electronic properties of Ni_{80}Pd_{20}P_{20} bulk metallic glasses. The calculations are carried out for large system sizes in order to probe structural features associated with the medium range order on the nanometer length scale. We discuss different approaches to modeling the glassy systems ranging from the cook-and-quench to the structural building block techniques. The nature of the medium range order on the nanometer length scale is examined using the theory of fluctuation electron microscopy. The localization nature of the electronic eigenstates and the dc conductivity (of the model configurations) will be discussed in relation to the real space atomic structure.

4:18PM W15.00100 Microscopic pathway of a polymorphic transformation in Al90Sn10 system by molecular dynamics simulations, YANG SUN, FENG ZHANG, ZHUO YE, MIKHAIL MENDELEV, RYAN OTT, MATTHEW KRAMER, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory — When as-quenched amorphous Al-10.4%Sn alloy is isochronally heated up, it can display a nearly perfect polymorphic transformation into a complex cubic phase. Knowledge about the pathway of this transformation plays a key role for understanding the phase selection in this system driven far from equilibrium. We successfully simulated the growth of this crystalline phase from the amorphous state using molecular dynamics, with the help of a preexisting crystalline seed. The as-grown structure is in good agreement with experimental X-ray diffraction measurement. By analyzing the atomic trajectories during growth, we show the microscopic pathway linking the amorphous and crystalline phases and how the transformation is controlled by the driving force, atomic diffusivities and structural topologies.

4:30PM W15.00111 Quasilattice-conserved molecular dynamics studies of the atomic structure of decagonal Al-Co-Ni quasicrystals, YU-JUN ZHAO, XIAOTIAN LI, South China University of Technology, ADVISOR- STUDENT COLLABORATION — The detailed atomic structure of quasicrystals has been an open question for decades. In this paper, we present a quasilattice-conserved molecular dynamics method (quasiMD), with particular quasiperiodic boundary conditions. As the atomic coordinates are described by basic cells and quasilattices, we are able to maintain the self-similarity characteristics of quasicrystals with the atomic structure of the boundary region updated timely following the relaxing region. Exemplified with the study of decagonal Al-Co-Ni (d-Al-Co-Ni), we propose a more stable atomic structure model based on Penrose quasilattice and our quasiMD simulations. In particular, ‘rectangle-triangle’ rules are suggested for the local atomic structures of d-Al-Co-Ni quasicrystals.

4:42PM W15.00112 Local density fluctuations and hyperuniformity in quasicrystals, ERDAL CELAL OĞUZ, SALVATORE TORQUATO, Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA — Local density fluctuations in many-body systems are of fundamental importance throughout various scientific disciplines, including physics, materials science, number theory and biology. In a point pattern, let the variance associated with the number of points contained in a spherical window of radius \( R \) be denoted by \( \sigma^2(R) \). Hyperuniform systems include all infinite periodic structures, aperiodic quasicrystals, and some special disordered systems. Previous investigations showed that the number variance for large \( R \) in hyperuniform systems serves as a useful metric to rank order systems according to the degree to which large-scale density fluctuations are suppressed. In this work, we investigate the number variance of two-dimensional quasicrystals with a variety of different rotational symmetries. We study how the number variance depends on the rotational symmetry and local isomorphism class of the quasicrystal. We compare these results to a number of different periodic systems as well as disordered hyperuniform systems.


4:54PM W15.00113 Growth of icosahedral quasicrystals, JOSHUA SOCOLAR, CONNOR HANN, Duke University, PAUL STEINHARDT, Princeton University — The discovery of an icosahedral quasicrystal that formed naturally in a rock sample originating from a meteorite highlights fundamental questions about quasi-crystal formation. The growth of a well-ordered quasicrystal through kinetics dominated by local energetics is known to be possible in principle for 2D systems: a Penrose tiling, for example, can be grown from a particular type of small seed by adding tiles only to surface sites where the tile type and orientation are unambiguously determined by already placed tiles that share a vertex. We consider the generalization of this result to icosahedral quasicrystal tilings comprised of Ammann rhombohedra. Numerical simulations strongly suggest that infinite, well-ordered, icosahedral quasicrystals can be generated. Unlike the 2D case, defects are generated outside the original seed, but the number of such defects appears to grow only linearly with the cluster radius. Analysis of the lift of the tiling to a 2D hypercubic lattice provides key insights into the growth mechanism.


5:06PM W15.00114 The Log-Lin Metric for Generic Responses in Logarithmic Structures, ANTONY J. BOURDILLON, Retired — The generic Log-Lin metric joins experimental quasicrystal data with its ideal structure. How does a periodic probe, e.g., an X-ray or electron beam, interact with an ‘aperiodic’ solid to produce sharp diffraction in geometric space? Based on the structure [1-2], and through its stretching factor in the hierarchical model, quasi-structure factors are expanded in geometric series. The Log-Lin metric is found to be a function of \( \tau^2 \) and \( \pi \) [3-4]. The solution is of special value in simulating not only icosahedral structures, but also defective logarithmic solids, and quasicrystals of lower symmetry. The metric, now analyzed and simulated, enables consistent measurement from the atomic scale to high order superclusters. It is essential in any wave interaction with logarithmic solids. The factor applies to physical clusters of extremely dense, binary, hard-sphere, icosahedral, unit cells.

2:30PM W16.00001 Extrinsic and Intrinsic Charge Trapping at the Graphene/Ferroelectric Interface, MOHAMMED HUMED YUSUF, BEN TIELSEN, MATTHEW DAWBER, XU DU, Stony Brook University — In previous works on graphene ferroelectric field effect transistors (GFeFETs), the characteristics of the devices were found to be largely affected by “anti-hysteresis” associated with charge trapping instead of ferroelectric domain switching. In this work, with PbTiO$_3$/SrTiO$_3$ (PTO/STO) superlattices, the effect of surface adsorbates was largely diminished by tuning the transition temperature of superlattices and depositing exfoliated graphene at an elevated temperature. With the removal of such extrinsic charge traps, the impact from the “intrinsic” defects of the ferroelectric substrate was revealed, inducing fast (~10 µs) charge-trapping and remaining active even at cryogenic temperatures. The defects manifested themselves as unit-cell deep square pits, which were evident from contact-mode Atomic Force Microscopy (AFM) of the interface. An asymmetry in electron and hole trapping was observed. Optimized superlattice growth conditions minimized the surface defects and subdued the charge trapping associated with it. The result was a robust, ramping speed independent, room temperature ferroelectric switching in GFeFETs. With an ideal interface, the work was further extended to study graphene transport across potential barriers/junctions.

This work was supported by NSF (Grant DMR-1105202). Part of this research was carried out at the Center for Functional Nanomaterials, Brookhaven National Laboratory.

2:42PM W16.00002 Sub-harmonic gap structure and Magneto-transport in suspended graphene—Superconductor ballistic junctions, PIRANAVAN KUMARAVADIVEL, XU DU, Stony Brook University — Inducing superconductivity in graphene via the proximity effect enables to study the rich transport of the massless Dirac fermions at the Superconductor(S) - Graphene(G) interface. Some of the predictions are pseudo diffusive transport in Ballistic SGS junctions at low carrier densities and the unique specular and retro Andreev reflections in graphene. One of the challenges in observing these experimentally is to fabricate highly transparent ballistic SGS junctions that can be probed at low carrier densities near the Dirac point. In this talk we will present our recent results on suspended graphene-Niobium Josephson weak links. Our devices exhibit a mobility of ~35 0000 cm$^2$/V$^{-1}$s$^{-1}$ with a carrier density as low as 10$^6$ cm$^{-2}$. Below the Superconducting transition temperature (T$_c$) ~ 9K, the devices show supercurrent and sub-harmonic gap structure due to Multiple Andreev reflections. In the vicinity of the Dirac point, the sub-harmonic gap structure becomes more pronounced, which as predicted, is indicative of pseudo-diffusive transport. With a fine scanning of gate voltage close to Dirac point we see emergence of some unusual sub-gap structures. We also report on our study of these samples below the upper critical field of Nb (~ 3.5T), where superconducting proximity effect coexists with Quantum Hall effect.

2:54PM W16.00003 Ultra-Short Channel Graphene Devices, M-JAVAD FARROKHJ, MATHIAS J. BOLAND, ABBISHAEK SUNDARARAJAN, DOUGLAS R. STRACHAN, Univ of Kentucky — Measurements and modeling of ultra-short nano-electronic devices consisting of metallic electrodes and graphene channels are presented. We will discuss the novel formation and characterization of these devices. The short channel of the devices permits the observation of high-field effects. This includes current saturation that has relevance to future size-scaling of atomically-thin nano-electronics in the sub-10 nm regime. Unusual features in the current-voltage characteristics are explained by an analytical ballistic model. In addition, we investigate the effect of contact induced energy level broadening of the electrodes and contact resistance on the current saturation.

3:06PM W16.00004 Ab initio simulation and design of graphene-based transistors at the atomic scale, WENCHANG LU, JERRY BERNHOLC, North Carolina State University, Raleigh, NC 27695 — Two-dimensional materials, such as graphene and molybdenum disulfide, have attracted much attention because of their unique properties. Graphene’s high mobility make it a very promising material for next generation electronics, but its zero band gap is a big hurdle for digital transistors. However, graphene nanoribbons can exhibit band gaps due to quantum confinement, and their electronic properties differ depending on the structures of their edges. Based on the real space multigrid method and the non-equilibrium Green functions technique for multi-probe systems, we have developed massively parallel DFT-based software to calculate quantum transport properties with several thousands atoms. We present results for transport properties of graphene-based transistors with different atomic structures and study the effects of nanoribbon length, width and gate structure.

3:18PM W16.00005 Low-Resistance Spin Filtering from Ferromagnet-Graphene-Ferromagnet Junctions, ENRIQUE COBAS, OLAOF VAN ‘T ERVE, SHU-FAN CHENG, BERRY JONKER, US Naval Research Laboratory — Nickel-graphene interfaces have been recently demonstrated to habor spin polarizations of up to 42% with Ni/Graphene/MgO/Co heterostructures exhibiting negative out-of-plane magnetoresistances of 31% [1]. These experiments agree qualitatively with theoretical predictions of spin filtering at planar Ni-Graphene and Co-Graphene interfaces [2]. We previously demonstrated room temperature magnetoresistance in vertical NiFe-Graphene-Co junctions [3]. Now we have fabricated high-quality NiFe(111)-Graphene-Co and NiFe(111)-Graphene-Fe junctions grown in-situ that exhibit high MR at room temperature while maintaining a very low interface resistance. Such junctions embody an excellent source of spin-polarized current for spintronics applications like fast and non-volatile magnetic random access memory.


3:30PM W16.00006 Plasma enhanced atomic layer deposition of ultrathin oxides on graphene, CHRISTIE J. TRIMBLE, ANNA M. ZANIEWSKI, MANPUNEET KAUR, ROBERT J. NEMANICH, Arizona State University — Graphene, a single atomic layer of sp2 bonded carbon atoms, possesses extreme material properties that point toward a plethora of potential electronic applications. Many of these possibilities require the combination of graphene with dielectric materials such as metal oxides. Simultaneously, there is interest in new physical properties that emerge when traditionally three dimensional materials are constrained to ultrathin layers. For both of these objectives, we explore deposition of ultrathin oxide layers on graphene. In this project, we perform plasma enhanced atomic layer deposition (PEALD) of aluminum oxide on graphene that has been grown by chemical vapor deposition atop copper foil and achieve oxide layers that are <1.5 nm. Because exposure to oxygen plasma can cause the graphene to deteriorate, we explore techniques to mitigate this effect and optimize the PEALD process. Following deposition, the graphene and oxide films are transferred to arbitrary substrates for further analysis. We use x-ray photoelectron spectroscopy, Raman spectroscopy, and atomic force microscopy to assess the quality of the resulting films.

This work is supported by the National Science Foundation under Grant # DMR-1206935.
3:42PM W16.00007 Energy gap formation and gap states analysis in bilayer graphene

KAOH KANAYAMA, The University of Tokyo, KOSUKE NAGASHIO, The University of Tokyo & PRESTO-JST — The targeted issue for bilayer graphene is low \( I_{on}/I_{off} \) at room temperature, which is explained by the variable range hopping in \( \text{gap states} \). However, there will be intrinsically no interface states in bilayer graphene because there is no dangling bonds, compared with \( \text{Pb} \) centers in \( \text{SiO}_2/\text{Si} \) system. The origin for the gap states is still open question. In spite of this, the detailed measurements on \( D_{\text{h}} \) and time constant for gap states have not been reported yet. One of reasons could be the leakage current through the top gate insulator since robust methodology is not established. Here, we demonstrates a considerable suppression of the low-field leakage in bilayer graphene by applying the high-pressure \( \text{O}_2 \) annealing to \( \text{Y}_2\text{O}_3 \) top gate insulator. The reliable \( \text{Y}_2\text{O}_3 \) top gate insulator provides the access to the carrier response issue in the largely-opened band gap. In this talk, we focus on the conductance measurements for bilayer graphene to extract \( D_{\text{h}} \), and time constant. Based on these measurements, two possible origins for the gap states, (i) border traps at the edge of \( \text{Y}_2\text{O}_3 \) and (ii) the local breakdown of A-B stacking in bilayer graphene, are discussed.

3:54PM W16.00008 ABSTRACT WITHDRAWN

4:06PM W16.00009 SrO(001) on graphene: a universal buffer layer for integration of complex oxides

ADAM AHMED, The Ohio State University, HUA WEN, University of California Riverside, IGOR PINCHUK, TIANCONG ZHU, ROLAND WAKAWAKI, The Ohio State University — We report the successful growth of high-quality crystalline SrO on highly-ordered pyrolytic graphite (HOPG) and single layer graphene by molecular beam epitaxy. The epitaxial SrO layers have (001) orientation as confirmed by x-ray diffraction (XRD), and atomic force microscopy measurements show rms surface roughness of optimal films to be 1.2 Å. Transport measurements of exfoliated graphene after SrO deposition show a strong dependence between the Dirac point and Sr oxidation. To show the utility of SrO as a buffer layer for complex oxide integration, we grew perovskite crystal \( \text{SrTiO}_3 \) on SrO, and it was also confirmed to have (001) orientation from x-ray diffraction. This materials advancement opens the door to integration of many other complex oxides to explore novel correlated electron physics in graphene.


JAMES HONE, Columbia University — Two-dimensional (2D) materials, such as graphene, hexagonal boron nitride (hBN), transition metal dichalcogenides, have shown great potential in nano-electronics because of their unique and superior physical properties. Among them, hBN has been known as an alternative crystal \( \text{SrTiO}_3 \) on SrO, and it was also confirmed to have (001) orientation from x-ray diffraction. This materials advancement opens the door to integration of many other complex oxides to explore novel correlated electron physics in graphene.

4:30PM W16.00011 Electronic transport in graphene structure: from weak to strong localization regimes

AURELIEN LHIBERI, Université catholique de Louvain, Institute of condensed matter and nanosciences, chemin des étoiles 8, 1348 Louvain-la-Neuve, Belgium — Graphene, often named the wonder material for its many fascinating properties, has sparked out intense research activities over the last decade. Electronic transport in graphene became rapidly an important research field because of the early reported extremely high charge carrier mobility which triggered large expectations for nanoelectronic devices. Besides mobilities, graphene samples can exhibit particularly long electronic coherence lengths which allow for phase-related quantum transport phenomena such as the weak and strong localization transport regimes. This makes graphene a remarkable playground for fundamental studies of localization theory in low-dimensional systems. In this presentation, using tight-binding models enriched by first principle calculations, and a real-space Kubo-Greenwood method, multiscale simulations of the electronic transport in various graphene-based systems will be discussed. Such an approach allows for computing transport properties of systems containing millions of atoms reaching therefore the experimental sample size. In order to tailor graphene properties, chemical and/or structural modifications are widely used. However, such modifications act as scattering defects and usually deteriorate transport properties. Open a band gap while maintaining good mobility is a typical illustration of this dual problem. The influence of various chemical and structural defects will be analyzed. In particular, the consequences of unbalanced sublattice nitrogen doping in graphene and the case of highly defective graphene structures exhibiting strong Anderson insulator behaviors will be examined. Defects being even more detrimental for transport in 1D structures, a synthesis method that is free of defects is highly desirable. A solution is provided by a bottom-up chemistry approach where precursor monomers are self-assembled. The electronic transport and the potential for nanoelectronics of such defect-free carbon ribbons will also be discussed.

5:06PM W16.00012 Aharonov-Bohm interference in gate-defined ring of high-mobility graphene

MINSOO KIM, HU-JONG LEE, Department of Physics, Pohang University of Science and Technology — Recent progress in preparing a high-quality graphene layer enables one to investigate the intrinsic carrier transport nature in the material. Here, we report the signature of conservation of the Berry’s phase with preserved valley symmetry in Aharonov-Bohm (AB) interferometers fabricated on monolayer graphene with high carrier mobility, where the graphene was sandwiched between two thin hexagonal boron nitride (h-BN) layers. In measurements, charge carriers were confined in an AB ring-shaped potential well formed by the dual-gate operation of the bottom and top gates and the four-terminal magneto-conductance (MC) was measured with varying magnetic flux through the ring. The signature of conservation of the Berry’s phase is clearly observed up to carrier density of \( 10^{12} \text{cm}^{-2} \) and MC agrees well with theoretical predictions. This is the first demonstration of Aharonov-Bohm interference in 2D materials.

5:18PM W16.00013 High-k Dielectric Nanosheets for Two-Dimensional material Electronics

YUFENG HAO, XU CUI, JUN YIN, GWAN-HYOUNG LEE, GHIDEWON AREFE, Columbia university, MINORU OSADA, TAKAYOSHI SASAKI, NIMS, Japan, JAMES HONE, Columbia University — Two-dimensional (2D) materials, such as graphene, hexagonal boron nitride (hBN), transition metal dichalcogenides, have shown great potential in nanoelectronics because of their unique and superior physical properties. Among them, hBN has been known as an alternative dielectric that is atomically flat and free of trapped charges, which drastically enhance the mobility of graphene or MoS2. However, low dielectric constant (\( k \sim 3.5 \)) of hBN limits its use in transistors as gate lengths are scaled down to tens of nanometers. Here we demonstrate high performance graphene and MoS2 field effect transistors by using ultrathin Ca2NaNb4O13 nanosheet as a dielectric and mechanically stacking 2D materials. We developed a facile transfer strategy to build 2D materials devices based on the Ca2NaNb4O13 nanosheets. We measured and found that the oxide nanosheet has high dielectric strength, along with high dielectric constant at thickness of a few tens of nanometer. Therefore, multiple-stacked heterostructure of 2D materials shows high mobility at small operating voltage. This study shows possibility of high-k dielectric nanosheets for 2D electronics.
2:30PM W17.00001 High Resolution Imaging of Graphene on SiC by Contact Resonance AFM: Experiment and Theory, QING TU, BJÖRN LANGE, Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC, USA; JOAO MARCELO LOPES, Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, D-10117 Berlin, Germany; STEFAN ZAUSCHER, VOLKER BLUM, Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC, USA — Contact resonance atomic force microscopy (CR-AFM) is a powerful tool for mapping differences of the mechanical properties of layered, 2D materials. The deconvolution of stiffness contributions arising from the different layers is, however, difficult. Here, density functional theory (DFT) calculations can help interpret experimental results. Few-layer graphene (FLG; mono-, bi-, or trilayer thickness) on silicon carbide (SiC) exhibits very clean and distinct surfaces and yields high-contrast CR-AFM images. To interpret the contributions from surface areas with different layer thickness and structure we use DFT to calculate atomic displacements for forces acting on FLG on SiC using the $\sqrt{3} \times \sqrt{3}$ and the $6\sqrt{3} \times 6\sqrt{3}$ structure models. Based on these displacements we calculate an effective modulus using a spring model. The resulting moduli can then be compared with those extracted from experimental CR-AFM measurements of FLG on SiC.


2:42PM W17.00002 Charging Ring Spectroscopy and Defect Identification in Graphene/Boron Nitride Through Scanning Tunneling Microscopy, JUWON LEE, DILLON WONG, JAIRO VALESCO, LONG JU, SALMAN KAHN, HHSINZON TSAI, CHAD GERMANY, Univ of California - Berkeley, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Material Science, ALEX ZETTL, FENG WANG, MICHAEL CROMMIE, Univ of California - Berkeley — Tip-induced ionization of defects in semiconductors and surface adatoms is known to cause ring-like structures in scanning tunneling spectroscopy (STS). We report the observation and investigation of charging ring structures in bulk single crystalline graphene grown on SiC. These rings provide quantitative information on the energy levels of the partially filled BN defects, providing insight into their chemical identities. This new technique suggests exciting possibilities for quantitative spectroscopic studies of defects in other insulating systems.

2:54PM W17.00003 Scanning tunneling microscopy studies of graphene and hydrogenated graphene on Cu(111), SHAWNA M. HOLLEN, GRADY GAMBREL, STEVEN TJUNG, NANCY M. SANTAGATA, EZEKIEL JOHNSTON-HALPERIN, JAY A. GUPTA, The Ohio State University — Because of the innate sensitivity of 2D material surfaces, it is increasingly important to understand and characterize surface functionalization and interactions with environmental elements, such as substrate, metallic contacts, and adatoms. Here we have developed a method for reproducible, epitaxial growth of pristine graphene islands on Cu(111) in UHV and use scanning tunneling microscopy and spectroscopy (STM) to study the interaction of these graphene islands with the Cu substrate. Tunneling spectroscopy measurements of the electronic surface states over the graphene islands indicate a lower work function, decreased coupling to bulk Cu states, and a decreased electron effective mass. Additionally, we support the novel field electron dissociation technique to form hydrogen-terminated graphene at low temperatures and in UHV. This technique produced what may be the first STM images of crystalline hydrogenated graphene. The pristine graphene island is then recovered by scanning at a high tip-sample bias. The hydrogenation and its reversibility suggest writing lateral 2D devices using the STM tip. Toward this end, we are developing the capability to repeat the hydrogenation on working graphene devices.

3:18PM W17.00005 Probing Graphene by Low-Energy Electrons under Non-normal Incidence, JOHANNEZ JOBST, JAAP KAUTZ, DANIEL GEELEN, Leiden University, Huygens-Kamerlingh Onnes Laboratory, RUDOLF M. TROMP, IBM T.J. Watson Research Center, SENSE JAN VAN DER MOLEN, Leiden University, Huygens-Kamerlingh Onnes Laboratory — Low-energy electron microscopy (LEEM) is a powerful surface analysis tool for investigating samples in real and reciprocal space. Moreover, spectroscopic information can be obtained by measuring LEEM-IV, i.e., the energy dependence of the reflected electron intensity. Here, we focus on the study of monolayer and bilayer graphene grown on silicon carbide. The bilayer structure gives rise to minima in the LEEM-IV, which are used to unambiguously determine the layer thickness as the number of minima is equal to the number of conducting graphene layers. In a typical LEEM experiment it is crucial to align the sample such that the electrons impinge perpendicular on the surface in order to guarantee ideal imaging conditions. In this study we, however, present a systematic analysis of the effect of beam tilt on the LEEM-IV. We find pronounced changes in shape depending on the tilt angle with respect to crystallographic axes. These changes can be related to the band structure of few-layer graphene.

3:30PM W17.00006 Resonant Modes in Circular Graphene pn Junctions Created by STM Probes, JONATHAN WYRICK, Center for Nanoscale Science and Technology NIST, YUE ZHAO, Center for Nanoscale Science and Technology NIST; Maryland NanoCenter UMD, FABIAN NATTERER, Center for Nanoscale Science and Technology NIST, JOAQUIN RODRIGUEZ NIEVA, Department of Physics, Massachusetts Institute of Technology, CYPRIAN LEWANDOWSKI, Department of Physics, Imperial College London, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, LEONID LEVITOV, Department of Physics, Massachusetts Institute of Technology, NIKOLAI ZHITENEV, JOSEPH STROSCIO, Center for Nanoscale Science and Technology NIST — Electronic states in graphene (and similar 2D materials) are susceptible to yield 2 types of resonances in the tunneling spectrum: first as oscillations in the otherwise linear graphene dispersion, and second when they are pulled across the Fermi-level due to tip gating. Tunable with tip height/radius, and tip work-function, the oscillations act as fingerprints of an induced pn junction. We compare experimental results to theory for confined states in circular geometries, characterizing energy and spatial characteristics of these modes.
3:42PM W17.00007 Stacking defects and transport in bilayer graphene1, FRANCISCO GUINEA, CSC — 

Pristine bilayer graphene behaves in some instances as an insulator with a transport gap of a few meV. Intriguingly, however, some samples of similar mobility exhibit good metallic properties, with a minimal conductivity of the order of 2e^2/h. Here we propose an explanation for this dichotomy, which is unrelated to electron interactions and based on the reversible formation of boundaries between stacking domains (‘solitons’). We argue, using a numerical analysis, that the hallmark features of the previously inferred insulating state can be explained by scattering on boundaries between domains with different stacking order (AB and BA). We furthermore present experimental evidence, reinforcing our interpretation, of reversible switching between a metallic and an insulating regime in suspended bilayers when subjected to thermal cycling or high current annealing.

1 work done in collaboration with P. San-Jose, R. V. Gorbachev, K. S. Novoselov, and A. K. Geim

4:18PM W17.00008 Examination of Humidity Effects on Measured Thickness and Interfacial Phenomena of Exfoliated Graphene on SiO_2 via AC-AFM, KATHERINE JINKINS, JORGE CAMACHO, LEE FARINA, YAN WU, Univ of Wisconsin, Platteville — Tapping (AC) mode Atomic Force Microscopy (AFM) is commonly used to determine the thickness of graphene samples. However, AFM measurements have been shown to be sensitive to environmental conditions such as adsorbed water, in turn dependent on relative humidity (RH). In the present study, AC-AFM is used to measure the thickness and loss tangent of exfoliated graphene on silicon dioxide (SiO_2) as RH is increased from 10% to 80%. We show that the measured thickness of graphene is dependent on RH. Loss tangent is an AFM imaging technique that interprets the phase information as a relationship between the stored and dissipated energy in the tip-sample interaction. This study demonstrates the loss tangent of the graphene and oxide regions are both affected by humidity, with generally higher loss tangent for graphene than SiO_2. As RH increases, we observe the loss tangent of both materials approaches the same value. We hypothesize that there is a layer of water trapped between the graphene and SiO_2 substrate to explain this observation. Using this interpretation, the loss tangent images also indicate movement and change in this trapped water layer as RH increases, which impacts the measured thickness of graphene using AC-AFM.

4:30PM W17.00009 Visualization of Photo-induced Doping patterns in Graphene/Boron Nitride Heterostructures via Scanning Tunneling Microscopy1, JAIRO VELASCO JR., LONG JU, DILLON WONG, JUWON LEE, SALMAN KAHN, HSIN-ZON TSAI, CHAD GERMANY, University of California at Berkeley, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS, ALEX ZETTL, FENG WANG, MIKE CROMMIE, University of California at Berkeley — Photo-induced doping in graphene-boron nitride (G/BN) heterostructures enables flexible and repeatable writing and erasing of charge doping in graphene using optical irradiation. So far, however, this phenomenon has been explored using spatially averaging probes such as electron transport, and there have been no local studies into the underlying microscopic behavior. Here we report a combined scanning tunneling microscopy (STM) and optoelectronic measurement scheme that has been utilized to investigate the microscopic mechanisms at work in this process. We will discuss the latest experimental progress towards the visualization of light-induced charge doping patterns on G/BN heterostructures via STM.

1 J.V acknowledges support from the UC President’s Postdoctoral Fellowship

4:42PM W17.00010 A Correlation of Raman and Single and Multiple Layer Graphene Conductivity As Detected With A Cryogenic Multiprobe AFM With On-line Raman, NSOM and Other SPM Modalities, AARON LEWIS, Hebrew University of Jerusalem, Benin School of Engineering & Applied Science, Jerusalem, Israel, OLEG ZINOVIEV, ANATOLY KOMISSAR, ERAN MAAYAN, DAVID LEWIS, Nanonics Imaging Ltd., Jerusalem, Israel — It is a challenge to study 2D materials, such as Graphene, MoS_2, WeSe_2, etc. at temperatures down to 10^3K when considering the wide variety of physical phenomena that must be applied for a full picture of the functionality of these materials. This involves questions of structure, nanometric photoconductivity, electrical properties, thermal properties, near-field optical in the apertured & scattering modes, Kelvin probe, and Raman. These phenomena are common not only to 2D materials but also to carbon nanotubes and related nanomaterials. This presentation will describe the instrumental development of such a multiprobe cryogenic system that allows for state of the art on-line optical measurements and will also include a review of the probe developments that permit such multifunctional multiprobe operation with on-line full optical access. This system has a completely free optical axis from above and below not obscured by electrical or other probes that have been developed for multiprobe operation. This permits on-line Raman and Tip Enhanced NanoRaman Scattering. With such a system we have investigated graphene and HFO2 using multiprobe electrical, Kelvin probe, NSOM and on-line Raman. The results have yielded new insights into chemical changes correlated to electrical conductivity.

4:54PM W17.00011 Electron Tunneling Spectroscopy of Single and Bilayer Graphene with Hexagonal Boron Nitride Tunneling Barrier, SUYONG JUNG, JAESUNG PARK, CHANYONG HWANG, DONGHAN HA, Korea Research Institute of Standards and Science, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, PILKYUNG MOON, New York University Shanghai, YOUNG-WOO SON, Korea Institute for Advanced Study — We have performed electron tunneling spectroscopy measurements on gated single and bilayer graphene devices with thin hexagonal boron nitride (h-BN) as a tunneling barrier. We can directly probe electronic structures of graphene devices by varying charge density and tunneling bias voltage. The evolution of bilayer energy gap identified as dI/dV dip in tunneling spectra is observed as the electric field between bottom gate and top tunneling probe varies. In addition, we can identify several spectra features which are in good agreement with the vibrational excitations; phonons of graphene and h-BN and a signature of local plasmonic excitation. Upon increasing external magnetic field, the development of Landau levels (LL) is observed as early as 0.2T and we are able to discern individual LL as many as 20 as an index for both filled and empty states, which is unprecedented in previous tunneling spectroscopy studies on graphene devices.

5:06PM W17.00012 Thermal mirror buckling transitions in a pristine freestanding graphene membrane investigated by scanning tunneling microscopy, KEVIN SCHOEIZ, University of Arkansas, VINCENT MEUNIER, Rensselaer Polytechnic Institute, PRADEEP KUMAR, University of Arkansas, MEHDHI NEEK-AMAL, Universiteit Antwerpen, PAUL THIBADO, University of Arkansas, FRAANCOIS PEETERS, Universiteit Antwerpen — Freestanding graphene membranes are not flat, but rather display an array of ripples with alternating curvature. By applying a local force using a scanning tunneling microscope tip, we can pull out these ripples, causing the graphene membrane to reversibly rise and fall. By increasing the tunneling current and exploiting the negative coefficient of thermal expansion, we can increase the strain in the graphene membrane causing an irreversible transition from this flexible state to a rigid configuration. This transition typically happens when the graphene membrane reaches 60-70% of the total graphene height. We successfully model this transition as the transition of a spin-half Ising magnet where the ripples are modeled as Ising spins. The buckling transition can be interpreted as the transition from an antiferromagnetic state, to a ferromagnetic state. In addition, four critical exponents are measured. These results provide insight into the role of the negative thermal expansion of graphene.

Thursday, March 5, 2015 2:30PM - 5:30PM —
Session W18 QGI DAMOP: Invited Session: Novel Approaches for Quantum Information Processing With Polar Molecules Mission Room 103A - Sabre Kais, Qatar Environment and Energy Research Institute & Purdue University

3:06PM W18.00002 Quantum matter based on ultracold molecules, JUN YE, JILA, NIST and University of Colorado — Molecules cooled to ultralow temperatures provide fundamental new insights to strongly correlated quantum systems, molecular interactions and chemistry in the quantum regime, and precision measurement. Complete control of molecular interactions by producing a molecular gas at very low entropy and near absolute zero has long been hindered by their complex energy level structure. Recently, a range of scientific tools have been developed to enable the production of molecules in the quantum regime. Here, molecular collisions follow full quantum descriptions. Chemical reaction is controlled via quantum statistics of the molecules, along with dipolar effects. Further, molecules can be confined in reduced spatial dimensions and their interactions precisely manipulated via external electromagnetic fields. For example, by encoding a spin-1/2 system in rotational states, we realize a spin lattice system where many-body spin dynamics are directly controlled by long-range and anisotropic dipolar interactions. These new capabilities promise further explorations of strongly interacting and collective quantum effects in exotic quantum matter.

3:42PM W18.00003 Abelian and non-abelian topological phases with dipoles, ALEXEY GORSHKOV, Joint Quantum Institute — Topological phases of matter offer a pathway towards fault-tolerant topological quantum computers, in which quantum information is encoded in nonlocal (topological) degrees of freedom and is processed robustly by braiding (i.e. moving around one another) topological defects called anyons. In this talk, we will develop schemes for taking advantage of the tremendous degree of control recently achieved in atomic, molecular, and optical systems – particularly in systems of interacting dipoles – to realize exotic topological phenomena, such as parafermions, Ising anyons, and Fibonacci anyons, that ultimately allow for universal topologically protected quantum computing.

4:18PM W18.00004 Getting trapped molecules into the quantum toolkit, BRIAN ODOM, Northwestern University — Obtaining control over the rotational quantum state of trapped molecules is a prerequisite for quantum information processing applications. However, this task has presented a significant challenge because of the large number of initial states typically populated and because of unwanted excitations generally occurring during optical manipulation. Using a single spectrally filtered broadband laser simultaneously addressing many rotational levels, we have optically cooled trapped AlH+ molecules from room temperature to 4 Kelvins, corresponding to an increase in ground rotational-vibrational state population from 3% to 95%. We anticipate that the cooling timescale can be reduced from 100 milliseconds to a few microseconds and that the cooling efficiency can also be improved. Our broadband cooling technique should also be applicable to a number of other neutral and charged diatomic species. Trapped AlH+, in particular, is a good candidate for future work on ultracold chemistry, coherent control and entanglement of rotational quantum states, non-destructive single-molecule state readout by fluorescence, and searches for time-variations of the electron-proton mass ratio.

4:54PM W18.00005 Universal Matchgate Quantum Computing With Cold Polar Molecules, FELIPE HERRERA, Harvard University — Polar molecules in optical lattices are attractive for quantum simulation and computation due to the ability to implement a variety of spin-lattice models using static, microwave and optical fields to engineer the long-range dipolar interaction between molecular qubits. Quantum simulation of spin models requires global control over the molecular ensemble, while quantum computation requires control of individual molecules with sub-wavelength resolution. In this talk, we describe the implementation of a matchgate quantum processor with an ensemble of polar molecules in an optical lattice. The scheme uses few-body qubit encoding and sequential control of two-body dipolar interactions over small plaquetes on a square lattice to perform universal quantum computing without single-site addressing. Effective spin-spin interactions with matchgate symmetry between open-shell polar molecules (e.g., SrF, OH) are driven by two infrared control pulses in the absence of static electric fields. The resulting matchgates are robust with respect to realistic imperfections in the driving fields and lattice trapping. Applications of the architecture for the simulation of interacting fermions in quantum chemistry are discussed, considering an imperfect lattice filling.

Thursday, March 5, 2015 2:30PM - 5:30PM – Session W19 DCOMP: Invited Session: Frontiers of Electronic Structure Theory for Materials Mission Room 103B - Volker Blum, Duke University

2:30PM W19.00001 Exchange-Correlation and Electronic Excitation Energies from Pairing Matrix Fluctuations and the Particle-Particle Random Phase Approximation, WEITAO YANG, Duke Univ — We have developed an adiabatic connection to formulate the ground-state exchange-correlation energy in terms of pairing matrix linear fluctuations, opening a new channel for density functional approximations. This resulting method has many highly desirable properties. It has minimal delocalization error with a nearly linear energy behavior for systems with fractional charges, describes van der Waals interactions similarly and thermodynamic properties significantly better than the conventional RPA, and eliminates static correlation error for single bond systems. It is the first known functional with closed-form dependence on orbitals, which captures the energy derivative discontinuity in strongly correlated systems. We also adopted pp-RPA to approximate the pairing matrix fluctuation and then determine excitation energies by the differences of two-electron addition/removal energies. This approach captures many types of interesting excitations: single and double excitations are described accurately, Rydberg excitations are in good agreement with experimental data and CT excitations display correct 1/R dependence.
3:06PM W19.00002 Towards a unified description of ground and excited state properties: GW vs RPA and beyond , PATRICK RINKE, Aalto University, School of Science, 00076 Aalto, Finland — In the quest for finding an "optimal" first principles electronic structure method, that combines accuracy and tractability with transferability across different chemical environments and dimensionalities (e.g. molecules, wires/tubes, surfaces, solids), the treatment of exchange and correlation in terms of "exact-exchange plus correlation in the random-phase approximation (EX+CPA)" offers a promising avenue. Likewise one can express the same level of theory in the Green's function context through the GW approximation, which has the additional advantage that quasiparticle spectra as measured by direct and inverse photoemission become accessible. In this talk I will contrast both approaches and present the latest results from our continuous assessment. We find that self-consistent (sc) GW provides excellent charge densities [1], which is particularly important for charge transfer systems [2]. Spectral properties for closed shell molecules are generally in good agreement with photoemission spectra, although a judicious choice of the starting point in perturbative GoH calculations can outperform scGW [1,3]. Other ground state properties do not improve over EX+CPA calculations [1]. EX+CPA, on the other hand, provides a good description of the ground state [4] even for challenging cases like chemical reaction barrier heights [5] and the f-electron metal cerium [6]. The notorious underbinding of EX+CPA can be corrected by going beyond RPA to renormalised second order perturbation theory (rPT2) [7] that gives the overall most balanced performance. I will also discuss the associated rPT2 self-energy that goes beyond GW.


3:42PM W19.00003 Range-separated Hybrid Functionals for Molecules and Interfaces , THOMAS KÖRZDÖRFER, University of Potsdam, Germany — Density functional theory (DFT) and its time-dependent extension (TD-DFT) are powerful tools enabling the theoretical prediction of the ground- and excited-state properties of many-electron systems with reasonable accuracy at affordable computational costs. The DFT treatment of particular electronic and structural properties, however, reveals severe qualitative failures of standard out-of-the-box functionals. Important examples include the wrong level alignment and spurious charge-transfer at organic-organic interfaces as well as the underestimation of bond-length alternations and excited-state energies in polymers. These failures can be traced back to the delocalization error inherent to semilocal and global hybrid functionals. In this talk, I will discuss recent efforts to reduce the delocalization error by using range-separated hybrid functionals combined with a non-empirical tuning procedure for the range-separation parameter [1-3]. The benefits and drawbacks of using range-separated hybrid functionals for the description of the ground and excited states of molecules and interfaces will be discussed. It will be demonstrated that this approach provides for robust and efficient means of calculating ionization potentials and electron affinities, for characterizing the electronic couplings in organic mixed-valence systems, for the calculation level alignment at organic/organic interfaces, and for the reliable prediction of the optical band-gap of low band-gap polymers. I will further motivate why RSH functionals provide for a superior starting point for non-self-consistent GW calculations as compared to standard semilocal or global hybrid functionals.


4:18PM W19.00004 New Developments in Diffusion QMC for materials , FERNANDO REBOREDO, Materials Science & Technology Division Oak Ridge National Laboratory — No abstract available.

4:54PM W19.00005 Stochastic Quantum Chemistry for extended systems , GEORGE BOOTH, Department of Chemistry University of Cambridge — No abstract available.

Thursday, March 5, 2015 2:30PM - 5:30PM — Session W20 DPOLY: Invited Session: Physics of Biomacromolecules Ballroom B - Patrick Underhill, Rensselaer Polytechnic Institute

2:30PM W20.00001 Electrostatic self-assembly of biomolecules1 , MONICA OLVERA DE LA CRUZ, Northwestern Univ — Charged filaments and membranes are natural structures abundant in cell media. In this talk we discuss the assembly of amphiphiles into biocompatible fibers, ribbons and membranes. We describe one- and two-dimensional assemblies that undergo re-entrant transitions in crystalline packing in response to changes in the solution pH and/or salt concentration resulting in different mesoscopic morphologies and properties. In the case of one-dimensional structures, we discuss self-assembled amphiphiles into highly charged nanofibers in water that order into two-dimensional crystals. These fibers of about 6 nm cross-sectional diameter form crystalline arrays with inter-fiber spacings of up to 130 nm. Solution concentration and temperature can be adjusted to control the inter-fiber spacings. The addition of salt destroys crystal packing, indicating that electrostatic repulsions are necessary for the observed ordering. We describe the crystallization of bundles of filament networks interacting via long-range repulsions in confinement by a phenomenological model. Two distinct crystallization mechanisms in the short and large screening length regimes are discussed and the phase diagram is obtained. Simulation of large bundles predicts the existence of topological defects among bundled filaments. Crystallization processes driven by electrostatic attractions are also discussed.

1 Funded by Center for Bio-Inspired Energy Science (CBES), which is an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0000989.

3:06PM W20.00002 Theory and Computational Design of Protein Materials , JEFFERY SAVEN, University of Pennsylvania — Protein design opens routes to arrive at novel molecules, materials and nanostructures. Recent theoretical methods can identify the properties of amino acid sequences consistent with desired structures and functions. Such methods leverage concepts from statistical mechanics and address the structural complexity of proteins and their many possible amino acid sequences. Computationally designed protein-based systems have been experimentally realized to encapsulate nonbiological cofactors and assemble into predetermined crystalline structures.
diagonal wavevector (2013) to include a direct antiferromagnetic exchange coupling between the Cu sites. As in previous work, we invariably find that the primary instability has a

SCHROEDER, University of Illinois at Urbana-Champaign — Single molecule techniques allow for the direct observation of polymer dynamics under highly non-equilibrium conditions. Until recently, however, these methods have been largely confined to linear semi-flexible DNA molecules as "model" polymer chains. This talk will show recent work from our group in extending the field of single polymer dynamics to new materials, including branched polymers and truly flexible polymer chains. In this way, we explore new questions in classical polymer physics such as the role of architecture, topology, and backbone flexibility on chain dynamics at the molecular level. Recently, we used single molecule methods to directly visualize comb-shaped DNA polymers. Macromolecular DNA combs are synthesized utilizing a hybrid enzymatic-synthetic approach, wherein chemically modified DNA branches and DNA backbones are generated in separate polymerase chain reactions, followed by graft-onto reactions via "click" chemistry. This method allows for the synthesis of dual-color DNA combs, such that the backbone and side branches can be engineered to interact with each other to achieve specific mechanical, physical, and chemical properties. This is in contrast to many other physical hydrogels, where predictable tuning of bulk mechanics from the molecular level remains elusive due to the reliance on non-specific and non-stoichiometric chain interactions for network formation. Furthermore, the hydrogel network can be easily modified to deliver a variety of bioactive payloads including growth factors, peptide drugs, and hydroxyapatite nanoparticles. Through a series of in vitro and in vivo studies, we demonstrate that these materials may significantly improve transplanted stem cell retention and function.

HEILSHORN, Stanford University — Stem cell transplantation is a promising therapy for a myriad of debilitating diseases and injuries; however, current delivery protocols are inadequate. Transplantation by direct injection, which is clinically preferred for its minimal invasiveness, commonly results in less than 5% cell viability, greatly inhibiting clinical outcomes. We demonstrate that mechanical membrane disruption results in significant acute loss of viability at clinically relevant injection rates. As a strategy to protect cells from these damaging forces, we show that cell encapsulation within hydrogels of specific mechanical properties will significantly improve viability. Building on these fundamental studies, we have designed a reproducible, bio-resorbable, customizable hydrogel using protein-engineering technology. In our Mixing-Induced Two-Component Hydrogel (MITCH), network assembly is driven by specific and stoichiometric peptide-peptide binding interactions. By integrating protein science methodologies with simple polymer physics models, we manipulate the polypeptide chain interactions and demonstrate the direct ability to tune the network crosslinking density, sol-gel phase behavior, and gel mechanics. This is in contrast to many other physical hydrogels, where predictable tuning of bulk mechanics from the molecular level remains elusive due to the reliance on non-specific and non-stoichiometric chain interactions for network formation. Furthermore, the hydrogel network can be easily modified to deliver a variety of bioactive payloads.

Thursday, March 5, 2015 2:30PM - 5:30PM — Session W21 DCMP: Density Waves in Superconductors and Other Systems

2:30PM W21.00001 Charge ordering in three-band models of the cuprates, ALEXANDRA THOMSON, SUBIR SACHDEV, Harvard University — We examine trends in the wavevectors and form-factors of charge density wave instabilities of three-band models of the underdoped cuprates. For instabilities from a high temperature state with a large Fermi surface, we extend a study by Bulut et al. (Phys. Rev. B 88, 155132 (2013)) to include a direct antiferromagnetic exchange coupling between the Cu sites. As in previous work, we invariably find that the primary instability has a diagonal wavevector (+Q0, ±Q0) and a d-form factor. The experimentally observed wavevectors along the principal axes (+Q0, 0), (0, ±Q0) have higher energy, and their form factor is found to be predominantly d. Next, we gap out the Fermi surface in the anti-nodal regions of the Brillouin zone by including static, long-range antiferromagnetic order at the wavevector (τ, π): this is a simple model of the pseudogap in which we assume the antiferromagnetic order averages to zero by 'renormalized classical' thermal fluctuations in its orientation, valid when the antiferromagnetic correlation length is large. The charge density wave instabilities of this pseudogap state are found to have the optimal wavevector (±Q0, 0), with the magnitude of the d-form factor decreasing with increasing magnetic order.


1Supported by DOE Grant DE-FG02-07ER46352.
2:54PM W21.00003 Charge-order in the underdoped cuprates: a window into the normal state, DEBANJAN CHOWDHURY, SUBIR SACHDEV, Harvard University — Recent experiments in the underdoped regime of the hole-doped cuprates have found evidence for an incommensurate charge density wave state. We present an analysis of the charge ordering instabilities in a metal with antiferromagnetic correlations, where the electronic excitations are coupled to the fractionalized excitations of a quantum fluctuating antiferromagnet on the square lattice [1]. The resulting charge density wave state emerging out of such a fractionalized Fermi-liquid (FL*) is remarkably similar to the one observed in experiments on a number of different families of the cuprates [2]. Our results show that the observed charge density wave appears as a low-energy instability of a fractionalized metallic state linked to the proximity to an antiferromagnetic insulator, and the pseudogap regime can be described by such a metal at least over intermediate length and energy scales. We also describe the transition from a Fermi-liquid with a large Fermi-surface to a FL* around optimal doping via a Higgs-transition of a SU(2) gauge-theory. The implications of such Higgs criticality in two-dimensional metals on the physics of strange metal will be discussed.


3:06PM W21.00004 dc Resistivity at the Onset of Spin Density Wave Order in Two-dimensional Metals, AVISHKAR PATEL, SUBIR SACHDEW, Harvard Univ — The theory for the onset of spin density wave order in a metal in two dimensions flows to strong coupling, with strong interactions not only at the “hot spots,” but on the entire Fermi surface. We advocate the computation of dc transport in a regime where there is rapid relaxation to local equilibrium around the Fermi surface by processes which conserve total momentum. The dc resistivity is then controlled by weaker perturbations which do not conserve momentum. We consider variations in the local position of the quantum-critical point, induced by long-wavelength disorder, and find a contribution to the resistivity which is linear in temperature (up to logarithmic corrections) at low temperature. Scattering of fermions between hot spots, by short-wavelength disorder, leads to a residual resistivity and a correction which is linear in temperature.

3:18PM W21.00005 Are there quantum oscillations in an incommensurate charge density wave? YI ZHANG, AKASH MAHARAJ, STEVEN KIVELSON, Stanford University — Because a material with an incommensurate charge density wave (ICDW) is only quasi-periodic, Bloch’s theorem does not apply and there is no sharply defined Fermi surface. We will show that, as a consequence, there are no quantum oscillations which are truly periodic functions of 1/B (where B is the magnitude of an applied magnetic field). For a weak ICDW, there exist broad ranges of 1/B in which approximately periodic variations occur, but with frequencies that vary inexorably in an unending cascade with increasing 1/B. For a strong ICDW, e.g. in a quasi-crystal, no quantum oscillations survive at all. Rational and irrational numbers really are different. The duality between quasi-periodic systems in different dimensions can be straightforwardly generalized beyond the quantum oscillations and provides an accurate and efficient perspective.

3:30PM W21.00006 Short-range incommensurate d-wave charge order from a two-loop renormalization group calculation of the fermionic hot spot model, HERMANN FREIRE, VANUILDO DE CARVALHO, Universidade Federal de Goiás — The two-loop renormalization group (RG) calculation is considerably extended here for a two-dimensional (2D) fermionic effective field theory model, which includes only the so-called “hot spots” that are connected by the spin-density-wave (SDW) ordering wavevector on a Fermi surface generated by the 2D t − t’ Hubbard model at low hole doping. We compute the Callan-Symanzik RG equation up to two loops describing the flow of the single-particle Green’s function, the corresponding spectral function, the Fermi velocity, and some of the most important order-parameter susceptibilities in the model at lower energies. As a result, we establish that — in addition to clearly dominant SDW correlations — an approximate (pseudospin) symmetry relating a short-range incommensurate d-wave charge order to the d-wave superconducting order indeed emerges at lower energy scales, which is in agreement with recent works available in the literature addressing the 2D spin-fermion model. We derive implications of this possible electronic phase in the ongoing attempt to describe the phenomenology of the pseudogap regime in underdoped cuprates.


3:42PM W21.00007 Charge Density Wave and Superconductivity in Cu_xTiSe_2 Single Crystals, GORAN KARAPETROV, P. HUSANIKOVA, Drexel University, V. CAMBEL, IEE, Slovak Academy of Sciences, Bratislava, Slovakia, P. SZABO, P. SAMUELY, IEP, Slovak Academy of Sciences and Safarik University, Kosice, Slovakia, J. FEDOR, M. IAVARONE, Temple University, Philadelphia — We investigate atomic scale scanning tunneling microscopy and spectroscopy in Cu_xTiSe_2 single crystals at low temperatures. We map the CDW and superconducting phase diagram as a function of copper doping. STM measurements reveal coexistence of chiral charge density wave and superconductivity. In case of optimally doped and overdoped cases we find that the amplitude of charge density wave modulation is strongly suppressed with respect to strongly underdoped case (x < 0.06) with the chiral domain size remaining approximately the same. Superconductivity exhibits BCS character at a variety of dopings with 2Delta/k_B ~ 3.4 ± 0.7 indicating an intermediate coupling strength. Application of the external magnetic field introduces the Abrikosov vortex lattice that is weakly pinned. The size of the vortex core extracted from vortex images corresponds to the one extracted from the magnetization measurements. Our results suggest that, if charge density wave quantum critical point exist, it should be well above the optimal copper concentration of x=0.08.

This work is supported by the Army Research Office Grant #W911NF-14-1-0567.

3:54PM W21.00008 Chiral Symmetry Breaking and Mott Physics from Gauge/Gravity Duality, GARRETT VANACORE, PHILIP PHILLIPS, University of Illinois, Urbana-Champaign — We use holographic techniques to address the origin of the Mott gap and Fermi arcs in the cuprates. We first show that dynamically generated gaps of the Mott kind arise in holographic settings from a bulk coupling that breaks chiral symmetry. We then explore a bulk coupling which breaks rotational symmetry but preserves chiral symmetry and show that Fermi arcs arise in the dual system at the boundary. We draw further lessons for the cuprates through the unambiguous interpretation of chiral symmetry as a combination of particle-hole and time reversal symmetry in the cuprates, and suggest that the interplay of these symmetries may be the key to understanding the transition between the Mott insulating phase and the pseudogap.

We thank the NSF DMR-1104909 for support of this work.

4:06PM W21.00009 Quantum Critical Transitions in Spin and Charge Ordered Systems, CORENTIN MORICE, University of Cambridge, PREMALA CHANDRA, Rutgers University, STEPHEN E. ROWLEY, SIDHARTH S. SAXENA, University of Cambridge — The talk will focus on search and discovery of novel forms of quantum order in ferroelectric and multiferroic systems. Materials tuned to the proximity of a zero temperature phase transition often show the emergence of novel quantum phenomena. Much of the effort to study these new emergent effects, like the breakdown of the conventional Fermi-liquid theory in metals has been focused in narrow band electronic systems. But Spin or Charge ordered phases in insulating systems can also be tuned to absolute zero. Close to such a zero temperature phase transition, physical quantities like susceptibility change into unconventional forms due to the fluctuations experienced in this region giving rise to new kinds ordered states.
4:18PM W21.00010 Ferromagnetic of the undoped cuprate superconductor Pr$_3$CuO$_4$. ROSS MCDONALD, Los Alamos National Laboratory, NICHOLAS BREZNAZ, NITYAN NAIR, JAMES ANALYTIS, UC Berkeley, ZENGWEI ZHU, KIMBERLEY MODIC, Los Alamos National Laboratory, YOSHIIHARU KROCKENBERGER, NTT Basic Research Laboratories, LANL COLLABORATION, UC BERKELEY COLLABORATION, NTT COLLABORATION—Recent advances in molecular beam epitaxy growth and preparation of cuprate thin films indicate that annealing can be employed to minimize apical oxygen defects. For Pr$_3$CuO$_4$, the resulting square planar coordinated structure exhibits a 25 K superconducting transition in the absence of doping. This calls into question whether a Mott insulating groundstate is the relevant description of the square-planar parent phase of the electron-doped cuprate superconductors. We present high field (\textasciitilde 90 T) measurements of magnetic quantum oscillations—the first observation of it's kind for a cuprate thin film. The oscillation frequency and effective mass are consistent with the reconstructed Fermi surface of the electron-doped cuprate Nd$_{2-x}$Ce$_x$CuO$_4$. The combination of a reconstructed bandstructure and the occurrence of metallicity at zero doping is consistent with a Slater picture of band magnetism, indicating that the “doped Mott insulator” paradigm may not apply in this system.

4:30PM W21.00011 Influence of Ti doping on the incommensurate charge density wave in 1T-TaS$_2$. JIAOQIAN CHEN, Brookhaven National Laboratory, CHRISTOPHER NUGROHO, ANNA J. MILLER, ANSHUL KOGAR, EDUARDO FRADKIN, DALE J. VAN HARLINGEN, PETER ABBAMONTE, Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, YOUNG IL JOE, National Institute of Standards and Technology, JOEL D. BROCK, Cornell University, JOCHEN GECK, Leibniz Institute for Solid State and Materials Research—Using x-ray scattering and transport, we studied the temperature dependence of the transition between incommensurate (IC) and nearly commensurate (NC) phases of the charge density wave (CDW) in Ti doped 1T-TaS$_2$. Our results showed a first order phase transition from IC to NC-CDW phase in all doping levels with decreased transition temperature, as Ti doping was increased. During this transition, the angle of the CDW in the basal plane rotates from 11.9° to 16.4° at 12% Ti doping, while the in-plane component of the CDW wave vector does not change significantly. In addition, we observed that at 8% Ti doping, the CDW diffraction peak position and resistivity resemble that of pure TaS$_2$ in its commensurate CDW state. With our data, we revisit the resistive anomaly originally observed by DiSalvo [F. J. DiSalvo et al., Phys. Rev. B 12, 2220 (1975)] at 8% doping. DeSalvo explained this anomaly as arising from the pinning of the CDW on the crystal lattice. Our study shows that the commensuration effects in the NC phase is the cause of this anomaly.

4:42PM W21.00012 Scanning Tunneling Spectroscopy study of the Charge Density Wave driven Mott Insulator 17-TaS$_2$. DOOHHEE CHO, CALDES, IBS, POSTECH, Pohang, Korea, YONG-HEUM CHO, Department of Physics, POSTECH, Pohang, Korea, SANG-WOOK CHEONG, Rutgers University, New Jersey, USA, KI-SEOR KIM, Department of Physics, POSTECH, Pohang, Korea, HANWOONG YEOM, CALDES, IBS, POSTECH, Pohang, Korea—Exotic ground states can be generated by competition or interplay between various interactions, such as electron-phonon (\(e-\phi\)) and electron-electron (\(e-e\)) coupling. 17-TaS$_2$ is a prime example to study such interplay since a Mott gap coexists with charge density waves (CDW) at low temperatures. Our scanning tunneling spectroscopy measurements with high spatial and energy resolution determine the CDW and the Mott gap as 0.20 – 0.24 eV and 0.32 eV, respectively, by analyzing the phase difference between the real space electron densities across multiple energy gaps. In addition, we observe a peculiar reduction of the Mott gap in the vicinity of defect sites. The effect of competition between \(e-\phi\) and \(e-e\) coupling on the Mott gap size will be discussed within the Hubbard-Holstein picture.

4:54PM W21.00013 Wavevector dependent electron–phonon coupling drives the CDW formation in TbTe$_3$. S. ROSENKRANZ, Argonne National Laboratory, M. MASCHKE, F. WEBER, R. HEID, Karlsruhe Institute of Technology, A.H. SAID, Argonne National Laboratory, P. GIRALDO-GALLO, I.R. FISHER, Stanford University—The charge density wave (CDW) transition in the rare-earth tritellurides RTe$_3$ (R=rare earth) is commonly assumed to originate from a textbook Fermi surface nesting instability. Contrary to this weak coupling scenario, our investigation of the soft phonon mode in TbTe$_3$ provides direct evidence that the periodicity of the CDW superstructure in this canonical compound is determined by a strong momentum dependence of the electron-phonon coupling. Our high-resolution inelastic x-ray measurements reveal a renormalization of the soft-phonon energy and a strong broadening of the soft-phonon linewidth over a large part of reciprocal space adjacent to the CDW ordering vector. Our detailed theoretical calculations reproduce these observations very well and show that the position in reciprocal space of the phonon renormalization, and with it the CDW order wavevector, is not related to Fermi surface nesting. Our results demonstrate the importance of strongly momentum dependent electron-phonon coupling in defining the CDW order, which could also be relevant to many other systems.

5:06PM W21.00014 Anisotropic symmetry breaking in two-dimensional charge density waves of ErTe$_3$ investigated by femtosecond electron crystallography. FARAN ZHOU, TIMOFEY GOLUBEV, BIN HWANG, CHONG-YU RUAN, PHIL DUXBURY, Michigan State Univ, CHRISTOS MALLIKIAS, MERCOURI KANATZIDIS, Northwestern University, CHONG-YU RUAN GROUP TEAM, DUXBURY GROUP COLLABORATION, KANATZIDIS GROUP COLLABORATION— Electron-phonon interactions can give rise to various charge-ordered states, especially at low dimensions, where Fermi surface is more prone to form nesting. Rare earth tritellurides compound ErTe$_3$ develops charge density waves (CDW) along two perpendicular directions at different temperatures. By directly probing the order parameters of the two CDWs using femtosecond electron crystallography under different temperatures and driving phononic energy, we investigated the emergences of competing CDW orders in a dynamical phase diagram. The anisotropic symmetry breaking and the role of electron-phonon coupling, and photo-doping effect are discussed in reference to other CDW systems.

5:18PM W21.00015 Electronic band structure of Charge Density Wave PdxHoTe$_3$. SHANCAI WANG, YIPENG CAI, ZHONGHUA LIU, LEILEI JIA, YANG HE ZHAO, Department of Physics, Renmin Univ. of China, T. QIAN, HONG DING, Institute of Physics, China academy of Sciences, JUNBAO HE, Department of Physics, Renmin Univ. of China, GENFU CHEN, Institute of Physics, China academy of Sciences—The origin of superconductivity and interplay between superconductivity and different ground states remains challenging. The Pd-intercalated HoTe$_3$, suppresses the charge density wave (CDW) order and leads to the superconductivity. Here we report the detailed Angle-resolved photoemission spectroscopy (ARPES) study of the electronic structure on Pd$_x$Ho$_{1-x}$Te$_3$. In the CDW parent phase (HoTe$_3$), we found out the Fermi surface topology, CDW gap symmetry have 2 fold symmetry, with further Pd-intercalations, the system evolves from 2-fold symmetry to 4-fold symmetry with two CDW vectors, and eventually into superconducting state. The evolution of the CDW gap symmetry, gap size and CDW caused shadow bands are discussed at different phases.
conducting carbon nanotubes in aligned array field effect transistors and photovoltaics. MICHAEL ARNOLD, University of Wisconsin-Madison — Recent advances in (1) achieving highly monodisperse semiconducting carbon nanotubes without problematic metallic nanotubes and (2) depositing these nanotubes on useful, organized arrays and thin flexible substrates have created new opportunities for studying the physics of these one-dimensional conductors and for applying them in electronics and photonics technologies. In this talk, I will present on two topics that are along these lines. In the first, we have pioneered a scalable approach for depositing aligned arrays of ultrahigh purity semiconducting SWCNTs (prepared using polyfluorene-derivatives) called floating evaporative self-assembly (FESA). FESA is exploited to create FETs with exceptionally high combined on-conductance and on-off ratio of 261 µS/µm and 2x10^7, respectively, for a channel length of 240 nm. This is 1400x greater on-off ratio than SWCNT FETs fabricated by other methods, at comparable on-conductance per width of 250 µS/µm, and 30-100x greater on-conductance per width, at comparable on-off ratio of 10^7-10^8.

3:06PM W22.00002 Performance Enhanced Photoconductive Channels Based on (Carbon Nanotube)-(CdS Nanowire) Hybrid Nanostructures, MYUNGJAE YANG, HYUNGWOO LEE, Department of Physics and Astronomy, Seoul National University, KWANG HEO, Interdisciplinary Program in Nano-Science and Technology, Seoul National University, ABBAS MAA-ROOF, Department of Physics and Astronomy, Seoul National University, YONGJU PARK, SEUNGUK NOH, School of Electrical Engineering and Computer Science, Seoul National University, JUNE PARK, Department of Physics, Chung-Ang University, JIKANG JIANG, School of Physical Science and Technology, Xingjiao University, CHANGHEE LEE, School of Electrical Engineering and Computer Science, Seoul National University, MAE-JG SEONG, Department of Physics, Chung-Ang University, SEUNGHUN HONG, Department of Physics and Astronomy, Seoul National University — Previous researches showed that the performance of photocoercive channels based on individual CdS nanowires (NWs) is improved compared to the CdS bulk or thin-film-based channels. However, the assembly of a single NW is usually complex and time-consuming. Herein, we report a high-performance photoconductive channel based on CNT–CdS NW hybrid nanostructures, which can be easily prepared on both flat and curved substrates. In our experiments, the CNT-network-based channel was fabricated using an array of SWCNTs. We found that our channels exhibit a much larger photoresponse and faster photoresponse than those of previously reported CNT or CdS NW-based channels. In addition, we fabricated the channels on a curved surface.

3:18PM W22.00003 Impact of SWCNT characteristics and processing on the performance of nanotube-silicon solar cells. JOHN M. HARRIS, NDSU, ROBERT J. HEADRICK, Rice University, MATTHEW R. SEMLER, NDSU, MATTEO PASQUALI, Rice University, JEFFREY A. FAGAN, NIST, ERIK K. HOBBIE, NDSU — Single-wall carbon nanotubes (SWCNTs) sorted by length, electronic type and chirality are used to understand the influence of SWCNT characteristics on the performance of SWCNT-silicon solar cells. Solution-processed SWCNT films are deposited on n-doped silicon substrates and p-doped to yield photovoltaic devices that are competitive in terms of photo-conversion efficiency, fill factor and open-circuit voltage. The temperature dependence of the dark-current and the transient reverse-bias recovery technique are used to clarify the nature of the devices as a function of SWCNT type and chirality as well as device manufacturing method, where the latter ranges from the vacuum filtration of aqueous colloidal suspensions to the flow-deposition of super-acid solutions.

3:30PM W22.00004 15% Power Conversion Efficiency from a Gated Nanotube/Silicon Nanowire Array Solar Cell, MAUREEN K. PETTERSON1, MAXIME G. LEMAITRE, YU SHEN, Pooja WADHWA2, JIE HOU, SVELTANA V. VASILIEVA, Dept. of Physics, University of Florida, IVAN I. KRAVCHENKO, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, ANDREW G. RINZLER, Dept. of Physics, University of Florida — Despite their enhanced light trapping ability the performance of silicon nanowire array solar cells have, been stagnant with power conversion efficiencies barely breaking 10%. The problem is understood to be the consequence of a high photo-carrier recombination at the large surface area of the Si nanowire sidewalls. Here, by exploiting 1) electronic gating via an ionic liquid electrolyte to induce inversion in the n-type Si nanowires and 2) using a layer of single wall carbon nanotubes engineered to contact each nanowire tip and extract the minority carriers, we demonstrate silicon nanowire array solar cells with power conversion efficiencies of 15%. Our results allow for discrimination between the two principle means of avoiding front surface recombination: surface passivation and the use of local fields. A deleterious electrochemical reaction of the silicon due to the electrolyte gating is shown to be caused by oxygen/water entrained in the ionic liquid electrolyte. While encapsulation can avoid the issue a non-encapsulation based solution is also described.

1We gratefully acknowledge support from the National Science Foundation under ECCS-1232018
2Presently at Applied Materials
3Presently at INTEL

3:42PM W22.00005 Carbon nanotube fiber based flexible, lightweight and broadband photodetector, AHMED ZUBAIR, ECE Department, Rice University, NAOKI FUJIMURA, Department of Physical Electronics, Tokyo Institute of Technology, DIMITRI E. TSENTALOVICH, COLIN C. YOUNG, ChBE Department, Rice University, XIAOHEI HE, XUAN WANG, WEI LU GAO, ECE Department, Rice University, YUKIO KAWANO, Department of Physical Electronics, Tokyo Institute of Technology, MATTEO PASQUALI, ChBE Department, Rice University, JUNICHIRO KONO, ECE Department, Rice University — Ultrabroadband absorption properties of carbon nanotubes (CNTs) make them attractive materials for solar cell and photodetector applications. In particular, CNT fibers, which have the unique properties of flexibility and high mechanical strength combined with excellent electrical and optical properties, hold the promise as flexible, broadband photodetectors with inherent polarization sensitivity. Here, we explore the optoelectronic properties of high-performance multifunctional fibers of CNTs towards the development of lightweight, flexible, and broadband photodetectors. We present a photothermal electric-effect-based flexible CNT-fiber photodetector fabricated using a novel technique. The spatial variation of doping in CNT fibers creates a Seebeck coefficient gradient, leading to a photothermoelectric signal. The current-voltage characteristics of the fiber photodetector produced polarization-sensitive short-circuit currents and open-circuit voltages in response to light in a wide wavelength range, from the visible to the far-infrared. In the terahertz frequency range, the device showed responsivities as high as 2.1 mA/W.
3:54PM W22.00006 Polarization-dependent terahertz spectroscopy of macroscopic films of aligned single-wall and multiwall carbon nanotubes, XIAOWEI HE, JOHN ROBINSON, WEILU GAO, AHMED ZURBAIR, Rice University, NØE ALVAREZ, University of Cincinnati, ROBERT H. HAUGE, JUNICHIRO KONO, Rice University — The light absorption properties of carbon nanotubes are strongly anisotropic, especially in the terahertz (THz) region of the electromagnetic spectrum due to their inherently one-dimensional intraband carrier dynamics. Macroscopic films of aligned carbon nanotubes are thus ideal for developing high-performance, low-cost THz polarizers. Here, we present results of polarization-dependent time-domain THz spectroscopy studies of large-area films of aligned single-wall carbon nanotubes (SWCNTs) and multiwall carbon nanotubes (MWCNTs) in a frequency range of 0.15-1 THz by varying the polarization of the incident beam with respect to the carbon nanotube alignment direction. The nematic order parameter ($S$), the extinction ratio (ER), and the degree of polarization (DOP) were calculated to establish the performance of the films as polarizers. We found the $S$ of the SWCNT film to be 0.96. The ER of the SWCNT was found to be -12 dB. The measured value of the $S$ for the MWCNT was 0.77, with an ER of -11 dB.

4:06PM W22.00007 Revisiting length-dependent Raman spectroscopy of single-wall carbon nanotubes using single chirality, length-refined populations, YANMEI PIAO, STEPHANIE LAM, ANGELA HIGHT WALKER, JEFFREY FAGAN, National Institute of Standards and Technology (NIST) — As-synthesized, single-wall carbon nanotube (SWCNT) populations contain a wide variety of diameter and length nanotubes. This structural diversity with its accompanying property variation, especially in optical properties, provides a great challenge to the characterization for these materials. Given the tremendous effort to understand the diameter-dependent optical properties of SWCNTs, it is perhaps surprising that little recent work has re-examined the consequences of length, a correspondingly important factor in terms of characterization, to our understanding of the science. Early work demonstrated that for SWCNTs of mixed chirality, the variation in length drove a degradation at short lengths in the optical responses. Since then, identification that morphological impurities and defect density were highly correlated with length in singly sorted samples prompted a reexamination of those results. In this work we probe the length-dependent optical properties of SWCNTs using extremely high-quality SWCNT populations based on multiple aqueous-two-phase separations followed by size exclusion chromatography length-separations. Our results reveal significant and varying dependencies on properties including the G peak intensity and D/G ratio as measured by resonant Raman spectroscopy with the length of single species SWCNT populations, and in other optical properties including absorption and fluorescence.

4:18PM W22.00008 Wide dynamic range stretchable electrical interconnect using carbon nanotube sheets and elastomer, YOURACK LEE, VIET THONG LE, YONG HEE LEE, DONGSEOK SUH, Center for Integrated Nanostructure Physics, Institute for Basic Science. — Stretchable electric conductor has been investigated for bendable electronics and wearable devices. Nanoscale conducting materials such as silver nanowires, gold nanoparticles, graphenes, and carbon nanotubes had been employed for stretchable conductor. Various structural designs like wrinkle, coil and even fabric had been adopted to reduce a direct stress applied to conducting materials for structural stability. Once such conducting materials are stretched, however, their resistance increased enormously because of the dimensional change related to Poisson ratio and the percolation based electrical conduction. In this study, we fabricated a stretchable conductor by combining carbon nanotube sheets and highly stretchable elastomer, which only has 10% of resistance change while it is stretched up to 600% strain. And we found out that the resistance change can be decreased less than 1%, even though it is stretched up to 600% strain, by using a proper capping method that prevents the contacts between folded regions of conducting materials. We expect that this method can help the practical usage of this stretchable conductor as a stretchable electrical interconnect applications.

4:30PM W22.00009 Enhanced Electrical Conductivity of Aluminum by Carbon Nanotube Hybrid Dilution, SHELBY STIGERS, The Pennsylvania State University-Altoona College, ALEXANDER SAVADELIS, KATHRYN CARRUBA, KILEY JOHNS, The Pennsylvania State University, KOFI ADU, The Pennsylvania State University-Altoona College — Carbon nanotubes (CNTs) have been recognized as potential candidate for reinforcements in lightweight metals. A composite consisting of CNTs embedded in an Al-matrix might work as an ultra-low-resistive material with the potential of having a room-temperature resistivity far below Al, Cu and Ag. While several advances have been made in developing Al-CNT composites, three major challenges: (1) interfacial bond strength between CNT and the Al matrix, (2) homogeneous dispersion of the CNTs in the Al matrix and impurity (CNTs) scattering centers, continue to limit progress in Al-CNT composites. Several conventional methods including powder metallurgy, melting and solidification, thermal spray and electrochemical deposition have been used to process Al and CNT to form composites. We present preliminary results that address these challenges: (a) multiphase in-situ 3D alignment of CNTs in an Al matrix, (b) high-quality Al-CNT composites using CNT hybrid as reinforcement and an inductive melting technique that takes advantage of the induced eddy current in the melt to provide in-situ stirring.

4:42PM W22.00010 Carbon Nanotube Networks Reinforced by Silver Nanowires with Improved Optical Transparency and Conductivity, PATRICIA MARTINE1, University of Texas, Dallas, AZIN FAKHIMI, Surrey University Guildford, UK, LING LIN2, University of Texas, Dallas, IZABELA JUREWICZ, ALAN DALTON, Surrey University Guildford, UK, ANVAR A. ZAKHIDOV3, RAY H. BAUGHMAN1, University of Texas, Dallas — We have fabricated highly transparent and conductive free-standing nanocomposite thin film electrodes by adding silver nanowires (AgNWs) to dry-spun Multiwall Carbon Nanotube (MWNT) aerogels. This nanocomposite exhibits desirable properties such as high optical transmittance, excellent flexibility and enhanced electrical conductivity. The incorporation of the AgNWs to the MWNT aerogels was accomplished by using a spray coating method. The optical transparency and sheet resistance of the nanocomposite was tuned by adjusting the concentration of AgNWs, back pressure and nozzle distance of the spray gun to the MWNT aerogel during deposition. As the solvent evaporated, the aerogel MWNT bundles densified via surface tension which caused the MWNT bundles to collapse. This adjustable process was responsible in forming well defined apertures that increased the nanocomposite’s transmittance up to 90 percent. Via AgNWs percolation and random interconnections between separate MWNT bundles in the aerogel matrix, the sheet resistance decreased from 1 K ohm/sq to less than 100 ohm/sq.

1This work was supported by the Institute for Basic Science (IBS-R011-D1) and the Basic Science Research Program through the NRF of Korea, funded by the Ministry of Science, ICT & Future Planning (No. 2013R1A1A1070606).

2This Work is Supported by Penn State Altoona Undergraduate Research Sponsored Program and Penn State Materials Research Institute, University Park

3Alan G. MacDiarmid NanoTech Institute
4Alan G. MacDiarmid NanoTech Institute
5Alan G. MacDiarmid NanoTech Institute
6Alan G. MacDiarmid NanoTech Institute
The interplay of interactions and disorder within the typical medium dynamical cluster approximation using the Anderson-Hubbard model. By the typical medium theory (TMT), and showed that the typical (not average) DOS is critical at the transition. While the TMT is able to capture the localized distribution, for which the most probable and the typical values differ noticeably from the average value. Dobrosavljevic et.al., incorporated such ideas in their potential approximation and its cluster extensions [1] fail to describe the Anderson transition, as the average density of states (DOS) employed in such theories...
matrices per site: the G show that product states over Matrix Product Operators of small bond dimension is the corresponding natural language for describing the MBL phases. In this (MBL) phases. The natural language for representing the spectrum of the Anderson insulator is that of product states over the single-particle modes. We interacting disordered systems which have localized single particle eigenstates. The interacting analogue of Anderson insulators are the Many-Body Localized operators [4] M. E. Flatté, Nature Phys. 7, 285-286 (2011).


3:30PM W23.00004 Study of multiband disordered systems using the typical medium dynamical cluster approximation , YI ZHANG, Louisiana State Univ - Baton Rouge, HANNA TERLETSKA, Ames Laboratory, CONRAD MOORE, CHINEDU EKUMA, KA MING TAM, JUANA MORENO, MARK HARRELL, Louisiana State University — We generalize the typical medium dynamical cluster approximation to disordered systems with multiple bands. Using our extended formalism, we perform a systematic study of the non-local correlation effects induced by disorder on the density of states and the mobility edge of the Anderson localized states. We apply our method to three dimensional multiband Anderson model with both inter- and intra-band hopping and disorder potential and find fast convergence with increasing cluster size. Our results are consistent with the ones obtained by the transfer matrix and the kernel polynomial methods. Our findings show that the typical medium dynamical cluster approximation method can be used to study the Anderson localization in real materials.

3:42PM W23.00005 Benchmarking Multiband Cluster Typical Medium Theory , CONRAD MOORE, YI ZHANG, KA MING TAM, JUANA MORENO, MARK HARRELL, Louisiana State University — We perform transfer matrix calculations on a non-interacting multiple band disordered system with diagonal and off-diagonal disorder. The mobility edge is determined by finite size scaling. We compare with mobility edge predictions from the Typical Medium Dynamical Cluster Approximation (TMDCA). From these results, we discuss the applicability of TMDCA to study localization in realistic disordered systems.

3:54PM W23.00006 Disorder Problem In Diluted Magnetic Semiconductors, RYKLY NELSON, CHINEDU EKUMA, HANNA TERLETSKA, Louisiana State University, VIDHYADHIRAJA SUDHINDRA, Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, 560064, India, JUANA MORENO, MARK HARRELL, Louisiana State University — Motivated by experimental studies [1-4] addressing the role of impurity disorder in diluted magnetic semiconductors (DMS), we investigate the effects of disorder using a simple tight-binding Hamiltonian with random impurity potential and spin-fermion exchange which is self-consistently solved using the typical medium theory. Adopting the typical density of states (TDoS) as the order parameter, we find that the TDoS vanishes below a critical concentration of the impurity, which indicates an Anderson localization transition in the system. Our results qualitatively explain why at concentrations lower than a critical value DMS are insulating and paramagnetic, while at larger concentrations are ferromagnetic. We also compare several simple models to explore the interplay between ferromagnetic order and disorder induced insulating behavior, and the role of the spin-orbit interaction on this competition. We apply our findings to (Ga,Mn)As and (Ga,Mn)N to compare and contrast their phase diagrams.

4:06PM W23.00007 Encoding the structure of many-body localization with matrix product operators, DAVID PEKKER, University of Pittsburgh, BRYAN K. CLARK, University of Illinois at Urbana Champaign — Anderson insulators are non-interacting disordered systems which have localized single particle eigenstates. The interacting analogue of Anderson insulators are the Many-Body Localized (MBL) phases. The natural language for representing the spectrum of the Anderson insulator is that of product states over the single-particle modes. We show that product states over Matrix Product Operators of small bond dimension is the corresponding natural language for describing the MBL phases. In this language all of the many-body eigenstates are encode by Matrix Product States (i.e. DMRG wave function) consisting of only two sets of low bond-dimension matrices per site: the $G_i$ matrix corresponding to the local ground state on site $i$ and the $E_i$ matrix corresponding to the local excited state. All $2^n$ eigenstates can be generated from all possible combinations of these matrices.

4:18PM W23.00008 Typical density of states as an order parameter for the Anderson localization , KA-MING TAM, CONRAD MOORE, JUANA MORENO, MARK HARRELL, Louisiana State University — The typical medium theory and its recently proposed extensions for models with off-diagonal disorder and multiple bands are significant progress towards the study of localization phenomenon in real materials. The fundamental assumption of these methods is that the typical density of states can be treated as an order parameter. However, its justifications in lattice model is largely lacking. This is predominantly due to two factors. First, the lattice sizes amenable for exact diagonalization is rather limited. Second, the small lattice sizes lead to a very sensitive dependence on the broadening factor. In this work, we use the kernel polynomial method to perform simulation for large system sizes. By adapting the method for the study of criticality, we find that the typical density of states has a well defined finite size scaling behavior. In particular, from the kurtosis, Binder ratio, of the distribution of the density of states for different lattice sizes, we find a clear crossing to identify the critical point. This provides further support that the typical density of states can be used as an order parameter for the localization transition.

Thursday, March 5, 2015 2:30PM - 5:30PM — Session W24 DCOMP: Electronic Structure Methods V 203AB - Eric Shirley, National Institute of Standards and Technology
The work was supported by the Center for Defect Physics, an Energy Frontier Research Center of DoE.

1National High Magnetic Field Laboratory

3:30PM W24.00006 Projector Augmented-Wave formulation of response to strain and electric field perturbation within the density-functional perturbation theory. ALEXANDRE MARTIN, CEA-DIF, Arpajon, France, MARC TORRENT, CEA-DIF, Arpajon, France, RAZVAN CARACAS, CNRS - ENS Lyon, France — A formulation of the response of a system to strain and electric field perturbations in the pseudopotential-based density functional perturbation theory (DFPT) has been proposed by D.R Hamman and co-workers. It uses an elegant formalism based on the expression of DFT total energy in reduced coordinates, the key quantity being the metric tensor and its first and second derivatives [1]. We propose to extend this formulation to the Projector Augmented-Wave approach (PAW). In this context, we express the full elastic tensor including the strain tensor (the response to electric field change (piezoelectric tensor and effective charges). With this we are able to compute the elastic tensor for all materials (metals and insulators) within a fully analytical formulation. The comparison with finite differences calculations on simple systems shows an excellent agreement. This formalism has been implemented in the planewave code ABINIT. We apply it to the computation of elastic properties and seismic-wave velocities of iron with impurity elements. By analogy with the materials contained in meteorites, tested impurities are light elements (H, O, C, S, Si).


3:42PM W24.00007 Constructing Wannier functions with automatically selected trial orbitals, JAMAL I. MUSTAFA, SINISA COH, MARVIN L. COHEN, STEVEN G. LOUIE, University of California at Berkeley, Lawrence Berkeley National Lab — Maximally localized Wannier functions (MLWFs) are widely used in electronic structure theory. Some applications include analysis of chemical bonding, electric polarization, orbital magnetization, and Wannier interpolation. The state of the art method for constructing MLWFs of N composite bands is based on the method of Marzari and Vanderbilt (MV) and is implemented in the Wannier90 code. One of the practical difficulties in constructing Wannier functions using the MV method is choosing the set of starting atomic orbitals and then selecting an optimal subspace of them. We propose a new approach which puts conditions only on the density and potentials. This approach allows a proof that if the density is continuous and nowhere vanishing, then a representing potential in $L^2 + L^\infty$ is unique up to an overall constant.

This work was supported by NSF Grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at LBNL's NERSC facility.

2:42PM W24.00002 a new approach to Hohenberg-Kohn theorem. PAUL LAMMERT, Pennsylvania State Univ — The Hohenberg-Kohn theorem is a cornerstone of electronic density functional theory, and yet in order to carry through its proof one must assume that ground state wavefunctions never vanish on a set of nonzero Lebesgue measure. This is a particularly unsatisfactory situation since DFT is supposed to avoid need of knowing the many-body wavefunction. I propose a new approach which puts conditions only on the density and potentials. This approach allows a proof that if the density is continuous and nowhere vanishing, then a representing potential in $L^2 + L^\infty$ is unique up to an overall constant.

2:54PM W24.00003 Enhanced transferability for Bethe-Salpeter Calculations, ERIC L. SHIRLEY, NIST — We have systematized projector-augmented-wave methods to reliably augment plane-wave/pseudopotential Bloch functions in atomic core regions for purposes of performing screening calculations, evaluating transition matrix elements, and evaluating Slater integrals in the condensed matter environment. This has improved the accuracy of core-hole screening, adherence to sum rules, and control of the strength of absorption features. This also ensures that transition matrix elements and concomitant core excitation spectra are reliable over significant energy ranges. To accomplish this, we improve the quality of the pseudopotentials (which become harder), extending norm conservation, and increasing the number of “valence electrons.” We present results for both insulators and metals, and for both core and valence excitations. Comparison to experimental data is a key part of this work. We also emphasize what approximations remain to be tackled in the treatment of electronic excitation spectra, many of which are more difficult to treat than what is within the scope of this work.

3:06PM W24.00004 A convergence test of the full potential KKR method, G.M. STOCKS, Oak Ridge National Laboratory, YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University — The full-potential Korringa-Kohn-Rostoker (KKR) method is a powerful tool for the ab initio study of the electronic structure of solids. In this method, the expansion of crystal wave functions, the LDA potential, and the charge density are determined by three angular momentum parameters respectively. Essentially, these three angular momentum parameters are an important key for controlling the convergence of an electronic structure calculation. In this presentation, we demonstrate the convergence character of the full potential KKR method by running the electronic structure calculation for a set of transition metals. We will discuss the implication of the results, and show the optimal choice of the angular momentum parameters, which are the one that requires the least computational cost for the desired accuracy for the total energy.
Different parametrizations are examined. The ability to distinguish metallic and Mott insulating solutions is analysed. In DMFT applications, a key issue is the choice of descriptor, the data representation used as input for ML, which is not dependent on the impurity solver. That ML can be used efficiently for the Anderson impurity model (AIM) [1] and present preliminary results on its use as a solver for dynamical mean field theory (DMFT) framework, it is shown that the dielectric matrix parametrization, which is usually applied to calculate the random phase approximation (RPA) correlation energy, can also be used for alternative RPA expressions including exchange effects. Within this framework we derive a simple effective theory for the correlation energy within the second order screened exchange (SOSEX), an approximate time-dependent Hartree-Fock (TDHF), and second order Möller-Plesset (MP2) levels of theory. The accuracy of these approaches can be further improved by the effect of screening to obtain an approximate formulation of the Bethe-Salpeter equation for correlation energies. The proposed formalism is particularly suitable for implementation in periodic boundary condition plane-wave codes, in particular by using a compact basis set to represent dielectric matrices [1,2]. To demonstrate the accuracy of these approaches the binding curves of several diatomic molecules will be shown.

but does not meet the analytic upper bound of a linear scaling with relative density that is predicted for stretching dominated geometries like the octet-truss.

Combining novel nanoscale mechanical properties with a 3-dimensional architecture enables the creation of new classes of materials with tunable properties. These structures can be made on length scales spanning multiple orders of magnitude, from tens of nanometers to hundreds of microns. The smallest features are controllable on length scales where materials have been shown to exhibit size effects in their mechanical response. In contrast to the traditional ground state structure prediction method where the total energy was solely used as the fitness function, we adopted a new fitness function in combination with the first-principles calculation to select the optimal solutions for a description of given chemical systems. The result suggested that our approach is reliable and can be widely applied into design of new electrides.

This work was supported by the Austrian Spezialforschungsbereich Vienna Computational Materials Laboratory (SFB ViCoM) and the Deutsche Forschungsgruppe (FOR) 1346.

5:18PM W24.00015 Self-consistent GW(QP)+Vertex calculations for the insulating oxides of transition (rare earth) metals, ANDREY KUTFEPPOV, VLADIMIR ANTROPOV, Ames Lab, Ames, IA, SERGEY SAVRASOV, University of California, Davis, CA, GABRIEL KOTLIAR, Rutgers University, Piscataway, NJ — Searching for a methodology with predictive power we have developed recently a new approach incorporating many-body vertex corrections into GW-based numerical schemes. Here we apply it to study the electronic structure of the following materials: SrTiO3, TiO2, NiO, and CeO2. We compare four different variations of the scheme: GW, GW+Vertex, QP (quasi-particle), and QP+Vertex. All calculations have self-consistency, at either the full or the QP level. Whereas vertex corrected GW approximation only partially corrects the GW results the QPGW approximation supplemented with first order vertex corrections to both polarizability and self energy allows us to improve essentially the agreement between calculated and experimental spectra. The addition of vertex correction diagrams to the GW method is straightforward. We discuss the subtleties involved in the addition of vertex corrections to the QPGW method. Formally our approach can be considered as fully self-consistent GW(QP)+DMFT with a perturbative impurity solver and the implications for GW(QP)+DMFT will be discussed.

Thursday, March 5, 2015 2:30PM - 5:18PM
Session W25 DMP: Focus Session: Cooperative Phenomena in Plasticity III

2:30PM W25.00001 ABSTRACT MOVED TO F23.00009 –

2:42PM W25.00002 Dsigen of Inorganic Electrodes, ZHANG YUNWEI, PENG FENG, MA YANMING, Stake Key Laboratory of Superhard Materials, Jilin University — Electrodes, in which all of or part of the valence electrons occupy interstitial regions in the crystal and behave as anions, have been synthesized at ambient or high-pressure conditions [1]. Their loosely bound anionic electrons make electrodes good candidates for electroactive materials. Here, we report a developed methodology to systematically design electrodes for given chemical systems. The new approach is based on the swarm-intelligence CALYPSO algorithm on structure prediction [2-3] and requires only the chemical compositions to predict the electrode phases. In contrast to the traditional ground state structure prediction method where the total energy was solely used as the fitness function, we adopted a new fitness function in combination with the first-principles calculation to select the optimal solutions for a description of given chemical systems. The result suggested that our approach is reliable and can be widely applied into design of new electrodes.


2:54PM W25.00003 Spontaneous thermally-induced delamination of polymer films, PUNIT KOHLI, KEXIN JIAO, CHUANHONG ZHOU, JARED WYNNE, ANISH POUDE, PHILIP CHU, Southern IL Univ-Carbondale, CHEMISTRY AND BIOCHEMISTRY — In this talk, we will discuss spontaneous thermally-induced biaxial delamination of thin polymer films from flat surfaces. The delamination results in the formation of ultra-high aspect ratio (up to 1000) of micro-ribbons of polydimethylsiloxane. The thickness, width, and length of the micro-ribbons is about 10 µm, 100 µm, and up to many centimeter respectively. We will demonstrate that the formation of polymer micro-ribbons can be experimentally controlled. Specifically, the thickness and mechanical properties of polymer, and geometrical and physical properties of the substrate played crucial roles in defining the delamination process. From the practical viewpoint, we demonstrate the use of the micro-ribbons for imaging and separation applications.

[1] NSF, NIH, and SIUC

3:06PM W25.00004 Mechanical properties of 3D ceramic nanolattices, LUCAS MEZA, California Institute of Technology — Developments in advanced nanoscale fabrication techniques have allowed for the creation of 3-dimensional hierarchical structural meta-materials that can be designed with arbitrary geometry. These structures can be made on length scales spanning multiple orders of magnitude, from tens of nanometers to hundreds of microns. The smallest features are controllable on length scales where materials have been shown to exhibit size effects in their mechanical properties. Combining novel nanoscale mechanical properties with a 3-dimensional architecture enables the creation of new classes of materials with tunable and unprecedented mechanical properties. We present the fabrication and mechanical deformation of hollow tube alumina nanolattices that were fabricated using two-photon lithography direct laser writing (DLW), atomic layer deposition (ALD), and oxygen plasma etching. Nanolattices were designed in a number of different geometries including octet-truss, octahedron, and 3D Kagome. Additionally, a number of structural parameters were varied including tube wall thickness (t), tube major axis (a), and unit cell size (L). The resulting nanolattices had a range of densities from 0 = 4 to 250 mg/cm³. Uniaxial compression and cyclic loading tests were performed on the nanolattices to obtain the yield strength and modulus. In these tests, a marked change in the deformation response was observed when the thickness was reduced below 20nm: thick-walled nanolattices (>20nm) underwent catastrophic, brittle failure, while thick-walled nanolattices (>20nm) underwent catastrophic, brittle failure. Thick-walled nanolattices also exhibited no recovery after compression, while thin-walled structures demonstrated notable recovery, with some recovering by 98% after compression to 50% strain and by 80% when compressed to 90% strain. Across all geometries, unit cell sizes, and wall thicknesses, we found a consistent power law relation between strength and modulus with relative density of E ∝ ρα and σ ∝ ρβ. This scaling marks an improvement over the formation of lightweight and ultralight materials, which normally scale as E ∝ ρ2 or E ∝ ρ3, but does not meet the analytic upper bound of a linear scaling with relative density that is predicted for stretching dominated geometries like the octet-truss.

3:42PM W25.00005 ABSTRACT WITHDRAWN –
The graphene film. The amplitude data was used to calculate the mechanical resistance and slip time for water molecules sliding on the graphene surface. The measurements were performed with the QCM mounted in vacuum, and then water vapor was slowly introduced into the vacuum chamber until it reached saturation, while simultaneously monitoring the frequency and amplitude of the QCM. Negative shifts in frequency were observed, indicating that water vapor formed a film on the graphene film. The amplitude data was used to calculate the mechanical resistance and slip time for water molecules sliding on the graphene surface. The low slip time indicates a relatively low friction between a water film and graphene. Funding provided by NSF DMR.

3:54PM W25.00006 Shock induced chemistry in granular Ni/Al nanocomposites. MATHEW CHERUKARA, Purdue Univ, TIMOTHY GERMANN, EDWARD KOBER, Los Alamos National Lab, ALEJANDRO STRACHAN, Purdue Univ — Intermolecular reactive composites find diverse applications in defense, microelectronics and medicine, where strong, localized sources of heat are required. However, fundamental questions of the initiation and propagation mechanisms on the nanoscale remain to be addressed, which is a roadblock to their widespread application. Motivated by experimental work which has shown that high-energy ball milling can significantly improve the reactivity as well as the ease of ignition of Ni/Al inter-metallic composites, we present large scale (~ 41 million atom) molecular dynamics simulations of shock-induced chemistry in granular Ni/Al nano-composites, which are designed to capture the microstructure that is obtained post milling. Shock propagation in these granular composites is observed to be extremely diffuse at low piston velocities, leading to a large inhomogeneity in the local stress states of the material. At higher piston velocities, the shock front is more homogeneous as a consequence of a change in the compaction mechanism; from plastic deformation mediated pore collapse at low piston velocities, to fluid filling of the pores at higher impact velocities. The flow of molten ejecta into the pores subsequently leads to the formation of vortices, where the reaction progresses much faster than in the bulk.

4:06PM W25.00007 Stoichiometric Control of DNA-Grafted Colloid Self-Assembly. THI VO, VENKAT VENKATASUBRAMANIAN, SANAT KUMAR, Columbia University, BABJI SRINIVASAN, Indian Institute of Technology - Gandhinagar, SUCHETAN PAL, YUGANG ZHANG, OLEG GANG, Brookhaven National Lab — There have been recent surges of interest in understanding the self-assembly of DNA-grafted colloids into different crystallographic lattices, namely CsCl, AIB2, Cr3Si, and Cs6SiC60. Conventional approaches view the number of grafted linkers and effective size of each colloid as the major governing design parameters. It is generally assumed that the mixed stoichiometries need to match those defined by the target structures in order to obtain the desired lattice. Thus, contributions from stoichiometry are considered secondary and its exact effects on lattice formation remains an open question. Theoretical extensions to the popular complementary contact model show that the equilibrium lattice structure can be tuned through direct control of stoichiometry. Our results are also validated through experimental observations of the equilibrium crystal morphologies at differing stoichiometric ratios. These findings strongly suggest that stoichiometry is a new handle that can be used to control DNA-grafted colloidal self-assembly.

4:18PM W25.00008 Computational Study of Nanoparticle Clustering via DNA Hyperdyzation1. XIU MA, MARK J. BOWICK, Syracuse University, RASTIKO SKNEPNEK, University of Dundee — We use molecular dynamics simulation to study the self-assembly of small clusters through DNA hybridization in a binary mixture of spherical nucleic acid gold nanoparticles(SNA-GNPs) system. The resultant structures are self-assembled clusters with a varying number of large SNA-GNPs clusters around the small ones, forming dimers, trimmers, tetramers etc. The outcome structures can be tuned by adjusting external factors including temperature, particle hydrodynamics size ratio.

3:54PM W25.00006 Shock induced chemistry in granular Ni/Al nanocomposites. MATHEW CHERUKARA, Purdue Univ, TIMOTHY GERMANN, EDWARD KOBER, Los Alamos National Lab, ALEJANDRO STRACHAN, Purdue Univ — Intermolecular reactive composites find diverse applications in defense, microelectronics and medicine, where strong, localized sources of heat are required. However, fundamental questions of the initiation and propagation mechanisms on the nanoscale remain to be addressed, which is a roadblock to their widespread application. Motivated by experimental work which has shown that high-energy ball milling can significantly improve the reactivity as well as the ease of ignition of Ni/Al inter-metallic composites, we present large scale (~ 41 million atom) molecular dynamics simulations of shock-induced chemistry in granular Ni/Al nano-composites, which are designed to capture the microstructure that is obtained post milling. Shock propagation in these granular composites is observed to be extremely diffuse at low piston velocities, leading to a large inhomogeneity in the local stress states of the material. At higher piston velocities, the shock front is more homogeneous as a consequence of a change in the compaction mechanism; from plastic deformation mediated pore collapse at low piston velocities, to fluid filling of the pores at higher impact velocities. The flow of molten ejecta into the pores subsequently leads to the formation of vortices, where the reaction progresses much faster than in the bulk.

4:06PM W25.00007 Stoichiometric Control of DNA-Grafted Colloid Self-Assembly. THI VO, VENKAT VENKATASUBRAMANIAN, SANAT KUMAR, Columbia University, BABJI SRINIVASAN, Indian Institute of Technology - Gandhinagar, SUCHETAN PAL, YUGANG ZHANG, OLEG GANG, Brookhaven National Lab — There have been recent surges of interest in understanding the self-assembly of DNA-grafted colloids into different crystallographic lattices, namely CsCl, AIB2, Cr3Si, and Cs6SiC60. Conventional approaches view the number of grafted linkers and effective size of each colloid as the major governing design parameters. It is generally assumed that the mixed stoichiometries need to match those defined by the target structures in order to obtain the desired lattice. Thus, contributions from stoichiometry are considered secondary and its exact effects on lattice formation remains an open question. Theoretical extensions to the popular complementary contact model show that the equilibrium lattice structure can be tuned through direct control of stoichiometry. Our results are also validated through experimental observations of the equilibrium crystal morphologies at differing stoichiometric ratios. These findings strongly suggest that stoichiometry is a new handle that can be used to control DNA-grafted colloidal self-assembly.

4:18PM W25.00008 Computational Study of Nanoparticle Clustering via DNA Hyperdyzation1. XIU MA, MARK J. BOWICK, Syracuse University, RASTIKO SKNEPNEK, University of Dundee — We use molecular dynamics simulation to study the self-assembly of small clusters through DNA hybridization in a binary mixture of spherical nucleic acid gold nanoparticles(SNA-GNPs) system. The resultant structures are self-assembled clusters with a varying number of large SNA-GNPs clusters around the small ones, forming dimers, trimmers, tetramers etc. The outcome structures can be tuned by adjusting external factors including temperature, particle hydrodynamics size ratio.

1Soft Matter Program, Syracuse University

3:40PM W25.00009 Tetrahedrally bonded carbonates and aqueous carbonate anions under extreme conditions1. DING PAN, GIULIA GALLI, Institute for Molecular Engineering, the University of Chicago, DEEP CARBON OBSERVATORY COLLABORATION — The carbonate ion, CO3<sup>-2</sup>, has a trigonal planar structure composed of carbon bonded with three oxygen atoms. The existence of tetrahedrally bonded carbonate units, CO3, analogous to SiO4 in silicates, has long been under debate. Using a combination of first-principles calculations and in situ infrared spectroscopy measurements [1], we provided definitive evidence that in magnesite, at pressures above 80 GPa, sp<sup>3</sup> bonded CO3 trigonal groups transforms into sp<sup>2</sup> bonded CO3 tetrahedral units. These units were found to be asymmetric, with two longer and two shorter C-O bonds. In addition, using first principles molecular dynamics we investigated carbonate anions in water at high temperature and pressure, corresponding to Earth’s upper mantle conditions. We found significant quantities of bicarbonate ions dissolved in the liquid. The relevance of our simulation results for geophysical models of hydrous carbonates in the Earth will be discussed.


3:42PM W25.00010 ABSTRACT MOVED TO S23.00008 —

4:42PM W25.00010 ABSTRACT MOVED TO S23.00008 —

4:54PM W25.00011 Fluorescent probes for shock compression spectroscopy. ALEXANDR BANISHEV, JAMES CHRISTENSEN, DANA DLOTT, University of Illinois at Urbana-Champaign — We have demonstrated the capability of using Rhodamine 6G dye as an ultrafast emission probe in high-speed shock compression of condensed matter. The ultimate time response of the probe, which functions as a high-speed pressure sensor, is limited by fundamental photophysical processes such as radiative rates, internal conversion rates and intersystem crossing rates. The time response has been greatly improved by encapsulating the dye in silica nano or microparticles. This probe was used to observed nanosecond viscoelastic shock compression of a polymer (PMMA), and has been used to monitor the response of individual grains of sand to high-speed impact.

5:06PM W25.00012 Sliding friction levels of water films on graphene measured by means of QCM. ZIJIAN LIU, SAMUEL KENNY, ZACHARY FREDRICKS, JACQUELINE KRIM, North Carolina State University — Diffusion and sliding friction of water on graphene is a matter of great current interest [1]. To study the surface friction of water on graphene, we recorded water film adsorption on a graphene film coated quartz crystal microbalance (QCM). Graphene films were deposited on QCMs via evaporation in vacuum on nickel substrates. Measurements were performed with the QCM mounted in vacuum, and then water vapor was slowly introduced into the vacuum chamber until it reached saturation, while simultaneously monitoring the frequency and amplitude of the QCM. Negative shifts in frequency were observed, indicating that water vapor formed a film on the graphene film. The amplitude data was used to calculate the mechanical resistance and slip time for water molecules sliding on the graphene surface. The low slip time indicates a relatively low friction between a water film and graphene. Funding provided by NSF DMR.


Thursday, March 5, 2015 2:30PM - 5:30PM — Session W26 DCP: Computational Applications and Methods II 204A - Ryan Steele, University of Utah
2:42PM W26.00002 ABSTRACT WITHDRAWN –

2:54PM W26.00003 Ultrafast Electron-Ion Dynamics Near Aluminum Surfaces, ANDRE SCHLEIFE, KAI WELLS, SAM KNEWSTUB, University of Illinois - Urbana — Computational physics and materials research have greatly benefited from high-performance computing; modern first-principles simulations allow insight with unprecedented accuracy and detail. Here we use a recently highly parallel implementation of Ehrenfest molecular dynamics based on real-time time-dependent density functional theory to describe non-adiabatic ultrafast electron-ion dynamics using accurate first-principles calculations. We experiment aluminum subject to highly energetic particle radiation (hydrogen projectile) and study energy deposition due to the fast projectiles. Their high velocity makes it necessary to overcome the Born-Oppenheimer approximation. Using our first-principles calculations we study the behavior of fast ions near the surface of aluminum slabs and investigate, for instance, the influence of velocity and impact angle of the projectile ion. From the emerging non-adiabatic electron-ion dynamics we gain insight into the material on an atto-second time scale.

3:06PM W26.00004 New spectroscopic approaches for periodic systems, SANDRA LUBER, University of Zurich — Knowledge about local properties is extremely helpful for the analysis of structures and interactions. Moreover, it is a valuable source of information for the characterisation of dynamic processes and facilitates the interpretation of experimental data. In case of vibrational spectroscopy, for example, it is desirable to determine the impact of certain atoms/molecules on the bands in the experimental spectra. This may be straightforward for simple systems but becomes more and more complex for larger systems. Calculations provide additional insight allowing the targeted study of specific structures. In this way, it is possible to quantify the contributions of, for instance, solute and solvent molecules or adsorbates on solids. We present novel, computationally efficient methods for the calculation of properties for periodic systems such as liquids and solids. These are applied to calculate, among others, vibrational spectra via ab initio molecular dynamics [2,3]. References: [1] S. Luber, J. Phys. Chem. A 117 (2013) 2760. [2] S. Luber, M. Iannuzzi, J. Hutter, J. Chem. Phys. 141 (2014) 094503.[3] S. Luber, submitted.

3:18PM W26.00005 Polarons in rutile TiO2 surfaces: a non-adiabatic excited-state dynamics study, GRIGORY KOLESOV, School of Engineering and Applied Sciences, Harvard University, DMITRY VINICHENKO, Department of Chemistry and Chemical Biology, Harvard University, GEORGIOS TRITSARIS, School of Engineering and Applied Sciences, Harvard University, CYNTHIA FRIEND, Department of Chemistry and Chemical Biology, Harvard University, EFFTHIMIOS KAXIRAS, School of Engineering and Applied Sciences, Department of Physics, Harvard University — Titanium dioxide is one of the most thoroughly studied photocatalytic materials with numerous proposed applications ranging from hydrogen production to cleanup of environmental pollutants. Photocatalytic methoxy splitting on rutile TiO2 (110) surfaces that leads to formation of formaldehyde has been previously observed in STM and TPD experiments. Due to complexity of such photocatalytic reactions the computational simulations of these reactions are requisite for providing insight into their underlying mechanisms and are crucial for the rational design of new photocatalysts. Because such simulations are necessarily computationally expensive we developed an efficient methodology based on time-dependent density functional theory (TDDFT) and localized basis set. Our recent non-adiabatic simulations of the photo-catalytic methoxy splitting on titania surface demonstrate an extremely important role played in these reactions by surface and subsurface polarons. Here the polarons serve as electron acceptor sites that participate in driving the reaction and are required to stabilize the reaction products and allow for their subsequent desorption from the surface. In this work we focus on the polarons in rutile titanium surfaces and study dynamics of their formation and their properties.

3:30PM W26.00006 TDDFT+DMFT analysis of excitations and relaxation dynamics in alpha-Ce, SYED ISLAMUDDIN SHAH, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics, University of Central Florida — We apply a combination of time-dependent density functional theory and dynamic mean-field theory (TDDFT+DMFT) to study the excitation spectrum and response of bulk alpha-Ce to an external perturbation by a laser pulse. The excitation spectrum is obtained by solving TDDFT Casida equation with the “free electron” spectrum calculated from density functional theory and the exchange-correlation (XC) kernel extracted from the DMFT charge susceptibility. We pay special attention to the complex role of the hybridization of the f- with the s-, p-, and d-electron states in the system spectrum. The nonequilibrium solution of the TDDFT equations shows that the short-lived local moments of f-electrons get suppressed as the hybridization strength between the f- and other orbitals increases. We also calculate the effective scattering times for the scattering of the f-electrons from the s-, p-, and d-states at different values of the local Coulomb repulsion and exchange J parameters from the corresponding expression for the orbital-resolved XC kernel, and analyze how these scattering processes may affect the dynamics of the system relaxation.

3:42PM W26.00007 Auger Relaxation of Hot Electrons in CdSe Quantum Dots using GFSH, DHARA TRIVEDI, Department of Physics & Astronomy, University of Rochester, LINJUN WANG, OLEG PREZHDO, Department of Chemistry, University of Southern California — We carry out ab initio nonadiabatic molecular dynamics (NAMD) simulations to study the fast relaxations of hot electrons in a CdSe quantum dot (QD). The reviewed system is a promising candidate for QD-sensitized semiconductor solar cells and the presence of well-separated conduction electron states opens the possibility of energy selectivity for hot carriers. We examine the intraband relaxation of the photoexcited electrons in the QD and the role of surface ligand in the process. A novel global flux surface hopping (GFSH) approach is adopted. We investigate the electron relaxation from the 1Pe to 1Se state in pure and 1.6-hexanediol ligated CdSe QD. The intraband relaxation is accelerated due to the Auger-type relaxation in the pure QD. The ligand forms a hole trapping state, which competes with the Auger-type relaxation impeding the electron-hole energy exchange. The present study establishes the basic theoretical model describing the relaxation processes in both scenarios. The obtained interplay between the competing phonon-assisted Auger and ligand-induced trapping mechanisms has given us a comprehensive picture of the complex photoinduced dynamic related to QDs.
3:54PM W26.00008 New Developments in Ab Initio Multiple Spawning for Efficient Nonadiabatic Molecular Dynamics\textsuperscript{1}, BASILE F.E. CURCHOD, AARON SIETO, DAVID R. GLOWACKI, TODD J. MARTÍNEZ, Stanford University — Ab initio multiple spawning (AIMS) describes the nonadiabatic dynamics of nuclear wavepackets by means of a linear combination of frozen Gaussian states. While the Gaussian centers follow classical trajectories, the expansion coefficients are propagated according to the time-dependent Schrödinger equation. As a result of the coupling between Gaussian functions, AIMS accurately describes coherence and decoherence effects close to nonadiabatic regions. This accuracy has further been validated by the excellent agreement reported between AIMS dynamics and experimental observations. In this Contribution, we will discuss new techniques used to extend the applicability of AIMS to (i) larger molecules, (ii) long-time simulations, and (iii) dynamics involving an important number of electronic states. We present different examples of nonadiabatic molecular dynamics in organic and atmospheric photochemistry, resulting from the interface between AIMS and the GPU-accelerated electronic structure code TeraChem. New methods improving the AIMS efficiency for larger systems will be discussed, such as the stochastic-selection AIMS. Finally, we will highlight early results on the extension of AIMS to the combined description of both internal conversion and intersystem crossing phenomena.

\textsuperscript{1}B.F.E.C. acknowledges the Swiss National Science Foundation (fellowship P2ELP2_151927) for financial support.

4:06PM W26.00009 Effects of Thermal and Quantum Fluctuations on Dipole-moment distribution of \(H_2O\) molecules in ice \(I_h\)\textsuperscript{1}, PEDRO MOREIRA, UFScar, MAURICE DE KONING, Unicamp — Molecular dipole moments are the fundamental entities that underpin the dielectric behavior of molecular materials. Here, we discuss the molecular dipole distributions of water molecules in ice \(I_h\), considering the roles of proton-disorder, as well as the effects of thermal and quantum fluctuations. For this purpose we employ ab initio Born-Oppenheimer and Path-Integral Molecular Dynamics simulations and compute molecular dipole moments using maximally-localized Wannier functions. We discuss trends in the dipole-moment distributions as a function of temperature.

\textsuperscript{1}P.A.F.P.M. and M.K. acknowledge financial support from the Brazilian agencies Fapesp, Capes, and CNPq. All calculations were performed at CCJDR, IFGW, Unicamp.

4:18PM W26.00010 Screened Hybrid Exact Exchange Schemes to Adsorption Energies on Perovskite Oxides, ELTON SANTOS, Department of Chemical Engineering, Stanford University, Stanford, California 94305, USA — ALEKSANDRA VOJVODIC, SLAC National Accelerator Laboratory, Menlo Park, CA, 94305, JENS K. NORSKOV, Department of Chemical Engineering, Stanford University, Stanford, California 94305, USA — The bond formation between an oxide surface and oxygen, which is one of the important intermediates for oxygen evolution reaction, is investigated using hybrid functionals. We show that there exists a linear correlation between the adsorption energies of oxygen on LaM\textsubscript{O3} (M=Sc-Cu) oxides at hybrid calculations to those computed using semilocal density functionals through the magnetic properties of the bulk phase. The energetics of the spin-polarized surfaces follow the same trend as corresponding bulk systems, which can be treated at a much lower computational cost. The difference in adsorption energy due to magnetism is linearly correlated to the magnetization energy of bulk, i.e., the energy difference between the spin-polarized and the non-spin-polarized solutions. This suggests that one could estimate the correction to the semilocal density functional adsorption energies directly from the hybrid bulk magnetization energy.

4:30PM W26.00011 Kinetic compensation effect in thermal desorption, NAYEUL ZUNIGA-HANSEN, Austin Peay State University, LEONARDO E. SILBERT, Southern Illinois University Carbondale, MERCEDES CALBI, University of Denver — The parameters which characterize the rates of many thermally activated processes are often extracted using the Arrhenius equation. A series of closely related thermally activated processes exhibit systematic variations in the energies of activation, \(E_a\), and preexponential factor, \(\theta\), in response to a perturbation, which leads to the concept of 'kinetic compensation', such that the different parameters in the Arrhenius equation balance each other out thereby leading to an implicitly assumed constant rate. However, the compensation effect has not been generally demonstrated and its origins are not completely understood. Using kinetic Monte Carlo simulations on a model interface, we explore how site-adsorbate and adsorbate-adsorbate interactions, and surface structural changes influence surface coverage and the kinetic parameters during a typical temperature programmed desorption process. We find that the concept of the compensation effect for interacting species breaks down and the time consuming desorption increases with increasing interaction strength due to an increase in the effective activation energy. At the 'molecular' level the changes are the result of enhanced site correlations with increasing adsorbate interaction strength suppressing the onset of desorption.

4:42PM W26.00012 First principles molecular dynamics simulations of the static, dynamic and electronic properties of the liquid silver-tin alloy\textsuperscript{1}, LAZARO CALDERIN, The Pennsylvania State University, PA, USA, DAVID GONZALEZ, LUIS E. GONZALEZ, Universidad de Valladolid, Valladolid, Spain — We report an ab-initio molecular dynamics study of several structural and dynamic properties of the liquid Ag-Sn alloy at three concentrations and a temperature of 1273 K. The calculated structural results show good agreement with the available experimental data and accurately reproduce the measured total static structure factors \[1\]. The heterocoordinating tendencies in the alloy have been analyzed in terms of some short range order parameters. As for the dynamical properties, the single particle dynamics in the liquid alloy has been studied by evaluating several velocity correlation functions and the associated diffusion coefficients. Results are also reported for other transport coefficients, such as the adiabatic sound velocities and shear viscosities. Finally, from the spectra of the longitudinal current correlation functions, the longitudinal dispersion curves have been computed. \[1\] I Kaban, W Hoyer, A Ilinski, O Slukhovskii and S Slyusarenko, J. Non-Cryst. Solids, 331, 254-262 (2003)

\textsuperscript{1}We acknowledge financial support from Spanish MSI (project FIS2012-33126).

5:04PM W26.00013 Orbital-free ab initio molecular dynamics study of the free liquid surface of Sn. From pseudopotential generation and dynamic properties\textsuperscript{1}, BEATRIZ GONZALEZ DEL RIO, LUIS ENRIQUE GONZALEZ TESEDO, Universidad de Valladolid — We report results of an orbital-free ab initio molecular dynamics (OF-AIMD) study of the free liquid surface of Sn at 1000 K. A key ingredient in the OF-AIMD method is the local ionic pseudopotential describing the ions-valence electrons interaction. We have developed a force-matching method \[1\] to derive a local ionic pseudopotential suitable to account for a rapidly varying density system, such as in a free liquid surface. We obtain very good results for several structural properties. We have also studied the evolution of some dynamical properties when going from the central region (where the system behaves like the bulk liquid) towards the free liquid surface.


5:44PM W26.00014 ABSTRACT WITHDRAWN –

5:18PM W26.00015 ABSTRACT WITHDRAWN –
and average responses in junctions that include destructive interference and circular currents.

In this talk, we will introduce the formalism for Noise spectroscopy and illustrate our findings within simple numerical models, displaying time-dependent measurements can be used to detect and quantify intra-molecular processes that occur in the picosecond timescale during the transient regime. In this work, Noise spectroscopy is an intuitive and technically accessible method to model time-dependent transport phenomena in molecular junctions that are driven by electric fields or fluctuating time dependence in the molecular Hamiltonian and is restricted to time-dependent voltages that are adiabatically slow. The method is trivial to computationally functions (NEGF) theory. As shown, the method applies to junctions that can be described by an effective independent-fermion Hamiltonian, admits arbitrary approximations that underlie the method are revealed via a derivation of the effective equations of motion within the framework of non-equilibrium Green's functions. Our method is based on a general analytical solution of the biphasic rate equations. Our method can be used to determine the underlying biphasic interaction mechanism from the analysis of the SPR data, and to extract the rate constants with high confidence levels.

Two-photon absorption (TPA) transition bands of these branched- or butterfly-configured molecules are similar to those in their linear absorption. The molecular TPA cross sections in an excitation environment reach around 50-130 GM, and peak within the available wavelength ranges of a Ti:Sapphire femtosecond oscillator. We also observe that two-photon absorptivity increases progressively with the addition of donor/acceptor moieties on the TPE backbone. This phenomenon is presumably attributed to the improved conjugation length and enhanced intramolecular charge transfer, hence better delocalization of π-system. In UV plasmonics.

We present an aggregation enhancement in two-photon-excited absorption (TPA) transition bands of these branched- or butterfly-configured molecules are similar to those in their linear absorption. The molecular TPA cross sections in an excitation environment reach around 50-130 GM, and peak within the available wavelength ranges of a Ti:Sapphire femtosecond oscillator. We also observe that two-photon absorptivity increases progressively with the addition of donor/acceptor moieties on the TPE backbone. This phenomenon is presumably attributed to the improved conjugation length and enhanced intramolecular charge transfer, hence better delocalization of π-electrons. For each compound, the aggregation enhancement in TPA may also offers clues of aggregation effect on the molecular electronic structure.

Our method is based on a general analytical solution of the biphasic rate equations. Our method can be used to determine the underlying biphasic interaction mechanism from the analysis of the SPR data, and to extract the rate constants with high confidence levels.

Two-photon optical properties of D-TPE-A molecules are introduced into these D-π-A molecules via tetraphenylethylene (TPE), which is used as their π-bridge. Detailed analysis shows that the TPEF of these molecules are enhanced in aggregation environment with both fluorescence quantum efficiency and two-photon absorptivity concomitantly. The two-photon absorption (TPA) transition bands of these branched- or butterfly-configured molecules are similar to those in their linear absorption. The molecular TPA cross sections in an excitation environment reach around 50-130 GM, and peak within the available wavelength ranges of a Ti:Sapphire femtosecond oscillator. We also observe that two-photon absorptivity increases progressively with the addition of donor/acceptor moieties on the TPE backbone. This phenomenon is presumably attributed to the improved conjugation length and enhanced intramolecular charge transfer, hence better delocalization of π-electrons. For each compound, the aggregation enhancement in TPA may also offers clues of aggregation effect on the molecular electronic structure.

A simple method that accurately captures the dynamics of metal-molecule-metal junctions under the influence of time-dependent driving forces is presented. In it, the metallic contacts are modeled explicitly as a discrete set of levels that are dynamically broadened via an artificial damping term in the equations of motion. The approximations that underlie the method are revealed via a derivation of the effective equations of motion within the framework of non-equilibrium Green's functions (NEGF) theory. As shown, the method applies to junctions that can be described by an effective independent-fermion Hamiltonian, admits arbitrary time dependence in the molecular Hamiltonian and is restricted to time-dependent voltages that are adiabatically slow. The method is trivial to computationally implement, has a well defined range where the results are independent of artificial model parameters, and is numerically shown to quantitatively reproduce the time-dependent transport characteristics of a model molecular junction driven by laser fields as described by an exact NEGF method. As such it constitutes an intuitive and technically accessible method to model time-dependent transport phenomena in molecular junctions that are driven by electric fields or fluctuating environments.

Recent theoretical investigations have shown that Ultrafast Laser Pulse Pair Sequences applied to molecular junctions and dc current measurements can be used to detect and quantify intra-molecular processes that occur in the picosecond timescale during the transient regime. In this work, we have continued these investigations and found that while averaged current measurements can capture dynamics directly related to electron transport, one needs to go beyond and consider averaged Noise measurements in order to detect intra-molecular processes not directly participating in the electron transport. In this talk, we will introduce the formalism for this Noise spectroscopy and illustrate our findings within simple numerical models, displaying time-dependent and average responses in junctions that include destructive interference and circular currents.
Resonance Broadening in Molecular Junctions

Our analysis illustrates that interferences can be directly determined from the molecular Hamiltonian and the molecule-electrode couplings. Herein we use linear algebra and the Landauer-Büttiker theory for electron transport to derive a general rule for predicting the existence and locations of interferences in electrode-molecule-electrode transport junctions. We believe that a similar analysis may contribute to the understanding of many phenomena characteristic to the fields of nano- and molecular-electronics.

This work is supported by the DOE, and computational resources are provided by NERSC.

Quantum model of capacitance of nanostructures

We present new insights into the role dimensionality plays in the lead-molecule coupling scheme at molecular electronic junctions. A key ingredient of our approach is a transformation of the Hamiltonian matrix from an atomistic to a state representation of the molecular junction. This provides direct access to the different couplings between the molecular states and the energy manifold of the leads, which underlie the transport properties of molecular junctions. We explore several tight-binding junction models and predict the appearance of coupling bands that depend on the dimensionality and shape of the leads. We believe that a similar analysis may contribute to the understanding of many phenomena characteristic to the fields of nano- and molecular-electronics.

This work is supported by NSF-EPSCOR program (Grants 1002410 and 1010094) and an award from Research Corporation for Science Advancement. JQL is also grateful for the support from the Faculty of Arts and Sciences, University of Puerto Rico at Mayaguez.

Finding Destructive Interference Features in Molecular Transport Junctions

We present new insights into the role dimensionality plays in the lead-molecule coupling scheme at molecular electronic junctions. A key ingredient of our approach is a transformation of the Hamiltonian matrix from an atomistic to a state representation of the molecular junction. This provides direct access to the different couplings between the molecular states and the energy manifold of the leads, which underlie the transport properties of molecular junctions. We explore several tight-binding junction models and predict the appearance of coupling bands that depend on the dimensionality and shape of the leads. We believe that a similar analysis may contribute to the understanding of many phenomena characteristic to the fields of nano- and molecular-electronics.

This work is supported by the DOE, and computational resources are provided by NERSC.

The role of dimensionality on the molecule-lead coupling in molecular electronic junctions

We present new insights into the role dimensionality plays in the lead-molecule coupling scheme at molecular electronic junctions. A key ingredient of our approach is a transformation of the Hamiltonian matrix from an atomistic to a state representation of the molecular junction. This provides direct access to the different couplings between the molecular states and the energy manifold of the leads, which underlie the transport properties of molecular junctions. We explore several tight-binding junction models and predict the appearance of coupling bands that depend on the dimensionality and shape of the leads. We believe that a similar analysis may contribute to the understanding of many phenomena characteristic to the fields of nano- and molecular-electronics.

‘Soft’ amplifier circuits based on field-effect ionic transistors

We present new insights into the role dimensionality plays in the lead-molecule coupling scheme at molecular electronic junctions. A key ingredient of our approach is a transformation of the Hamiltonian matrix from an atomistic to a state representation of the molecular junction. This provides direct access to the different couplings between the molecular states and the energy manifold of the leads, which underlie the transport properties of molecular junctions. We explore several tight-binding junction models and predict the appearance of coupling bands that depend on the dimensionality and shape of the leads. We believe that a similar analysis may contribute to the understanding of many phenomena characteristic to the fields of nano- and molecular-electronics.

We establish a theoretical framework in terms of the curl flux, population landscape, and coherence for non- equilibrium quantum systems at steady state, through exploring the energy and charge transport in molecular processes. The curl quantum flux plays the key role in determining transport properties and the system reaches equilibrium when flux vanishes. The novel curl quantum flux reflects the degree of non-equilibriumness and the time irreversibility. We found an analytical expression for the quantum flux and its relationship to the environmental pumping (non-equilibriumness quantified by the voltage away from the equilibrium) and the quantum tunneling. Furthermore, we investigated another quantum signature, the coherence, quantitatively measured by the non-zero off diagonal element of the density matrix. Quantum flux is promoted by the coherence in the regime of small tunneling while reduced by the coherence in the regime of large tunneling, due to the non-monotonic relationship between the coherence and tunneling. For the systems coupled to bosonic (photonic and phononic) reservoirs the flux is significantly promoted at large voltage while for fermionic (electronic) reservoirs the flux reaches a saturation after a significant enhancement at large voltage.

EPR Studies of orthorhombic Jahn-Teller effect in single crystal of ferroelectric Cu(II)Cds(NH4)2(SO4)3

The isotropic EPR spectra of the 2D ion (in regular octahedral symmetry) at higher temperature becomes anisotropic at low temperature with clear manifestation of orthorhombic g and hyperfine tensors at 15 K. The static Jahn-Teller(JT) effect can only be explained theoretically by assuming the three JT potential wells energetically inequivalent, unlike the potential wells in most of the Cu(II) doped crystalline materials where JT effect manifests. The measured splitting of the JT potential wells in this ferroelectric crystal fall in the sub millimeter wave region pointing to possible application of the material.
5:18PM W27.00015 Probing molecular dynamics at the nanoscale via an individual paramagnetic center TOBIAS STAUDACHER, 3rd Institute of Physics and Research Center SCOPE, University Stuttgart, NICOLE RAATZ, SEBASTIEN PEZZAGNA, JAN MEIJER, Institute for experimental physics II, University of Leipzig, FRIEDMANN REINHARD, Walter Schottky Institut, Technical University Munich, CARLOS MERILES, CUNY-City College of New York, JOERG WRACHTTRUP, 3rd Institute of Physics and Research Center SCOPE, University Stuttgart — We use shallow NVs to probe mesoscale proton ensembles from different substances deposited on the diamond surface. We resort to a form of correlation spectroscopy to reconstruct the equivalent of a nuclear “free-induction-decay” (FID), which, unlike the NMR counterpart, does not require nuclear spin pre-polarization. This pseudo FID has a limit decay time governed by the NV spin-lattice relaxation time T1 (typically longer than the NV coherence lifetime T2), which allows us to attain spectral resolution superior to that possible with standard magnetometry techniques. Upon applying this scheme to solid- and liquid-state substances we find substantial differences in the correlation signal lifetime, which we associate with the presumably different molecular dynamics governing these systems. In particular, we observe long-lived 1H signals from oil molecules, likely a consequence of the interplay between fast molecular tumbling and slow self-diffusion.

Thursday, May 5, 2015 2:30PM - 5:30PM —
Session W28 GMAG DMP FIAP: Focus Session: Spin Caloritronics 205 - Geoffrey Beach, Massachusetts Institute of Technology

2:30PM W28.00001 Spin-current phenomena at high magnetic fields and high temperatures KEN-ICHI UCHIDA, Institute for Materials Research, Tohoku University — In the field of spintronics, many experimental and theoretical studies have been focused on spin-transport phenomena in paramagnet/ferromagnet junction systems, where a spin current plays a central role. After the first demonstration of spin transport in insulator-based systems [1], a Pt/YIG junction system becomes one of the prototype samples. In this system, itinerant spins in Pt and localized magnetic moments in YIG interact with each other via the interface s-d interaction, i.e., the spin-mixing conductance: this interaction is the basic mechanism underlying various spin-current-related phenomena, such as the spin pumping [1], the spin Seebeck effect [2], and the recently-discovered spin Hall magnetoresistance (SMR) [3]. In this talk, we report the observation of the longitudinal spin Seebeck effect (LSSE) [4] and the SMR in Pt/YIG systems at high magnetic fields and high temperatures. The LSSE measurements in a high magnetic field range confirm that the observed voltage in the Pt/YIG systems is of magnon origin, providing a useful way to distinguish the LSSE from the anomalous Nernst effect induced by proximity ferromagnetism in Pt [5]. The LSSE and SMR at high temperatures highlight the importance of the temperature dependence of the spin-mixing conductance at the Pt/YIG interface [6]. These results will be helpful for obtaining full understanding of the mechanism of the LSSE and SMR.

We thank E. Saitoh, S. Maekawa, G. E. W. Bauer, H. Adachi, Y. Ohnuma, T. Kikkawa, S. Daimon, Y. Shiomi, and J. Shiomi for their support and valuable discussions.


3:06PM W28.00002 ABSTRACT WITHDRAWN –

3:18PM W28.00003 Spin current draining effect on heat-driven spin transport1, YADONG XU, BOWEN YANG, CHI TANG, ZI Long JIANG, JING SHI, UC Riverside, MICHAEL SCHNEIDER, RENU WHIG, Everspin Technologies — As a non-magnetic heavy metal is attached to a ferromagnet, a vertically flowing heat-driven spin current is converted to a transverse electric voltage, which is known as the longitudinal spin Seebeck effect. If the ferromagnet is a metal, this voltage is also accompanied by voltages from two other sources, i.e. the anomalous Nernst effect in both the ferromagnet and the proximity-induced ferromagnetic boundary layer. In this work, we have investigated these phenomena in NiFe/Cu/heavy metal multilayer structure. By identifying and carefully separating those effects, we find that in this pure spin current circuit the additional spin current drawn by the heavy metal generates another voltage in the ferromagnetic metal via the inverse spin Hall effect.

1The research was supported by the DOE BES award #DE-FG02-07ER46351 and DARPA/DMEA under H94003-10-2-1004.

3:30PM W28.00004 Mechanism of the two sign changes in the spin Seebeck effect of a compensated ferrimagnet, YUICHI OHNUMA, Tohoku University, HIROTO ADACHI, Japan Atomic Energy Agency, EIJI SAITO,H, Tohoku University, SADAMICHI MAEKAWA, Japan Atomic Energy Agency — Spin Seebeck effect is the mechanism of thermal spin injection from a precessing ferromagnet into an attached paramagnetic metal [Uchida et al., Nature 455, 778 (2008)]. We have theoretically investigated the spin Seebeck effect in compensated ferrimagnets [Ohnuma et al., Phys. Rev. B 87, 014423 (2013)] and predicted that the sign of the spin Seebeck signal changes at the compensation temperature, which is recently confirmed by an experiment [Gepr"ags et al., arXiv:1405.4971 (2014)]. Interestingly, the experiment found another sign change at a lower temperature. Here we explain its origin by taking account of sublattice dependence of the exchange coupling at the ferrimagnet/paramagnet interface.

3:42PM W28.00005 The effect of magnetic anisotropy on spin-dependent thermoelectric effects in nanoscopic systems1, MACIEJ MISIORY, Chammers University of Technology (Gothenburg, Sweden) and Adam Mickiewicz University (Poznañ, Poland), JóZEF BARNAS, Adam Mickiewicz University (Poznañ, Poland) — Harnessing of the interplay between transport of charge, spin and energy is a prospect route towards maximizing the functional potential of nanoscopic electronic and spintronic devices. Here, we investigate theoretically spin-related thermoelectric effects in electronic, linear-response transport through a nanoscopic systems exhibiting magnetic anisotropy. As an example, a magnetic tunnel junction with a large-spin impurity—either a magnetic atom or molecule—embedded in the barrier is considered. Conduction electrons traversing the junction can then scatter on the impurity, which effectively can lead to angular momentum and energy exchange between the electrons and the impurity. As we show, such processes have a profound effect on the thermoelectric response of the system. Since the scattering mechanism also involves processes when electrons are inelastically scattered back to the same electrode, one can expect the flow of spin and energy also in the absence of charge transport through the junction. This, in turn, results in a finite spin thermopower, and the magnetic anisotropy plays a key role for this effect to occur. [1] M. Misiorny and Barnañ, Phys. Rev. B 89, 235438 (2014). [2] M. Misiorny and Barnañ, arXiv:1411.2741 (submitted for publication).

1Work supported by the National Science Center in Poland as the Project No. DEC-2012/04/A/ST3/00372.
3:54PM W28.00006 Optical detection of Spin-Seebeck Effect in Ferromagnetic thin films. RYAN MCLAUGHLIN, DANI SUN, VALY VARDYEN, University of Utah — The field of Spin Caloritronics has attracted great interest because of the generation of spin currents in the presence of temperature gradients, mainly detected by means of an Inverse Spin Hall Effect (ISHE) voltage in metals with strong spin-orbit coupling. However, this method of electrical detection is difficult due to the subtle voltage generated by the ISHE combined with a large number of artifacts such as proximity effect, anisotropic magnetoresistance, anomalous Nernst effect, etc., which makes a quantitative understanding of the Spin Seebeck Effect elusive. Instead, here we demonstrate an optical detection of spin accumulation in Ferromagnetic thin films using a custom-built Kerr Rotation sensitive interferometer, enabling us to investigate the pure spin accumulation from Spin Seebeck in the absence of spurious effects.

4:06PM W28.00007 Separation of the inverse spin Hall effect and anomalous Nernst effect in a single ferromagnetic metal using on-chip spin Seebeck devices. STEPHEN WU, JASON HOFFMAN, JOHN PEARSON, ANAND BHATTACHARYA, Argonne National Laboratory — The longitudinal spin Seebeck effect is measured on the ferromagnetic insulator Fe3O4 with the ferromagnetic metal Co0.2Fe0.8B0.2 (CoFeB) as the spin detector in a micro-patterned device structure using an on-chip heater. By using a non-magnetic spacer material between the two materials (Ti), it is possible to decouple the two ferromagnetic materials and directly observe pure spin flow from Fe3O4 into CoFeB. It is shown, that in a single ferromagnetic metal the inverse spin Hall effect (ISHE) and anomalous Nernst effect (ANE) can occur simultaneously with opposite polarity. Using this and the large difference in the coercive fields between the two magnets, it is possible to unambiguously separate the contributions of the spin Seebeck effect from the ANE and observe the degree to which each effect contributes to the total response within a single experiment. Additionally, by using the spin detector layer as a thermometer, an accurate value for the thermal gradient across the device can be measured. These results match well with thermal simulations of our device structure.

3:54PM W28.00008 Thermal Hall Effect of Spins in a Paramagnet. HYUNYONG LEE, JUNG HOON HAN, Department of Physics, Sungkyunkwan University, Suwon 440-746, Korea, PATRICK LEE, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA — Theory of Hall transport of spins in a correlated paramagnetic phase is developed. By identifying the thermal Hall current operator in the spin language, which turns out to equal the spin chirality in the pure Heisenberg model, various response functions can be derived straightforwardly. Subsequent reduction to the Schwinger boson representation of spins allows a convenient calculation of thermal and spin Hall coefficients in the paramagnetic regime using self-consistent mean-field theory. Comparison is made to results from the Holstein-Primakoff reduction of spin operators appropriate for ordered phases.

4:30PM W28.00009 Ultrafast Time-correlated Measurements of Spin-Seebeck effect in Yttrium Iron Garnet. JOHN JAMISON, BRANDON GILES, Department of Materials Science and Engineering, The Ohio State University, Columbus, OH, ZHIHAO YANG, Department of Electrical and Computer Engineering, The Ohio State University, Columbus, OH, ROBERTO MYERS, Department of Materials Science and Engineering, The Ohio State University, Columbus, OH — Recently, the time dependence of the spin-Seebeck effect (SSE) has been measured using optical pulses. These measurements suggest a time response faster than 5ns[1]. Here we present time-correlated measurements of the spin-Seebeck effect in Yttrium Iron Garnet (YIG) using an ultrafast laser. The pulsed beam is split into two individually modulated beams with a controllable delay time with sub-picosecond time resolution. The laser pulses are absorbed by a top Pt contact which generates a transient thermal gradient resulting in a spin current crossing the interface. The spin current is detected as a transverse voltage arising from the inverse spin Hall effect in Pt. We will present measurements of the time-correlated SSE signal from the two pulses as a function of delay time out to 1 ns. [1] Roschewsky et al., Appl. Phys. Lett., 104, 202410 (2014).

4:42PM W28.00010 Spatiotemporal Imaging of Gigahertz Frequency Magnetization Dynamics Using the Time Resolved Anomalous Nernst Effect. JASON BARTELL, DARRYL NGAI, ZHAOQI LENG, G.D. FUCHS, Cornell University — We report on the first demonstration of spatiotemporal magnetic microscopy based on the Time Resolved Anomalous Nernst Effect (TRANE). In TRANE microscopy, pulsed laser light is used to create a transient thermal gradient perpendicular to the film plane. The anomalous Nernst effect generates a corresponding transient electric field that is proportional to the cross product of both the thermal gradient and the in-plane projection of the magnetic moment. We demonstrate TRANE microscopy and use it to study the magnetic configuration and excited magnetization dynamics of patterned YIG samples. We show that the time resolution exceeds 30 ps, allowing measurement of dynamics above 16 GHz. We observe that the spatial resolution using a thermal gradient generated from focused light matches the optical diffraction limit, indicating that lateral thermal diffusion does not limit resolution. Numerical simulations of the time-dependent thermal gradient indicate that the thermal spot can be confined to nanoscale dimensions using, for instance, a plasmon antenna. This could allow TRANE microscopy to achieve bench-top imaging of magnetization with spatial resolution comparable to the domain wall width and temporal resolution in the GHz range.

4:54PM W28.00011 Non-local thermal spin injection: Mapping the magnon spin diffusion length in Yttrium Iron Garnet (YIG). BRANDON L. GILES, Department of Materials Science and Engineering, The Ohio State University, ZHIHAO YANG, Department of Electrical and Computer Engineering, The Ohio State University, JOHN JAMISON, ROBERTO C. MYERS, Department of Materials Science and Engineering, The Ohio State University — The non-local spin detection geometry was developed to sample a pure electron spin current in the absence of an electric field, thereby removing parasitic transport effects [1]. Here we demonstrate the non-local detection of magnon spins that are thermally injected via the spin Seebeck effect in single crystal YIG. A laser is used to thermally generate a spin current under an electrically isolated Pt absorbing pad. The spin current is detected on a remote Pt strip via the inverse spin Hall effect (\(V_{\text{ISHE}}\)). Spatial maps of the spin current are acquired by measuring \(V_{\text{ISHE}}\) while scanning the laser to different absorbing pads. Temperature modeling shows the laser-induced temperature gradient contained within 50\(\mu\)m of the Pt absorbing pad [2]. Thus, the spin detector is isolated from thermal effects unrelated to the spin current. Although the thermal magnon diffusion length at 21K is \(\sim 1\,\mu\)m [3], \(V_{\text{ISHE}}\) is detected at displacements of more than 150\(\mu\)m with an exponential decay constant of 40 \(\mu\)m at 25K.

3:54PM W28.00008 Thermal Hall Effect of Spins in a Paramagnet. HYUNYONG LEE, JUNG HOON HAN, Department of Physics, Sungkyunkwan University, Suwon 440-746, Korea, PATRICK LEE, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA — Theory of Hall transport of spins in a correlated paramagnetic phase is developed. By identifying the thermal Hall current operator in the spin language, which turns out to equal the spin chirality in the pure Heisenberg model, various response functions can be derived straightforwardly. Subsequent reduction to the Schwinger boson representation of spins allows a convenient calculation of thermal and spin Hall coefficients in the paramagnetic regime using self-consistent mean-field theory. Comparison is made to results from the Holstein-Primakoff reduction of spin operators appropriate for ordered phases.

Work supported by the ARO-MURI W911NF-14-1-0016.
The spins diffuse laterally and are detected non-locally on a remote Pt detector via the inverse spin Hall effect (ISHE). This has been demonstrated, in which a laser is focused on an electrically isolated Pt absorbing pad on yttrium iron garnet (YIG), thermally generating a spin current in YIG. This work was supported by ARO MURI. The authors acknowledge the Brazilian agencies CNPq, CAPES, FAPERJ and INCT de Nanoestruturas de Carbono for financial support.
3:30PM W29.00004 Theory of spin relaxation in bilayer graphene.1, denis kochan, susanne irmer, Martin gmitra, jaroslav fabian, university of regensburg — We present a new spin relaxation mechanism based on resonant scattering off local magnetic moments. We apply this mechanism to mono [1] and bilayer graphene and show that it can account for the ultrafast spin relaxation observed in spin injection experiments. In particular, the model explains the opposite dependence of the spin relaxation on the carrier density in mono and in bilayer graphene. We also show that for bilayer graphene the model explains the observed temperature induced changes in the carrier density dependence. [1] D. Kochan, M. Gmitra, J. Fabian; Phys. Rev. Lett. 112, 116602 (2014).

3:42PM W29.00005 Spin-orbit coupling in fluorinated graphene1, susanne irmer, tobias frank, SebastiAn putz, Martin gmitra, denis kochan, jaroslav fabian, University of Regensburg — We theoretically study spin-orbit coupling effects of fluorine chemisorbed on graphene. Both dense and dilute limit reveal a giant local enhancement of spin-orbit coupling by a factor of 1000 in the vicinity of the adatom—spin-orbit strength of about 10 meV. We present results of fully converged first-principles calculations and analyze them by a tight-binding Hamiltonian based on symmetry arguments. Our work covers different limits of fluorine concentration from dense to intermediate to dilute coverage. We find that fluorine’s native spin-orbit coupling exceeds the effect of the sp3 distortion of the lattice. Moreover, we identify fluorine as a weak resonant scatterer giving rise to resonant signatures in the band structure off the Dirac point by about 0.3 eV. Our findings are important for studies on relaxation and transport. Details can be found in the following manuscript: http://arxiv.org/abs/1411.0016

3:54PM W29.00006 Simultaneous magnetic force microscopy and electrical transport measurements of a graphene non-local spin valve, Michael page, Andrew berger, Hua wen, Vidya bhallamudi, Roland Kawakami, P. Chris Hammel, Ohio State University — Non-local signals in graphene spin valves depend on the magnetization states of the ferromagnetic electrodes. Currently, determining the relative influence of each magnetic electrode relies on fitting the non-local signal to the one-dimensional spin diffusion model. We report imaging of the magnetization states of the spin valve electrodes using a custom magnetic force microscope, while simultaneously acquiring the non-local spin signal electrically. This allows direct correlation of the non-local signal features to the switching of the individual electrodes and determination of the relative contribution to the signal by the participating electrodes. We also image the formation and motion of domain walls near the graphene transport channel and correlate these with features in the non-local signal. This measurement technique supports the one-dimensional spin diffusion model and provides information necessary for reliable switching behavior in spin valves with magnetic electrodes.

4:06PM W29.00007 Spintronics in hybrid organic/inorganic heterojunctions1, Shayan hematicyan, institut fuer Physik, Johannes Gutenberg Universitaet Mainz, D-55099-Dept of Physics, Texas A&M University, College Station, Texas 7784-4242, USA, Erik Mcnellis, jairo sinova, institut fuer Physik, Johannes Gutenberg Universitaet Mainz, D-55099 Mainz, Germany — In this work, we present the results of extensive analytical and numerical calculations to investigate spin and charge transport inside organic semiconductors and also at the interface with ferromagnetic metals. Based upon these calculations, we will describe the underlying spin relaxation mechanisms with reference to the spin dependent characteristic parameters e.g. spin relaxation time and spin diffusion length of the organic semiconductors in connection with the ferromagnetic electrodes.

4:18PM W29.00008 Bias Dependence of Tunneling Spin Injection into Graphene, TianCong Zhu, Ohio State Univ - Columbus, Hua Wen, WALID AMAMOU, ZHISHENG LIn, JING Shi, University of California, Riverside, ROLAND KAWAKAMI, Ohio State Univ - Columbus — Bias dependence of spin injection into a spin channel typically exhibits unusual behavior, which has been challenging to understand. In this study, we investigate the bias-dependence of tunneling spin injection into graphene with lateral spin-valve geometry. Co/MgO/graphene is used as tunneling barrier contact and lock-in measurement is performed. By applying a DC bias to AC spin injection current, we observe a strong non-linearity of bias-dependent non-local voltage on both the electron and hole side of graphene. The non-local voltage also flips sign when a large negative DC bias is applied. We extracted the interfacial spin polarization as a function of DC bias. The data analysis suggests that the unusual behavior of bias-dependent tunneling spin injection in graphene is mainly due to the spin polarization changing at the ferromagnetic/graphene interface. To better understand this behavior, we also compare our data with several other existing models on bias-dependent spin injection.

4:30PM W29.00009 Tunable Magnetic Proximity Effects in Graphene Junctions1, Predrag Lazic, Department of Physics, University at Buffalo, State University of New York, Buffalo; New York 14260, USA, Kirill Belashchenko, Department of Physics and Astronomy University of Nebraska-Lincoln, Lincoln, NE 68588-0299, USA, Igor Zutic, Department of Physics, University at Buffalo, State University of New York, Buffalo, New York 14260, USA — The characteristic length of the magnetic proximity effects exceeds the thickness of a graphene layer leading to an important, but typically overlooked, modification of equilibrium and transport properties, as well as the implications for graphene spintronics [1,2]. Using the first-principles studies that integrate a real space density functional theory (GPAW) [3] with the state-of-the art boundary elements electrostatic code based on the Robin Hood method [4], we explore tunable structural and magnetic proximity effects in the ferromagnet/insulator/graphene junctions. We show that the inclusion of a finite-size gate electrodes and van der Walls interaction lead to nontrivial effects that could also be important in other two-dimensional materials beyond graphene.

4:42PM W29.00010 Giant Perpendicular Magnetic Anisotropy of Graphene-Co Heterostructures 1, HONGXIN YANG, ALI HALLAL, MAIRBEK CHSHIEV, Univ. Grenoble Alpes, INAC-SPIINTEC, F-38000 Grenoble, France; CNRS, SPIINTEC, F-38000 Grenoble, France, and CEA, INAC-SPIINTEC, F-38000 Grenoble, France, SPIINTEC THEORY TEAM  — We report strongly enhanced perpendicular anisotropy (PMA) of Co films by graphene coating via ab-initio calculations. [1] The results show that graphene coating can improve the surface anisotropy of Co film up to twice large of the bare Co case and keep the film effective anisotropy being out-of-plane till 25 Å of Co, in agreement with experiments [2,3]. Our layer resolved analysis reveals that PMA of Co (Co/Gr) films mainly originates from the adjacent 3 Co layers close to surface (interface) and can be strongly influenced by graphene. Furthermore, orbital hybridization analysis uncovers the origin of the PMA enhancement which is due to graphene-Co bonding causing an inversion of Co 3d_{x^2} and 3d_{y^2} Bloch states close to Fermi level. Finally, we propose to design Co-graphene heterostructures which possess a linearly increasing surface anisotropy and a constant effective anisotropy. These findings point towards a possible engineering graphene-Co junctions with giant anisotropy, which stands as a hallmark for future spintronic information processing. [1] H. X. Yang, et al. to submit. [2] C. Vo-Van, et al. New J. Phys. 12, 103040 (2010). [3] N. Rougemaille et al. Appl. Phys. Lett. 101, 142403 (2012).

3This work was supported by European Graphene Flagship, European Union-funded STREP project CONCEPT-GRAPHENE, French ANR Projects NANOSSM-GRAPHENE and NMGEM

4:54PM W29.00011 Spin and charge transport across cobalt/graphene interfaces. MAIRBEK CHSHIEV, SPIINTEC, UMR CEA/CNRS/IFJ/G-INP, ALAN KALITSOV, OLEG MRYASOV, Univ of Alabama - Tuscaloosa  — We report ballistic calculations of in-plane and out-of-plane spin and charge transport through graphene device attached to the hcp-Co electrodes. Our calculations are based on the Keldysh non-equilibrium Green Function formalism and the tight binding Hamiltonian model tailored to treat both lateral and vertical device configurations. We present results for (i) vertical device that consists of a one-side fluorinated C,F graphene sandwiched between two hcp Co electrodes and (ii) lateral device consisting of pristine graphene/C,F graphene bilayer with two top hcp-Co electrodes. Our calculations predict large magnetoresistance with small resistance-area product and significant deviation from sinusoidal behavior of spin transfer torque for the vertical device configuration.

5:06PM W29.00012 Blocking of spin transport between Ni_{10}Fe_{20} and Cu by a graphene interlayer, WILL GANNETT, MARK W. KELLER, TOM SILVA, HANS NEMBACH, ANN CHIARAMONTI DEBAY, National Institute of Standards and Technology, Boulder, CO  — By chemical vapor deposition on epitaxial thin films of Cu(111), we are able to produce continuous, large-grain monolayer graphene (Gr). We then sputter deposit Ni_{10}Fe_{20} (Py) in a different chamber to create large area Cu/Gr/Py samples. We are able to avoid damaging the graphene during this process by varying the Py deposition angle, and we confirm this with Raman spectroscopy. Ferromagnetic resonance measurements with a vector network analyzer show no change in damping with varying Py thickness, while Py deposited directly on Cu(111) shows the typical increase in damping associated with spin pumping between Py and Cu. We interpret these results in terms of spin pumping, interfacial conductivity, and magnetic proximity effects.

Thursday, March 5, 2015 2:30PM - 5:30PM  —
Session W30 GMAG DMP: Focus Session: Frontiers in Magnetism I 206B - Christian Binek, University of Nebraska

2:30PM W30.00001 Antiferromagnetic coupling in ferrimagnetic hard-soft core/shell nanoparticles 1, JOSEP NOGUES, ICREA and ICN2 - Institut Catala de Nanociencia i Nanotecnologia, Barcelona, Spain  — The coupling between different magnetic layers in thin film bi-layers and multilayer systems is usually ferromagnetic (FM) (layers parallel to each other). However, other types of couplings such as antiferromagnetic (AFM) (i.e., antiparallel layers) have also been reported. In contrast, the magnetic properties of bi-magnetic core/shell nanoparticles remain relatively unexplored. While Monte Carlo simulations have probed the effects of different types of interface couplings from the theoretical point of view (e.g., FM vs. AFM coupling), experimental work so far has only reported ferromagnetic coupling between the counterparts. Here we present the existence of an interfacial AFM coupling in ferrimagnetic (FM) soft/hard and hard/soft core/shell nanoparticles based on iron and manganese oxides [1]. Narrow size distribution Fe_3O_4/Mn_3O_4 and Mn_3O_4/Fe_3O_4 core/shell, soft/hard and hard/soft, were synthesized by seed-mediated growth. In contrast to conventional systems, the temperature dependence of the magnetization, M, and the ferromagnetic resonance field, H_R, show a downturn at the magnetic ordering temperature of the hard Mn_3O_4 phase (T_C(Mn_3O_4) = 40 K). This decrease in M and H_R can be linked to an antiferromagnetic coupling between both phases. Moreover, element selective X-ray magnetic circular dichroism (XMCD) spectra and hysteresis loops confirm that the magnetization of the Mn-containing phase lies opposite to the Fe-containing phase. Magnetometry hysteresis loops show that for small cooling fields the loop shifts towards negative fields similar to exchange bias in conventional FM/AFM systems. However, for large cooling fields the loops shift to the opposite direction, i.e., positive exchange bias. Finally, Monte Carlo simulations clearly confirm that an AFM interface coupling leads to a magnetization decrease at low temperatures and a positive exchange bias for large cooling fields.


1Partial support from the MAT2013-48628-R project

3:06PM W30.00002 Electronic, magnetic and oxidation properties of Co and Co_{1-x}Ni_{x} sub-nanosopic cylinders, EUGENIO VOGEL, Universidad de La Frontera, Chile, J. MARTIN MONTEJANO-CARRIZALES, FAUSTIN AGUILERA-GRANJA, Universidad Autonoma San Luis Potosi, Mexico  — One of the most convenient shapes among magnetic nanoparticles are cylinders (solid or hollow). They can be made out of different materials, they are easy to produce in different sizes, and they are relatively easy to handle. One of the present aims at present to make these particles as small as possible. Which is the minimum stable cylindrical shape possible? Can they grow from a seed to make large particles? What are their physical properties at this scale where quantum mechanics operate? Some of these questions have been recently answered for the case of cylinders formed by Co atoms [F. Aguileria-Granja, J.M. Montejano-Carrizales, E.E. Vogel, Eur. Phys. J. D (2014) 68:38]. In this presentation we want to get deeper into this problem in particular considering binary magnetic alloys like it is the case when Ni atoms substitute for Co in the original stable structures. We invoke program SIESTA to study different configurations. Among the results shown to be reported are the following: cylindrical clusters are stable to any length at this process; there is an insulator-conductor transition at a certain length; magnetic moments are not uniformly distributed; Ni atoms tend to go to the periphery; Ni alloys tend to be more resistant to oxidation.

3:18PM W30.00003 Structure and magnetic properties of Co/CoO core-shell nanowires, KINJAL GANDHA, KEVIN ELKINS, NARAYAN POUDYAL, J. PING LIU, Department of Physics, The University of Texas at Arlington  — Cobalt nanowires with high coercivity have been synthesized via a solvothermal chemical process. A record high room-temperature coercivity value of 12.5 Koe has been measured in aligned Co nanowires with a diameter of about 15 nm and a mean length of 200 nm. When the surface of the Co nanowires were oxidized, exchange-bias (EB) was detected at low temperatures owing to the exchange coupling between the ferromagnetic (FM) Co core and the antiferromagnetic (AFM) CoO shell of the nanowires. EB fields of ~2.0 kOe were measured at 10 K, along the parallel direction of nanowires. Manipulation and control of the EB in the nanowires may lead to a better understanding of the EB effect and the applications of the nanowires in future permanent magnets and recording media.
3:30PM W30.00004 Chemical Synthesis of Iron-Nickel Nanoparticles1, FRANK ABEL, University of Delaware, VASILIAS TZITZIOS, Institute of Materials science, demokritos, Greece, GEORGE HADJIPANAYIS, University of Delaware — Equiatomic FeNi alloys undergo a phase transformation, like FePt, from a disordered fcc structure to an ordered fct structure. However, unlike FePt in Fe-Ni this transformation is very sluggish and has been only observed in heavily irradiated thin films and in meteorite samples as was recently reported.1,2 In this study, we used a high temperature chemical synthesis route to investigate the possibility of fabricating fct FeNi nanoparticles. The Iron Nickel Boron nanoparticles were made using anhydrous Iron (II) Chloride and Nickel (II) Chloride using Sodium borohydride as a reducing agent in tetr获得ygm under a nitrogen hydrogen atmosphere. The high temperature of the reaction allowed for the formation of as made crystalline Iron Nickel nanoparticles without additional annealing. By changing the concentration of sodium borohydride we were able to prepare nanoparticles either in the pure fcc phase, or in a new mixed phase. The magnetic properties were improved by increasing the concentration of Iron precursor. We obtained FeNi nanoparticles with saturation magnetization of (56 emu/g) and coercivity of (190 Oe). The particle size distribution of the FeNi particles ranged from several hundred nanometers to a half micron. References: 1. L Neel, et al., Journal of Applied Physics, Volume 35, No. 3 (1964) 2. M Kotsugi, et al., Journal of Physics: Condensed Matter, 26 064206 (2014)

1Work Supported by DOE-BES-DMSE (Grants No. DE-FG02-04ER4612)

3:42PM W30.00005 Voltage-Tunable Magnetic Stability in a Ni Nanoparticle3, PATRICK GARTLAND, Georgia Institute of Technology, WENCHAO JIANG, GlobalFoundries, DRAGOMIR DAVIDOVIC, Georgia Institute of Technology — We study single nickel particles ≈ 2nm in diameter using single electron tunneling spectroscopy and find that such particles lie at the threshold of stable ferromagnetic order. We find that the application of a bias voltage can precisely tune the conditions for a stable magnetization orientation, and simulate the experimental configuration using a master equation. Due to the addition of anisotropy from a single electron, a new energy scale emerges which governs the stability of magnetization as a function of voltage bias conditions.

3:54PM W30.00006 Engineered diamond nanopillars as mobile probes for high sensitivity metrology in fluid3, P. ANDRICH, C.F. DE LAS CASAS, F.J. HEREMANS, D.D. AWSCHALOM, University of Chicago, B.J. ALEMAN, K. OHNO, UC Santa Barbara, J.C. LEE, E.L. HU, Harvard University — The nitrogen-vacancy (NV) center’s optical addressability and exceptional spin coherence properties at room temperature, along with diamond’s biocompatibility, has put this defec at the front of meterology applications in biological environments. To push the spatial resolution to the nanoscale, extensive research efforts focus on using NV centers embedded in nanodiamonds (NDs). However, this approach has been hindered by degraded spin coherence properties in NDs and the lack of a platform for spatial control of the nanoparticles in fluid. In this work[3] we combine the use of high quality diamond membranes with a top-down patterning technique to fabricate diamond nanopillars with engineered and highly reproducible shape, size, and NV center density. We obtain NDs, easily releasable from the substrate into a water suspension, which contain single NV centers exhibiting consistently long spin coherence times (up to 700 μs). Additionally, we demonstrate highly stable, three-dimensional optical trapping of the nanoparticles within a microfluidic circuit. This level of control enables a bulk-like DC magnetic sensitivity and gives access to dynamical decoupling techniques on contactless, miniaturized diamond probes.


4:06PM W30.00007 Controlling Quantum Nanomagnets with Atomic Exchange Bias, SHICHAO YAN, DEUNG-JANG CHOI, JACOB BURGESS, STEFFEN ROLF-PISSARCKY, SEBASTIAN LOTTH, 1. Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg; 2. Max Planck Institute for Solid State Research, 70569 Stuttgart — Miniaturizing spintronic devices to the point where magnetization of the device’s elements becomes quantized is a possible avenue to achieving quantum computation with magnetic elements. Critical to such an approach is the ability to exert local control over the quantum nanomagnets. Atomic exchange bias field has been proposed as a mechanism for localized control of individual nanomagnets. Here we demonstrate that exchange coupling with the magnetic tip of a scanning tunnelling microscope provides continuous tuning of spin dynamics in an individual nanomagnet. By directly measuring spin relaxation time with electronic pump-probe spectroscopy, we find that the exchange interaction acts analogous to a local magnetic field that can be applied to a specific atom. It can be tuned in strength up to several teslas and cancel external magnetic fields, thereby demonstrating the feasibility of complete control over individual quantum magnets with atomically localized exchange coupling.

4:18PM W30.00008 High temperature magnetic phase transitions and exchange bias effect of FeSiCr alloy, XIN WANG, University of Electronic Science and Technology of China, STATE KEY LABORATORY OF ELECTRONIC THIN FILMS AND INTEGRATED DEVICES COLLABORATION — We present magnetic properties of FeSiCr alloy which was synthesized by melting and crushing method followed by milling and heat treatment. The samples under different heat treatment temperature were characterized by using X-ray diffractometer, scanning electron microscopy, vibrating sample magnetometer and Mössbauer spectroscopy. The micro-structure undergo crystallization and grain growth process starting from as-crushed state, and gradually transform to B2 atomic disordered crystal phase. B2 phase is formed into DO3 atomic ordered phase with the increasing temperature. Mössbauer spectroscopy are well fitted into one or two subspectras correspond to DO3 structure and two subspectras to Fe(7) and Fe(4) structures.

2We would like to thank Fluxtrol, Inc. for their help with this project
4:42PM W30.00010 Ballistic Anisotropic Magnetoresistance of Single-Atom Contacts. F. OTTE, J. SCHÖNEBERG, A. WEISSMANN, R. BERNDT, S. HEINZE, University of Kiel, Germany; N. NÉEL, J. KRÖGER, TU Ilmenau, Germany; Y. MOKROSOV, Forschungszentrum Jülich, Germany. It has been predicted that the anisotropic magnetoresistance (AMR) is greatly enhanced in the ballistic transport regime. Results from break junctions in a magnetic field can be explained in terms of this ballistic AMR (BAMR), although the interpretation is controversial due to the unknown atomic geometry of the junction. Here, we demonstrate the emergence of BAMR in single-atom contacts. Single Co and Ir atoms are deposited on domains and domain walls of ferromagnetic Fe layers on W(110), which is used to control their magnetization directions. They are contacted with nonmagnetic tips in a low-temperature scanning tunneling microscope to measure the junction conductances. AMR is observed and changes drastically between tunneling and the ballistic regime. First-principles calculations and tight-binding modeling demonstrate that this change is a competition of delocalized and localized d states of different orbital symmetry.


4:54PM W30.00011 Quantum Molecular Magnetism. SYLVAIN BRECHET, FRANCOIS REUSE, KLAUS MASCHKE, JEAN-PHILIPPE ANSERMET, EPFL. Our theoretical description of quantum molecular magnetism is based on the quantum master equations, where the system consists of the electronic spin degrees of freedom and the bath consists of the remaining degrees of freedom. The system is weakly coupled and weakly correlated to the bath, which is at equilibrium on an appropriate time scale. The electrons satisfy the exclusion principle, which requires the tensorial product of the spin and orbital parts of the state to be antisymmetric under permutation. However, the symmetries of the parts of the state taken separately are determined by the irreducible unitary representations of the permutation group. The structure of the quantum master equations is also determined by these representations. The coupling between different isotropic components of the permutation group appearing in the quantum master equations leads to a description of magnetic dissipation at the molecular level and defines molecular spin selection rules. Thus, this theoretical description is expected to bring new and fundamental insight for molecular magnetism. In particular, it is expected to predict the non-trivial deflection of molecular clusters in a field gradient.

5:06PM W30.00012 Using the binding site to control the magnetic and spintronic properties of a single magnetic molecule in a tunnel junction. BEN WARNER, FADI E. HALLAK, HENNING PRUESER, TOBIAS G. GILL, UCL, UK; JOHN SHARP, University of Liverpool, UK; ANDREW J. FISHER, UCL, UK; M. PERSSON, University of Liverpool, UK; CYRUS F. HIRSELJACOBS, UCL, UK. Many proposals outline the use of single magnetic molecules in new applications in information technology and spintronics, with the intention of creating new devices based on phenomena that only manifest at the atomic scale. To create these devices it will be necessary to engineer the required properties, whether through controlling the molecule’s chemical makeup or its interaction with the external surroundings. The latter may involve using interactions with the supporting substrate surface, which have been shown to not only modify the molecule properties [1] but also create effects such as chirality [2]. Here we utilize the surface interaction to modify the properties of FePc on copper nitride, a thin insulator, above bulk Cu(001). Using scanning tunneling microscopy we show that the interaction with the surface is defined by the binding site of the central Fe atom in the molecule. By performing elastic and inelastic tunneling spectroscopy and comparing the results to DFT modeling, we explore how coupling to the surface can be used to control the molecular orbitals and the accessibility of the spin excitations. This demonstrates the importance of controlling molecule-substrate coupling down to the atomic scale for the development of single molecule devices.

1 N. Tsukahara et al, Phys. Rev. Lett. 102, 167203 (2009)

5:18PM W30.00013 Stability of spin-electric coupling in triangular single-molecule magnets under external contacts. FHKRUL ISLAM, Linnaeus University, Sweden; JAVIER NOSSA, Carnegie Institution of Washington, USA; CARLO CANALI, Linnaeus University, Sweden; MARK PEDERSON, Department of Energy, USA. Triangular single molecule magnets (SMMs) with antiferromagnetic exchange coupling exhibit Kramer degenerate chiral spin-doublet ground states, which can be efficiently coupled by an electric field, even in the absence of spin-orbit interaction. Recent first-principles calculations [1] show that unsupported V₃ SMM has giant spin-electric coupling corresponding to dipole moment of about one tenth of the water-molecule dipole moment. The corresponding Rabi time for electric switching between two chiral states can be on the order of one nano-second for reasonable electric fields, which makes these molecules very attractive candidates for storing and manipulating pairs of coupled spin-chiral qbits. However, for device applications of the spin-electric coupling, these frustrated SMMs need to be supported on a surface or between metallic leads. Preserving this effect in an external environment is a challenging problem requiring appropriate functionalization. In this talk we will discuss the stability of the spin-electric coupling in V₃ SMM when coupled to gold leads or deposited on a graphene surface. [1] J. F. Nossa et al., Electric control of spin states in frustrated triangular molecular magnets (unpublished)

Thursday, March 5, 2015 2:30PM - 5:30PM –
Session W31 GMAG DMP FIAP: Focus Session: Spin-Dependent Phenomena in Semiconductors: Spins in Quantum Dots and Impurities

2:30PM W31.00001 Extreme Harmonic Generation in Electrically Driven Spin Resonance. JIRI STEHLIK, Department of Physics, Princeton University, Princeton, NJ 08544, USA. InAs nanowire double quantum dots offer a rich platform for studying single spin physics in a material with large spin-orbit (SO) coupling. The large SO coupling allows all electrical control of the electron spin through electric dipole spin resonance (EDSR). Here an oscillating electric field of frequency f displaces the electron wave function, while a magnetic field with strength B is applied. Spin rotations occur when the resonance condition hν = gμBB is met. Here g is the electron g-factor, h is Planck’s constant, and μB is the Bohr magneton. We find that near zero interdot detuning efficient spin rotations also occur when hν = nμBB, with n being an integer as large as 6 in our system. The harmonics feature a striking odd/even dependence. While the odd harmonics show an enhancement of the leakage current, the even harmonics show a reduction. In contrast, we do not observe any measurable harmonics at large detuning. We link the presence of harmonics with additional anti-crossings present in the level diagram. This implies that harmonics are the result of Landau-Zener transitions occurring at multiple anti-crossings. Recent theoretical work supports this conclusion.

1 Research performed in collaboration with M. D. Schroer, M. Z. Maialle, M. H. Degani, and J. R. Petta. Research was supported by the Sloan and Packard Foundations, Army Research Office, DARPA QuEST and the NSF.
3:06PM W31.00002 Spin relaxation of conduction electrons by inelastic scattering with neutral donors1, LAN QING, HANAN DERY, University of Rochester, Rochester, New York 14627, JING LI, IAN APPELBAUM, University of Maryland, College Park, Maryland 20742. — At low temperatures, in narrow-gap semiconductor quantum dots, a significant fraction of shallow donor sites are occupied by electrons, neutralizing the impurity core charge in equilibrium. Inelastic scattering by externally-injected conduction electrons accelerated by electric fields can excite transitions within the manifold of these localized states. Promotion into highly spin-mixed excited states results in spin relaxation that couples strongly to the conduction electrons by exchange interaction. Through experiments with silicon spin transport devices and complementary theory, we reveal the consequences of this previously unknown depolarization mechanism both below and above the impact ionization threshold and into the “deep inelastic” regime.

1This work is supported by NSF under contracts ECCS-1231570 and ECCS-1231855, by DTRA under contract HDTRA1-13-1-0013, and by ONR under contract N000141410317.

3:18PM W31.00003 Single-shot readout and relaxation measurements in exchange coupled31P electron spins in silicon, JUAN PABLO DEHOLLAINE, JUHA MUHonen, Kuan Tan, Centre for Quantum Computation and Communication Technology, University of New South Wales, ANDRE DE SARRANIA, Universidade Federal do Rio de Janeiro and University of Wisconsin-Madison, DAVID JAMIESON, Centre for Quantum Computation and Communication Technology, University of Melbourne, ANDREW DZURAK, ANDREA MORELLO, Centre for Quantum Computation and Communication Technology, University of New South Wales — We present the experimental observation of a large exchange coupling, $J \approx 3 \text{ meV}$, between two 31P electron spin qubits in silicon (Dehollain, PRL 112, 236801). The singlet and triplet states of the coupled spins are monitored in real time by a single-electron transistor, which detects ionization from tunnel-rate-dependent processes in the coupled spin system, yielding single-shot readout fidelities above 95%. The triplet to singlet relaxation time $T_1 \approx 4 \text{ ms}$ at zero magnetic field agrees with the theoretical prediction for the observed $J$-coupling energy in 31P dimers in silicon. The three order of magnitude increase in relaxation rate compared to single donors, is caused by a hyperfine interaction mediated mixing of the singlet and triplet states. Additionally, the time evolution of the two-electron state populations reveals an inversion in the energetic hierarchy of the valley-orbit excited states, which had been theoretically predicted for donor pairs with $< 6 \text{ nm}$ separation. These results pave the way to the realization of two-qubit quantum logic gates with spins in silicon and highlight the necessity to adopt gating schemes compatible with weak $J$-coupling strengths.

3:30PM W31.00004 g-Factors of Electrons, Holes and Excitons in Type-II ZnTe/ZnSe Submonolayer Quantum Dots, HAOJIE JI, SIDDHARTH DHOMKAR, the Graduate Center of CUNY; Queens College of CUNY, JONATHAN LUDWIG, DAMIR SMIRNOV, National High Magnetic Field Laboratory, MARIA TAMARGO, City College of CUNY; the Graduate Center of CUNY, IGOR KUSKOVSKY, Queens College of CUNY; the Graduate Center of CUNY — In recent years there has been intense interest in manipulating exciton spin states in semiconductor quantum dot (QDs) for application in spin electronics and quantum information processing. In these applications, the ability to enhance and control Zeeman spin splitting, which can be characterized by g-factors, plays a key role. Here we report our study of the g-factors of electrons, holes and excitons in type-II ZnTe/ZnSe submonolayer superlattices. Via analysis of left and right circularly polarized photoluminescence spectra, we determine the g-factor of type-II excitons. We obtain the g-factor of electrons by fitting the temperature dependence of degree of circular polarization. Thus, we find out the g-factor of holes confined in ZnTe QDs. This g-factor of confined holes is larger than those reported for bulk ZnTe. We propose that the enhancement of g-factor of holes is due to quantum confinement which leads to the admixture of the subband states.

3:42PM W31.00005 Competition between applied and exchange magnetic fields in (Zn,Mn)Se/ZnTe quantum dots1, BIPLO BARMAN, Y. TSAI, T. SCRACE, I. ZUTIC, B.D. MCCOMBE, A. PETROU, SUNY Buffalo, W-C CHOU, M-H TSOU, National Chiao Tung University, Taiwan, C-S YANG, Graduate Institute of Electro-Optical Engineering, Tatung University, Taiwan, I.R. SELLERS, University of Oklahoma, R. OSZWALDOWSKI, South Dakota School of Mines and Technology, SUNY BUFFALO COLLABORATION, NATIONAL CHIAO TUNG UNIVERSITY, TAIWAN COLLABORATION, TATUNG UNIVERSITY, TAIWAN COLLABORATION, UNIVERSITY OF OKLAHOMA COLLABORATION, SOUTH DAKOTA SCHOOL OF MINES AND TECHNOLOGY COLLABORATION — We have measured the peak energy of the photoluminescence (PL) emission and its circular polarization from type II (Zn,Mn)Se/ZnTe Quantum Dot structures in the Faraday and Voigt geometries. In the Faraday geometry the PL energy shows a 6 meV red shift at $B = 6$ tesla. This result verifies that the holes are confined in the non-magnetic ZnTe QDs, while the electrons move in the magnetic (Zn,Mn)Se matrix. The PL circular polarization saturates at 45%. In the Voigt geometry, the circular polarization is near-zero and the red shift is 2 meV. These results are discussed using a model that takes into account that electrons are influenced by the combination of the externally applied magnetic field and the exchange field due to the interaction between the Mn-spins and the carriers.

1This work is supported by DOE-BES and NSF-DMR.

3:54PM W31.00006 Spin structure of germanene quantum dot as a function of normal electric field1, APALKOV VADYM, VENKATA CHAGANTI, Georgia State University — Germanene quantum dot consisting of 13 germanium atoms is studied numerically within the nearest neighbor tight-binding model. Both the energy spectra and the spin structure of the corresponding Eigen-functions are obtained. Due to strong spin-orbit interaction in germanene the spin polarization of the germanene quantum dot strongly depends on the energy of the corresponding Eigen-state and on the external electric field, $E_z$. There are two states with energies close to zero, for which the direction of the spin is along z-axis, where z-axis is perpendicular of the quantum dot layer. For the higher energy levels the spin deviates from the z-axis with maximum angle $\theta_{\text{max}} = 3.9^\circ$ for the levels with energy 1128 meV (for electron channel) and -1128 meV (for hole channel) and zero electric field, $E_z = 0$. The angle $\theta_{\text{max}}$ increases almost linearly with $E_z$ and takes the value of $4.2^\circ$ at $E_z = 100 \text{ meV/A}$. The in-plane direction of spin is also sensitive to external electric field. With increasing electric field, the in-plane spin rotates in the anticlockwise and clockwise directions for the 1128 meV and -1128 meV levels, respectively. Due to such sensitivity of spin polarization to electric field, applying a bias voltage can control the spin current through germanene quantum dot.

4:06PM W31.00007 Structure determination of individual electron-nuclear spin complexes in a solid-state matrix, ABDELGHANI LARAOUI, DANIELA PAGLIERO, CARLOS MERILES, CUNY-City College of New York — A spin-based quantum computer will store and process information via “spin complexes” formed by a small number of interacting electronic and nuclear spins within a solid-state host. Unlike present electronic circuits, differences in the atomic composition and local geometry make each of these spin clusters distinct from the rest. Integration of these units into a working network thus builds on our ability to determine the cluster atomic structure, a problem we tackle herein with the aid of a magnetic resonance protocol. Using the nitrogen-vacancy (NV) center in diamond as a model system, we show analytically and numerically that the spatial coordinates of weakly coupled 13C spins can be determined by selectively transferring and retrieving spin polarization. The technique’s spatial resolution can reach up to 0.1 nm, limited by the NV spin coherence lifetime. No external magnetic field gradient is required, which makes this imaging scheme applicable to NV-13C complexes buried deep inside the crystal host. Further, this approach can be adapted to nuclear spins other than 13C, and thus applied to the characterization of individual molecules anchored to the diamond surface.

XIAYU LINPENG, TODD KARIN, University of Washington, RUSSEL BARBOUR, Spectrum Lab, MIKHAIL GLAZOV, Ioffe Institute, KAI-MEI FÜ, University of Washington — We observe an anomalous B-field dependence of the spin-flip time ($T_1$) of electrons bound to shallow donors which cannot be explained by current spin-relaxation theories. We conduct resonant pump-probe measurements in high-purity InP from the low to high magnetic field regimes, with a maximum $T_1$ (400 µs) observed near the turning point $gyB ≈ 30T$. At low $B$, the $T_1$ dependence on $B$ is consistent with an electron correlation time ($\tau_c$) in the tens of nanoseconds. The physical mechanism for the short $\tau_c$ in this high-purity sample ($n ≈ 2 \times 10^{14}$ cm$^{-3}$) is unclear, but a strong temperature dependence on $T_1$ can be further increased by lowering $T$ below the 1.5 K experimental temperature. At high $B$, a $B^{-3}$ dependence is observed, in contrast to the expected $B^{-5}$ predicted by single-phonon spin-orbit mediated interactions. An understanding of the anomalous $B$-field dependence is expected to elucidate the effect of electron transport (low-field) and phonons (high-field) on $T_1$ for shallow donors, which is of interest for both ensemble and single-spin quantum information applications.

1 This material is based upon work supported by the National Science Foundation under Grant No. 1150647, DGE-0718124 and DGE-1256082. InP samples were graciously provided by Simon Watkins at Simon Fraser University.

4:30PM W31.00009 Spin dynamics in a quantum point contact showing the 0.7-anomaly1, JAN VON DELFT, FLORIAN BAUER, JANHEYDER, DENNIS SCHIMMEL, Ludwig-Maximilians-University Munich, CENS/ASC TEAM — The 0.7-anomaly in the first conductance step of a quantum point contact is believed to arise from an interplay of geometry, spin dynamics and interaction effects. Various scenarios have been proposed to explain it, each evoking a different concept, including spontaneous spin polarization, or a quasi-localized state, or ferromagnetic spin fluctuations, or a van Hove ridge (a geometry-induced maximum in the density-of-states). Though these scenarios differ substantially regarding numerous details, they all imply anomalous dynamics for the spins in the vicinity of the QPC. We have performed a detailed study of this spin dynamics in the central region of a parabolic quantum point contact, by using the functional renormalization group to calculate the dynamical spin-spin correlation function $\chi(x, x', \omega)$ = $\int_0^\infty (S_z(x, t)S_z(x', 0)) e^{i\omega t}$. We will discuss its behavior as function of frequency, interaction strength and gate voltage and comment on the implications of these results for each of the above-mentioned scenarios.

1 We acknowledge support from the DFG through the NIM Excellence Cluster, SFB-TR12, and De730/4-3

4:42PM W31.00010 Optimal quantum control via numerical pulse shape optimization for two exciton qubits confined to semiconductor quantum dots, REUBLE MATHEW, HONG YI SHANG, KIMBERLEY HALL, Department of Physics and Atmospheric Science, Dalhousie University, Halifax, Nova Scotia, Canada — Optimal quantum control (OQC), which iteratively optimizes the control Hamiltonian to achieve a target quantum state, is a versatile approach for manipulating quantum systems. For optically-active transitions, OQC can be implemented using femtosecond pulse shaping which provides control over the amplitude and/or phase of the electric field. Optical pulse shaping has been employed to optimize physical processes such as nonlinear optical signals [1], photosynthesis [2], and has recently been applied to optimizing single-qubit gates in multiple semiconductor quantum dots [3]. In this work, we examine the use of numerical pulse shape optimization for optimal quantum control of multiple qubits confined to quantum dots as a function of their electronic structure parameters. The numerically optimized pulse shapes were found to produce high fidelity quantum gates for a range of transition frequencies, dipole moments, and arbitrary initial and final states. This work enhances the potential for scalability by reducing the laser resources required to control multiple qubits.


4:54PM W31.00011 Spin Manipulation through geometric phase in III-V semiconductor quantum dots1, SANJAY PRBAHAKAR, RODERICK MELNIK, Wilfrid Laurier University — A more robust technique is proposed to flip the spin completely through geometric phase in III-V semiconductor quantum dots (QDs). We transport the QDs adiabatically in a closed loop along the circular trajectory in the plane of two dimensional electron gas with the application of time dependent gate controlled electric fields and investigate the manipulation of Berry phase with the spin-orbit couplings. Here we show that both the Rashba and the Dresselhaus couplings are present for inducing a phase necessary for spin flip. If one of them is absent, the induced phase is trivial and irrelevant for spin-flip (Phys. Rev. B 89, 245310 (2014), Applied Physics Letters 104, 142411 (2014)).

1 We acknowledge the funding agency: Natural Sciences and Engineering Research Council of Canada and Canada Research Chair Program

5:06PM W31.00012 ABSTRACT WITHDRAWN —

5:18PM W31.00013 ABSTRACT WITHDRAWN —

Thursday, March 5, 2015 2:30PM - 5:30PM –

Session W32 GMAG DMP: Focus Session: Iridates 207B - Sae-Hwan Chun, Argonne National Laboratory

2:30PM W32.00001 Temperature and bias dependence of anisotropic magnetoresistance in antiferromagnetic Sr$_2$IrO$_4$. HEIDI SEINIGE, CHENG WANG, Physics Department, The University of Texas at Austin, GANG CAO, Center for Advanced Materials, University of Kentucky, JIAN-SHI ZHOU, JOHN B. GOODENOUGH, Texas Materials Institute, The University of Texas at Austin, MAXIM TSOI, Physics Department, The University of Texas at Austin — We study anisotropic magnetoresistance (AMR) in antiferromagnetic (AFM) Mott insulator Sr$_2$IrO$_4$. Such AMR is a promising candidate for monitoring the magnetic order parameter in AFM spintronics. Here we present temperature- and electrical bias-dependent measurements of the point-contact AMR in single crystals of Sr$_2$IrO$_4$. The point-contact technique allows to probe very small volumes and, therefore, look for electronic transport in Sr$_2$IrO$_4$ on a microscopic scale. Point-contact measurements at liquid nitrogen temperature revealed a large negative magnetoresistance (MR) for magnetic fields applied within IrO$_2$ a-b plane and electric currents flowing perpendicular to the plane. The observed MR decreases with increasing temperature and falls to zero at $T_{N_{AFM}}$ ~ 240 K. Interestingly, the temperature dependence of MR ratios differs qualitatively from that of the resistivity. The point-contact measurements also show a strong dependence of MR on the dc bias applied to the contact. The latter can be associated with correlations between electronic transport and magnetic order in Sr$_2$IrO$_4$.


1 This work was supported in part by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA, and by NSF grants DMR-1207577, DMR-1265162 and DMR-1122603.
2:42PM W32.00002 The Evolution of Electronic Structure in Electron and Hole-Doped Sr2IrO4, YUE CAO, XIUWEI ZHANG, HAOXIANGLI, XIAOQING ZHOU, University of Colorado at Boulder, RAJENDRA DHAKA, NICHOLAS PLUMB, Swiss Light Source, PSI, TONGFEI QI, JASMINKA TERZIC, University of Kentucky, ALEX ZUNGER, University of Colorado at Boulder, GANG CAO, University of Kentucky, D. S. DESSAU, University of Colorado at Boulder — How the electronic structure evolves in doped Mott insulators remains debated after decades of study, and affects the interpretations of many bulk and spectroscopic properties, including dc-conductance, quantum oscillations, etc. The recent discovery of the spin-orbital coupled J=1/2 Mott insulator Sr2IrO4 provides a new perspective into the above question. Combining angle-resolved photoemission spectroscopy and first-principles calculations, we present a unified description how the band dispersion, Fermi surface, chemical potential, and Mott gap change in electron and hole doped Sr2IrO4.

2:54PM W32.00003 Electrically tunable transport in antiferromagnetic Sr2IrO4, CHENG WANG, HEIDI SEINEIGE, Physics Department, The University of Texas at Austin, GANG CAO, Center for Advanced Materials, University of Kentucky, JIAN-SHI ZHOU, JOHN B. GOODENOUGH, Texas Materials Institute, The University of Texas at Austin, MAXIM TSOI, Physics Department, The University of Texas at Austin — Transport in antiferromagnetic (AFM) Mott insulators Sr2IrO4 is studied under high electric fields. Our goal is to address the question of electronic conduction in nano-scale AFM spintronic applications [1] where high biases and associated electric fields are routinely present. We use nano-scale contacts between a sharpened Cu tip and single crystal of Sr2IrO4 to achieve electric fields up to a few MV/m. When an electrical bias is applied to such a point contact, the electric potential drops essentially in a small contact region, thus leading to high electric fields and providing a means to probe electronic transport on a microscopic scale. Detailed measurements of point-contact voltage characteristics revealed that the contact resistance decreased significantly (50-70%) with an increasing dc bias. The observed bias dependence can be well fitted by an activation energy model that involves band structure modifications under strong electric fields. Our findings suggest a promising path towards band-gap engineering in 5th transition metal oxides, which may lead to appealing technical solutions in developing next generation’s electronic devices.


3:06PM W32.00004 A hidden non-dipolar magnetic order parameter in Sr2IrO4 observed using nonlinear optical measurements, LIUYAN ZHAO, Ins. for Q. Info. and Matt., California Institute of Technology, VSEVOLOD IVANOV, Department of Physics, California Institute of Technology, DARIUS TORCHINSKY, HAO CHU, Ins. for Q. Info. and Matt., California Institute of Technology, RON LIFSHITZ, Department of Physics and Astronomy, Tel Aviv University, REDDECA FLINT, Ins. for Q. Info. and Matt., California Institute of Technology — Iridium oxides are predicted to host a variety of exotic electronic phases arising from the interplay of electron correlations and spin-orbit coupling. One hidden non-dipolar order parameter in Sr2IrO4, originating from the hidden 5d orbital of Ir4+, is studied under high electric fields. Our goal is to address the question of electronic conduction in nano-scale AFM spintronic applications [1] where high biases and associated electric fields are routinely present. We use nano-scale contacts between a sharpened Cu tip and single crystal of Sr2IrO4 to achieve electric fields up to a few MV/m. When an electrical bias is applied to such a point contact, the electric potential drops essentially in a small contact region, thus leading to high electric fields and providing a means to probe electronic transport on a microscopic scale. Detailed measurements of point-contact voltage characteristics revealed that the contact resistance decreased significantly (50-70%) with an increasing dc bias. The observed bias dependence can be well fitted by an activation energy model that involves band structure modifications under strong electric fields. Our findings suggest a promising path towards band-gap engineering in 5th transition metal oxides, which may lead to appealing technical solutions in developing next generation’s electronic devices.


3:30PM W32.00006 23Na and 17O NMR studies of hyperkagome Na5Ir3O10, ABIGAIL SHOCKLEY, FABRICE BERT, JEAN-CHRISTOPHE ORAIN, Université Paris-Sud, YOSHIHIKO OKAMOTO, Nagoya University, PHILIPPE MENDELS, Université Paris-Sud — Na5Ir3O10 is a unique case of a 3D corner sharing triangular lattice which can be decorated with quantum spins. It has spurred a lot of theoretical interest as a spin liquid candidate of a new kind where the Hamiltonian might not be thought in terms of a simple Heisenberg case because of spin orbit coupling on the Ir 5d element. We present a comprehensive set of NMR data taken on both the 23Na and 17O sites. We have found that magnetic freezing of all Ir sites sets in below T1 ~ 7.5K ~ 0.019J with a clear hyperfine field transferred from Ir moments and a drastic decrease of 1/T1. Above T1, physical properties are expected to be a landmark of frustration in this exotic geometry. We will discuss our shift and relaxation data in the temperature range of 300K to 7.5 K in the light of published thermodynamic measurements (Y. Okamotoa et al, PRL 99 137207, 2007 and Y. Singh et al, PRB 88 220413(R), 2013) and comment on their implications for the already existing large body of theoretical work.

3:42PM W32.00007 55 Tesla coercive magnetic field in frustrated Sr3NiIrO10, JOHN SINGLETON, Los Alamos Natl Lab, JAE-WOOK KIM, Oxford University, CRAIG TOPPING, Oxford University, ANDERS HANSEN, Los Alamos Natl Lab, UNE-DEOK MUN, Simon Fraser University, SAMAN GHANNADZADEH, Oxford University, PAUL GODDARD, Warwick University, XUAN LUO, YOON SEOK OH, SANG-WOOK CHEONG, Rutgers University, VIVIEN ZAPF, Los Alamos Natl Lab — We have measured extremely large coercive fields of up to 55 T in Sr3NiIrO10 using low temperature nonlinear optical generation techniques [2,3]. We will discuss the significance of this novel order parameter in the context of cuprate high-Tc superconductivity and present comparative studies on non-perovskite families of iridium oxides.

Magnetic scattering, we find direct evidence of this frustration and follow its temperature dependence. We observe that three zigzag magnetic states with 

Ir-Ir bonds in the lattice. This result confirms the dominant role of the bond-directional interactions in the frustration.

Temperature driven by the cooperation of spin-orbit coupling and moderate Coulomb correlations. Transport measurements have shown a metal-insulator transition with electron doping in $\text{Sr}_x\text{La}_2\text{IrO}_6$ near $x = 0.12$. We will show how the electronic structure evolves through the metal to insulator transition and discuss these results in terms of strong correlations and how these evolve with doping.

Direct Observation of Magnetic Frustration via Bond-directional Interactions in a Honeycomb Lattice Iridate $\text{Na}_2\text{IrO}_3$ — SAE HWAN CHUN, H. ZHENG, C. STOUMPOS, C. MALLIAKAS, J. F. MØLHOL, A. ALI, Z. ISIBI, M. MOBREI, A. ŠALÁ, M. KRISCH, European Synchrotron Radiation Facility, J. CHALOPUKA, Central European Institute of Technology, Masaryk University, G. JACKELI, K. GHALIULILIN, B. J. KIM, Max Planck Institute for Solid State Research — Despite its long-range zigzag magnetic ground state, the honeycomb $\text{Na}_2\text{IrO}_3$ is considered as a model system for approaching a Kitaev quantum spin liquid due to a proposed bond-directional magnetic frustration. Using resonant x-ray magnetic scattering, we find direct evidence of this frustration and follow its temperature dependence.

We observe that three zigzag magnetic states with short-range antiferromagnetic coupling and moderate Coulomb correlations. Transport measurements have shown a metal-insulator transition with electron doping in $\text{Sr}_x\text{La}_2\text{IrO}_6$ near $x = 0.12$. We will show how the electronic structure evolves through the metal to insulator transition and discuss these results in terms of strong correlations and how these evolve with doping.

1:30PM W32.00008 Magnetic order and electron correlations in the frustrated Ising-like chain compound $\text{Sr}_3\text{NiIrO}_6$ — E. LEFRANÇOIS, Institut Laue-Langevin - Institut Néel, L. C. CHAPON, Institut Laue-Langevin, V. SIMONET, P. LEJAY, R. BALLOW, Institut Néel, S. RAYPAL, R. BRIGGS, J. T. ADROJA, ISIS Facility, STFC, Rutherford Appleton Laboratory, D. T. ADROJA, ISIS Facility, STFC, Rutherford Appleton Laboratory - University of Oxford — Oxides of the family $\text{A}_2\text{M}_2\text{O}_6$ ($\text{A}$ = alkali-earth metal, $\text{M}$ = transition metal) attracted a lot of attention because of their unconventional magnetic properties due to the interplay between low dimensionality, magnetic frustration and magnetocrystalline anisotropy. In these compounds, the $\text{M}$ ions form chains which are distributed on a triangular lattice. We studied the 5d-based system $\text{Sr}_3\text{NiIrO}_6$, which is in the strong spin-orbit coupling regime, by single crystal magnetization measurements and neutron powder diffraction. The magnetization revealed a large easy-axis of anisotropy confining the $\text{N}_2\text{M}_2$ and $\text{L}_2\text{M}_2$ magnetic moments along the chains. Besides, the zero-field-cooled and field-cooled measurements show that there are two characteristic temperatures: $T_1 = 75$ K and $T_2 = 17$ K. The first one is associated with the appearance of a magnetic order with a propagation vector $k = (0, 0, 1)$. At $T_2$, the susceptibility reaches a maximum followed by a sudden drop. The magnetic structure was determined from neutron powder diffraction only up to a global phase. However, symmetry arguments allowed determining the exact nature of the magnetic ground state below $T_2$, thus clarifying the universal magnetic properties of this family of compounds.
by the ribosome. More details can be found at doi:10.1529/biophysj.106.090944.

This study implicates alternative coordinates along which rearrangements are accurately described as diffusive movements across a one-dimensional free-energy profile. From this, we provide the theoretical foundation required for single-molecule techniques to uncover the energy landscape governing aa-tRNA selection events and accurately indicate when the aa-tRNA is on a transition path. While a currently-used coordinate in single-molecule experiments performs poorly, we have developed a coarse-grained model of a monomer that self-assembles into tubules. In this model the monomer has a wedge shape which promotes tubule formation. There are attractive binding sites on the vertical and lateral sides of the monomer. We previously performed molecular dynamics simulations to calculate the set of structures that form upon self-assembly as we vary the lateral and vertical interaction strengths. In this talk, we will present the results of mechanical studies of the coarse-grained tubule system. The persistence length and various elastic moduli have been calculated. Microtubules have some of the largest persistence lengths of polymers. We have found that the persistence length is indeed very long for this coarse-grained model system. We calculate elastic moduli for varying the interaction strengths of the lateral and vertical interactions. We gain insight into the values that occur in microtubules, with respect to mechanical stability and stiffness.

2:54PM W33.00003 Small-angle neutron and X-ray scattering reveal conformational changes in rhodopsin activation, UTSAB R. SHRESTHA, DEBISINGH KBHOMIK, Wayne State University, MI, SUCHITRHANGA M.C.D. PERERA, UDEEP CHAWLA, ANDREY V. STRUTS, University of Arizona, AZ, VITO GRAZIONI, Brookhaven National Laboratory, NY, SAI VENKATESH PINGALI, WILLIAM T. HELLER, SHOU QIAN, Oak Ridge National Laboratory, TN, MICHAEL F. BROWN, University of Arizona, AZ, XIANG-QIANG CHU, Wayne State University, MI — Understanding G-protein-coupled receptor (GPCR) activation plays a crucial role in the development of novel improved molecular drugs. During photo-activation, the retinal chromophore of the visual GPCR rhodopsin isomerizes from 11-cis to all-trans conformation, yielding an equilibrium between inactive Meta-1-like and active Meta-II-like states. The principal goal of this work is to address whether the activation of rhodopsin leads to a specific conformational ensemble, and how protein organizational structure changes with detergent environment in solution. We use both small-angle neutron scattering (SANS) and small-angle X-ray scattering (SAXS) techniques to answer the above questions. For the first time we observe the change in protein conformational ensemble upon photo-activation by SANS with contrast variation, which enables the separate study of the protein structure within the detergent assembly. In addition, SAXS study of protein structure within detergent assembly suggests that the detergent molecules form a belt of monolayer (micelle) around protein with different geometrical shapes to keep the protein in folded state.

3:06PM W33.00004 Effects of Uniaxial Strain on Shear Moduli of Semiflexible Polymer Networks, PAUL JANNEY, University of Pennsylvania — No abstract available.

3:42PM W33.00005 Emergence of attraction in simulations of coarse-grained double stranded DNA, SHAHZAD GHANBARIAN, JOERG ROTTLE, University of British Columbia — DNA condensation induced by multivalent counterions is believed to play an important role in DNA bundling and packing into the cell nucleus. We present a coarse-grained, implicit solvent representation of rigid ds-DNA molecules in the presence of divalent counterions. In order to include solvation effects arising from the discrete nature of the water molecules, short-ranged corrections are added to the pairwise interaction potentials. We find that the structure of counterions is consistent with results from corresponding explicit solvent simulations. The effective force between two DNA strands generated by these potentials provides an excellent match to that observed in the explicit solvent model. Importantly, this interaction features multiple minima and reproduces the like-charge attraction effect between DNA molecules observed in full atomistic simulations at significantly reduced computational expense. This result proves that it is possible to capture complex multibody interactions between polyelectrolyte strands with two-body potentials.

5:18PM W32.00015 Magnetotransport in BaIrO$_3$: JENNIFER TRINH, Univ of California-Santa Cruz, JOSHUA FLYNN, MAS SUBRAMANIAN, Oregon State University, ARTHUR RAMIREZ, Univ of California-Santa Cruz — The quasi-one-dimensional monolionic semiconductor BaIrO$_3$ possesses a transition at 177 K characterized by both charge-ordering and ferromagnetism. We have measured the magneto-transport on single crystal samples in fields of up to 7T. We find that the strongly hysteretic positive magnetoresistance (MR) possesses both linear and quadratic contributions. The linear contribution is positive in the full temperature range studied, with a peak below the transition temperature at 150 K. The quadratic MR changes sign at T_C, from positive above to negative below. The Hall effect is non-monotonic as a function of field below T_C and we will relate this to the FM order parameter.

This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE1339067.

Thursday, March 5, 2015 2:30PM - 5:30PM
Session W33 DBIO DPOYL: Focus Session: Conformations and Dynamics of Biopolymers III

2:30PM W33.00001 Non-Gaussian Distribution of DNA Barcode Extension In Nanochannels Using High-throughput Imaging, JULIAN SHEATS, WESLEY REINHART$^1$. Chemical Engineering and Materials Science, University of Minnesota, Minneapolis MN, USA, JEFF REIFENBERGER, BioNano Genomics, San Diego, CA, USA, DAMINI GUPTA, ABHIRAM MURALIDHAR, Chemical Engineering and Materials Science, University of Minnesota, Minneapolis MN, USA, HAN CAO, BioNano Genomics, San Diego, CA, USA, KEVIN DORFMAN, Chemical Engineering and Materials Science, University of Minnesota, Minneapolis MN, USA — We present experimental data for the extension of internal segments of highly confined DNA using a high-throughput experimental setup. Barcode-labeled E. coli genomic DNA molecules were imaged at a high areal density in square nanochannels with sizes ranging from 40 nm to 51 nm in width. Over 25,000 molecules were used to obtain more than 1,000,000 measurements for genomic distances between 2,500 bp and 100,000 bp. The distribution of extensions has positive excess kurtosis and is skewed left due to weak backfolding in the channel. As a result, the two Odijk theories for the chain extension and variance bracket the experimental data. We compared to predictions of a harmonic approximation for the confinement free energy and show that it produces a substantial error in the variance. These results suggest an inherent error associated with any statistical analysis of barcoded DNA that relies on harmonic models for chain extension.

$^1$Present address: Department of Chemical and Biological Engineering, Princeton University

2:42PM W33.00002 Simulation of Microtubules: Mechanical properties, MARK STEVENS, Sandia National Labs — In order to understand microtubule assembly and the necessary monomeric properties to design artificial polymers that possess features similar to those of microtubules, we have developed a coarse-grained model of a monomer that self-assembly into tubules. In this model the monomer has a wedge shape which promotes tubule formation. There are attractive binding sites on the vertical and lateral sides of the monomer. We previously performed molecular dynamics simulations to calculate the set of structures that form upon self-assembly as we vary the lateral and vertical interaction strengths. In this talk, we will present the results of mechanical studies of the coarse-grained tubule system. The persistence length and various elastic moduli have been calculated. Microtubules have some of the largest persistence lengths of polymers. We have found that the persistence length is indeed very long for this coarse-grained model system. We calculate elastic moduli for varying the interaction strengths of the lateral and vertical interactions. We gain insight into the values that occur in microtubules, with respect to mechanical stability and stiffness.

2:54PM W33.00003 Small-angle neutron and X-ray scattering reveal conformational changes in rhodopsin activation, UTSAB R. SHRESTHA, DEBISINGH KBHOMIK, Wayne State University, MI, SUCHITRHANGA M.C.D. PERERA, UDEEP CHAWLA, ANDREY V. STRUTS, University of Arizona, AZ, VITO GRAZIONI, Brookhaven National Laboratory, NY, SAI VENKATESH PINGALI, WILLIAM T. HELLER, SHOU QIAN, Oak Ridge National Laboratory, TN, MICHAEL F. BROWN, University of Arizona, AZ, XIANG-QIANG CHU, Wayne State University, MI — Understanding G-protein-coupled receptor (GPCR) activation plays a crucial role in the development of novel improved molecular drugs. During photo-activation, the retinal chromophore of the visual GPCR rhodopsin isomerizes from 11-cis to all-trans conformation, yielding an equilibrium between inactive Meta-1-like and active Meta-II-like states. The principal goal of this work is to address whether the activation of rhodopsin leads to a specific conformational ensemble, and how protein organizational structure changes with detergent environment in solution. We use both small-angle neutron scattering (SANS) and small-angle X-ray scattering (SAXS) techniques to answer the above questions. For the first time we observe the change in protein conformational ensemble upon photo-activation by SANS with contrast variation, which enables the separate study of the protein structure within the detergent assembly. In addition, SAXS study of protein structure within detergent assembly suggests that the detergent molecules form a belt of monolayer (micelle) around protein with different geometrical shapes to keep the protein in folded state.

3:06PM W33.00004 Effects of Uniaxial Strain on Shear Moduli of Semiflexible Polymer Networks, PAUL JANNEY, University of Pennsylvania — No abstract available.

3:42PM W33.00005 Emergence of attraction in simulations of coarse-grained double stranded DNA, SHAHZAD GHANBARIAN, JOERG ROTTLE, University of British Columbia — DNA condensation induced by multivalent counterions is believed to play an important role in DNA bundling and packing into the cell nucleus. We present a coarse-grained, implicit solvent representation of rigid ds-DNA molecules in the presence of divalent counterions. In order to include solvation effects arising from the discrete nature of the water molecules, short-ranged corrections are added to the pairwise interaction potentials. We find that the structure of counterions is consistent with results from corresponding explicit solvent simulations. The effective force between two DNA strands generated by these potentials provides an excellent match to that observed in the explicit solvent model. Importantly, this interaction features multiple minima and reproduces the like-charge attraction effect between DNA molecules observed in full atomistic simulations at significantly reduced computational expense. This result proves that it is possible to capture complex multibody interactions between polyelectrolyte strands with two-body potentials.

3:54PM W33.00006 Capturing Transition Paths and Transition States for Conformational Rearrangements in the Ribosome, JEFFREY NOEL, Center for Theoretical Biological Physics Rice University, JORGE CHAHINE, VITOR LEITE, Universidade Estadual Paulista, Rio Preto, Brazil, PAUL WHITFORD, Physics Dept Northeastern Univ — To reveal the molecular determinants of biological function, one seeks to characterize the interactions that are formed in conformational and chemical transition states. In other words, what interactions govern the molecule’s energy landscape? To accomplish this, it is necessary to identify which degrees of freedom can unambiguously identify each transition state. Here, we perform simulations of large-scale aminocyl-tRNA (aa-tRNA) rearrangements during accommodation on the ribosome and project the dynamics along experimentally-accessible atomic distances. From this analysis, we obtain evidence for which coordinates capture the correct number of barrier-crossing events and accurately indicate when the aa-tRNA is on a transition path. While a currently-used coordinate in single-molecule experiments performs poorly, this study implicates alternative coordinates along which rearrangements are accurately described as diffusive movements across a one-dimensional free-energy profile. From this, we provide the theoretical foundation required for single-molecule techniques to uncover the energy landscape governing aa-tRNA selection by the ribosome. More details can be found at doi:10.1529/biophysj.106.090944.
4:06PM W33.00007 Study on the stability of the DNA hairpin d(ATCCAT-GTTA-TAGGAT) employing molecular dynamics simulation, SANGWOOK WU, Department of Physics, Pukyong National University, Busan 608-737, Korea. HONGGU CHUN COLLABORATION — DNA hairpin plays a critical role in the regulation of gene expression and DNA recombination. We studied the conformation of the DNA hairpin (d(ATCCAT-GTTA-TAGGAT)) employing molecular dynamics (MD) simulation. Despite the non-canonical Watson-Crick base pair (G:A) in the tetraloop (GTGA), MD simulation reveals that the conformation of the DNA hairpin is remarkably stable. In this study, we discuss about the physical/chemical origin of the stability of the DNA hairpin.

1Department of Biomedical Engineering, Korea University, Seoul 136-703, Korea

4:18PM W33.00008 Effect of solvent viscosity on driven translocation of a semi-flexible polymer through a nanopore, RAMESH ADHIKARI, ANIKET BHATTACHARYA, University of Central Florida — We study the effect of solvent viscosity and pore diameter on the driven translocation of a semi-flexible chain using Langevin dynamics simulation. We observe that for a given chain stiffness the mean first passage time (MFPT) has a nonmonotonic dependence on the solvent viscosity. For moderate external biases, the MFPT decreases at very low solvent viscosity exhibiting a minimum before it increases linearly as a function of high solvent viscosity. We demonstrate a stiffer chain translocates faster than a flexible chain of same length at the low viscosity regime while the opposite is true at high viscosity regime. The effect of pore size on the translocation dynamics is more acute at low solvent viscosity (pore friction dominating regime), but has almost negligible effect at the high viscosity regime for the parameters used in our studies.

1Partially supported by UCF Office of Research and Commercialization & College of Science SEED grant

4:30PM W33.00009 Spontaneous curvature in chiral polar filaments near interfaces, PETER D. OLMSTED, Department of Physics, Georgetown University, EMILY E. RILEY, Department of Applied Mathematics and Theoretical Physics, Cambridge University, SOPHIA JORDENS, IVAN USOV, Department of Health Sciences & Technology, Laboratory of Food & Soft Materials, ETH Zurich, LUCIO ISA, Department of Materials, Laboratory for Surface Science & Technology, ETH Zurich, RAFFAELE MEZZENGA, Department of Health Sciences & Technology, Laboratory of Food & Soft Materials, ETH Zurich — Chiral filaments (actin, DNA, alpha helical strands, ...) are ubiquitous in biology, and they frequently come into contact with interfaces or inhomogeneous environments, either in biology (e.g. actin on membranes) or use and processing of biomaterials (fibrils at solvent boundaries or nanoparticle surfaces). Recent experiments have shown that amyloid fibrils can develop unusual curvatures at the air-water interface. Here we show that spontaneous curvature follows, on symmetry grounds, for chiral polar filaments placed in inhomogeneous environments such as near surfaces. We demonstrate this for simple model surface-fibril interactions, and discuss some of the implications.

3Financial support is acknowledged from: ETH Zurich (ETHHIRA TH 32-1), SNF (2-77002-11), and SNSF (IZK072.141955, PP00P2.144646/1, PZ00P2.142532/1).

4:42PM W33.00010 Adsorption of Helical Polymers on a Substrate, MATTHEW WILLIAMS, Univ of Georgia — Formation of tertiary structures made up of helical polymer segments is modified by the introduction of a substrate on which the polymer is adsorbed. The effect of a substrate on biological systems such as helical structures may be important in the formation of early life. We perform replica-exchange Monte Carlo simulations to study the effect of a substrate on formation of helical structures, comparing the structural phase space for both adsorbed and non-adsorbed helical polymers. For this purpose a generic, hybrid coarse-grained model for polymer adsorption has been employed.

4:54PM W33.00011 ABSTRACT WITHDRAWN —

5:06PM W33.00012 Elasticity of 3D networks with rigid filaments and compliant crosslinks, KNUT M. HEIDEMANN, Institute for Numerical and Applied Mathematics, Georg-August-Universität, Göttingen, Germany, ABHINAV SHARMA, FLORIAN REHFEIDT, CHRISTOPH F. SCHMIDT, Third Institute of Physics — Biophysics, Georg-August-Universität, Göttingen, Germany, MAX WARDETZKY, Institute for Numerical and Applied Mathematics, Georg-August-Universität, Göttingen, Germany — Disordered filamentous networks with compliant crosslinks exhibit a low linear elastic shear modulus at small strains, but stiffen dramatically at high strains. Here, we perform an analytical and numerical study on model networks in three dimensions. Our model consists of a collection of randomly oriented rigid filaments connected by flexible crosslinks that are modeled as wormlike chains. Under the assumption of affine deformations in the limit of infinite crosslink density, we show analytically that the nonlinear elastic regime in 1- and 2-dimensional networks is characterized by power-law scaling of the elastic modulus with the stress. In contrast, 3-dimensional networks show an exponential dependence of the modulus on stress. Independent of dimensionality, if the crosslink density is finite, we show that the only persistent scaling exponent is that of the single wormlike chain. Consequently, unlike suggested in prior work, the model system studied here cannot provide an explanation for the experimentally observed linear scaling of the modulus with the stress in filamentous networks.

1This work was funded by the Deutsche Forschungsgemeinschaft (DFG) within the collaborative research center SFB 755, project A3.

5:18PM W33.00013 Molecular Dynamics Investigations of the alpha-helix to Beta-barrel Conformational Transformation in RfaH, JEEVAN GC, YUBA BHANDARI, BERNARD GERSTMAN, PREM CHAPAGAIN, Florida International University — We used combination of replica exchange molecular dynamics simulations with implicit solvent and detailed all-atom simulations with explicit solvent to investigate the alpha-helix to beta-structure transformation of RfaH-CTD. While interacting with the N-terminal domain (NTD), the C-terminal domain (CTD) of RfaH folds to a alpha-helix bundle but it undergoes an all alpha to all beta conformational transformation when it does not interact with the NTD. The RfaH-CTD in the all alpha topology is involved in regulating transcription whereas in the all beta topology it is involved in stimulating translation by recruiting a ribosome to an mRNA. Calculations of free-energy landscape and transfer entropy elucidate the details of the RfaH-CTD transformation process. The importance of interfacial interactions between the two domains of RfaH is highlighted by the compromised structural integrity of the helical form of the CTD in the absence NTD. We also studied interdomain and intradomain interactions in RfaH using Steered Molecular Dynamics Simulations. We investigated the role of the interdomain salt-bridge interaction in the domain stability Potential mean force was calculated to obtain free energy profile using Jarzynski Equality.

Thursday, March 5, 2015 2:30PM - 5:06PM — Session W35 GSOFT: Colloidal Clusters, Interactions, and Synthesis

210B - Robert Hoy, University of South Florida
2:30PM W35.00001 Structure and dynamics of model colloidal clusters with short-range attractions, KRYSTLE QUINN, ROBERT HOY, University of South Florida — We examine the structure and dynamics of small isolated N-particle clusters interacting via short-ranged Morse potentials. Ideally prepared ensembles obtained via exact enumeration studies of sticky hard sphere packings serve as reference states allowing us to identify key statistical-geometrical properties as well as to quantitatively characterize how nonequilibrium ensembles prepared by thermal quenches at different rates T differ from their equilibrium counterparts. Our results provide a theoretical framework for extending recent experimental studies of small colloidal clusters to examine nonequilibrium phenomena.


2:42PM W35.00002 Ground States and Folding Dynamics of Colloidal Clusters, ELLEN KLEIN, W. BENJAMIN ROGERS, VINOTHAN N. MANOHARAN, Harvard University — We experimentally study colloidal clusters consisting of N<100 spherical particles with short range, isotropic interactions. These clusters are a model system for understanding colloidal self-assembly and dynamics, since the positions and motion of the particles can be observed in real space. For N ≤ 10 the ground states are degenerate; previous work has shown that the probabilities of observing specific clusters depend primarily on their rotational entropy, which is determined by symmetry. Thus, less symmetric structures are more frequently observed. However, for large N the ground state should be a highly symmetric close-packed lattice. We seek to understand how this transition occurs as a function of N.To do this, we coat colloidal particles with complementary DNA strands that induce a short-range, temperature dependent interparticle attraction. We then assemble and anneal an ensemble of clusters with N ≥ 10. We characterize the number of apparent ground states, their symmetries, and their probabilities as a function of N. We also observe how these clusters fold into minimal-energy configurations by subjecting them to an electric field that we then relax.

1 VENI grant from The Netherlands Organization for Scientific Research (NWO)

3:06PM W35.00004 Countermediated-Mediated Assembly of Spherical Nucleic Acid-Au Nanoparticle Conjugates (SNA-AuNPs), SUMIT KEWALRAMANI, LIANE MOREAU, GUILLERMO GUERRERO-GARCIA, CHAD MIRKIN, MONICA OLVERA DE LA CRUZ, MICHAEL BEDZYK, Northwestern University, AFOSR MURI TEAM — Controlled crystallization of colloids from solution has been a goal of material scientists for decades. Recently, nucleic acid functionalized spherical Au nanoparticles (SNA-AuNPs) have been programmed to assemble in a wide variety of crystal structures. In this approach, the assembly is driven by Watson-Crick hybridization between DNAs coating the AuNPs. Here, we show that counterions can induce ordered assembly of SNA-AuNPs in bulk solutions, even in the absence of base pairing interactions. The electrostatics-driven assembly of spherical nucleic acid-Au nanoparticle conjugates (SNA-AuNPs) is probed as a function of counterion concentration and counterion valency [±1 (Na+) or ±2 (Ca2+) ] by in situ solution X-ray scattering. Assemblies of AuNPs capped with single-stranded (ss) or double-stranded (ds) DNA are examined. SAXS reveals disordered (gas-like) → face-centered-cubic (FCC) → glass-like phase transitions with increasing solution ionic strength. These studies demonstrate how non-base-pairing interactions can be tuned to create crystalline assemblies of SNA-AuNPs. The dependence of the inter-SNA-AuNP interactions on counterion valency and stiffness of the DNA corona will be discussed.

3:18PM W35.00005 Measuring colloidal charges in low polar media from statistics of particle trajectories, DANIEL KRAFT, Leiden University — Controlling the geometry and yield of anisotropic colloidal particles remains a challenge for hierarchical self-assembly. I will discuss a synthetic strategy for fabricating colloidal clusters by creating order in randomly aggregated polymer spheres using surface tension and geometrical constraints. The technique can be extended to a variety of charge-stabilized polymer spheres and offers control over the cluster size distribution.

3:30PM W35.00006 Does Suspension Crowding Screen Hydrodynamic Interactions? , YU SU, ROSEANNA N. ZIA, Cornell University, JAMES W. SWAN, Massachusetts Institute of Technology — Resistance and mobility functions describe linear couplings between moments of the hydrodynamic traction on a suspended particle and the motion of that or other particles. For two isolated spheres, these functions are well known and have been applied directly to the precise measurements in the vicinities of dilute colloidal dispersions. We have devised a new stochastic technique to calculate an analogous set of functions for two spheres immersed in a suspension that are then used to model the near-equilibrium dynamics of concentrated suspensions, including viscoelasticity and long-time diffusion. Of interest is the degree of screening of hydrodynamic interactions by the intervening medium. We find that the mobility is unscreened at the pair level, even in suspensions of high concentration, confirming that hydrodynamic interactions are an essential part of the dynamics of crowded systems and cannot be neglected in favor of simple renormalization schemes. We compare our results for the hydrodynamic interactions between suspended particles to predictions from two-point microrheology. This technique can be used to infer the complex viscosity from long-ranged decay of the pair mobility in viscoelastic materials.

3:42PM W35.00007 Pair Interactions of Superhydrophobic Colloids at an Oil-Aqueous Phase Interface, COLM KELLEHER, New York University, ANNA WANG, Harvard University, IVAN GUERRERO, Northwestern University, BHASKAR KRISHNATREYA, ANDREW HOLLINGSWORTH, DAVID GRIER, New York University, VINOTHAN MANOHARAN, Harvard University, PAUL CHAIKIN, New York University — Superhydrophobic PMMA colloids, dispersed in oil, can become highly charged. In the presence of an interface with a conducting aqueous phase, image charge effects lead to strong binding of colloidal particles to the interface, despite the fact that the equilibrium contact angle θi > 170°. We present the results of a series of experiments designed to probe the attraction of individual colloids to the interface, and the repulsion between pairs of interfacially bound colloids. We show that these interactions are relatively uniform, reproducible, and time-independent, and can be described by a simple model in which the only parameters are the particle charge and the Debye screening length in the oil phase. These factors make this system a good candidate for studying various equilibrium and non-equilibrium phenomena in 2D condensed matter physics, for example defect formation and dynamics in 2D colloidal crystals, and structural rearrangements in sheared colloidal glasses.

3:54PM W35.00008 Precise measurement of surface plasmon forces at a metal-dielectric interface using a calibrated evanescent wave, LULU LIU, ALEX WOOLF, Harvard University — By observing the motion of an optically trapped microscopic colloid, sub-piconewton static and dynamical forces have been measured using a technique called photonice force microscopy. This technique, though potentially powerful, has in the past struggled to provide precise measurements of a reflective or metallic interface, due to distortions of the optical field. We introduce a new in-situ, contact-free calibration method for particle tracking using an evanescent wave, and demonstrate its expanded capability by the precise measurement of forces of interaction between a single colloid and the optical field generated by a propagating surface plasmon polariton on gold.
4:06PM W35.00009 Osmotic equation of colloidal nanoparticles transiently confined in an optical trap.  
JINXIN FU, Georgia Institute of Technology, H. DANIEL OU-YANG, Lehigh University — Equilibrium number density profile of colloidal particles in a potential force field depends on the particle number density, the force field and interactions between the particles. Einstein described the particle number density profile by an osmotic equilibrium equation relating colloidal osmotic pressure and the potential force in his 1905 paper on the Brownian motion. For a dilute suspension of colloids, when particle interactions are negligible, the osmotic equilibrium equation can be used to determine unknown potential energy profiles from the Boltzmann distribution of the particle number density. Using a known potential energy profile, one can determine the colloidal osmotic pressure as a function of particle density, i.e., the osmotic equation of state, from the density profiles of interacting colloids. We use particle density profiles determined by confocal imaging of fluorescent polystyrene nanoparticles transiently confined in an optical trap to determine the colloidal osmotic equation of state for colloids in the presence of KCl and neutral polymers. The osmotic compressibility and chemical potentials of the colloids are calculated from the osmotic equation of state to predict colloidal stability and phase transitions.

4:18PM W35.00010 Determination of colloidal osmotic equation of state by dielectrophoresis.  
JACOB MAZZA, HAO HUANG, H. DANIEL OU-YANG, Lehigh University — Osmotic equation of state $P(N,T)$ describes both the mechanical properties and phase behavior of a colloidal suspension. As an alternative to sedimentation, we propose a new approach to determine $P(N,T)$ by dielectrophoresis (DEP). Using fluorescence confocal microscopy, we obtain particle density profiles in order to determine the DEP force distribution when the particle concentration is low and the inter-particle interactions are negligible. From the known force distribution and Einstein’s osmotic equilibrium equation, we can calculate $P(N,T)$ from the particle density profile of interacting, charge-stabilized polystyrene latex particles under different salt concentrations and added neutral polymers. The osmotic equation of state for colloidal suspensions can then be crosschecked by sedimentation equilibrium.

4:30PM W35.00011 Differential Dynamic Microscopy of Weakly Scattering and Polydisperse Protein Rich Clusters.  
JACINTA CONRAD, MOHAMMAD SAFARI, PETER VEKILOV, University of Houston — Biological objects often scatter light weakly and are frequently smaller than the diffraction limit, complicating measurements of their dynamics. Differential dynamic microscopy (DDM) is a recently developed method to quantify dynamics of sub-$\mu$m particles in solutions from fluctuations in intensity in optical micrographs. DDM is well established for monodisperse particles but has not been applied to polydisperse biological nanoparticles. Here, we used DDM to measure dynamics of polydisperse nanoscale objects, protein-rich liquid clusters in protein solutions, whose size ranged from tens to hundreds of nanometers and whose total volume fraction was less than 10$^{-5}$. For solutions of two proteins, lysozyme and hemoglobin A, we measured the dynamics of clusters using DDM and evaluated their diffusion coefficients from the dependence of the diffusion lag time on the scattering wave vector. The average diffusion coefficient of clusters measured using DDM was consistently smaller than that obtained from dynamic light scattering at 90°. The apparent discrepancy between these results was explained by Mie scattering theory, which indicates that larger clusters preferentially scatter more light in the forward direction.

4:42PM W35.00012 Fast Holographic Characterization of Dimpled Spheres.  
MARK HANDEL, CHRISTINE MIDDLETON, DAVID GRIER, New York University — We present a method for quickly analyzing the radii and refractive indexes of dimpled spheres using Holographic Video Microscopy. Our method utilizes an azimuthal median to suppress the perturbation caused by the dimple on an otherwise radially symmetric hologram. The resulting one-dimensional radial profile is fit to Lorenz-Mie theory using Support Vector Machines (SVM). We then discuss the limitations of this method as well as the use of SVMs trained on different scattering geometries or theories.

4:54PM W35.00013 Highly uniform polyhedral colloids formed by colloidal crystal templating.  
YIFAN WANG, JAMES MCCGINLEY, JOHN CROCKER, Univ of Pennsylvania, CROCKER RESEARCH GROUP TEAM — We seek to create polyhedral solid particles by trapping oil droplets in a colloidal crystal, and polymerizing them in situ, resulting in polyhedral particles containing spherical dimples in an ordered arrangement. Specifically, highly monodisperse, micron-sized droplets of 3-methacryloxypropyl trimethoxysilane (TPM) were first prepared through a recently developed method used to quantify dynamics of sub-$\mu$m particles in solutions from fluctuations in intensity in optical micrographs. DDM is well established for monodisperse particles but has not been applied to polydisperse biological nanoparticles. Here, we used DDM to measure dynamics of polydisperse nanoscale objects, protein-rich liquid clusters in protein solutions, whose size ranged from tens to hundreds of nanometers and whose total volume fraction was less than 10$^{-5}$. For solutions of two proteins, lysozyme and hemoglobin A, we measured the dynamics of clusters using DDM and evaluated their diffusion coefficients from the dependence of the diffusion lag time on the scattering wave vector. The average diffusion coefficient of clusters measured using DDM was consistently smaller than that obtained from dynamic light scattering at 90°. The apparent discrepancy between these results was explained by Mie scattering theory, which indicates that larger clusters preferentially scatter more light in the forward direction.


2:30PM W36.00001 Quantifying fermionic decoherence in many-particle systems.  
ARNAB KAR, IGNACIO FRANCO, Univ of Rochester — Decoherence or the loss of quantum correlations in a system arises due to the interaction of the system with its environment. Our aim is to construct measures of decoherence that are applicable to multi-electron systems and, using them, understand the relationship between electronic correlations and decoherence. Usual measures of decoherence are of limited applicability in many body systems because they are based on the hierarchy of particle reduced density matrices [1-2]. Given a single particle basis, these measures can be used to succinctly capture relevant coherences and interpret decoherence dynamics in driven and non-driven many body systems. The distilled purity measures will be exemplified using the dynamics of the Su-Schrieffer-Heeger Hamiltonian for trans-polyacetylene. The advantages and limitations of these distilled purity measures will also be discussed.


2:42PM W36.00002 High Resolution Neutral Atom Microscope.  
IGHL BUCAY, RODRIGO CASTILLO-GARZA, GEORGIOS STRATIS, MARK RAIZEN, University of Texas at Austin — We are developing a high resolution neutral atom microscope based on metastable atom electron spectroscopy (MAES). When a metastable atom of a noble gas is near a solid, a surface electron will tunnel to an empty energy level of the metastable atom, thereby ejecting the excited electron from the atom. The emitted electrons carry information regarding the local topography and electronic, magnetic, and chemical structures of most hard materials. Furthermore, using a chromatic aberration corrected magnetic hexapole lens we expect to attain a spatial resolution below 10 nm. We will use this microscope to investigate how local phenomena can give rise to macroscopic effects in materials that cannot be probed using a scanning tunneling microscope, namely insulating transition metal oxides.
2:54PM W36.00003 Feshbach Modulation Spectroscopy1. JAMES FREERICHS, Georgetown Univ, ANDREAS DIRKS, Volume Graphics, HULILAK KRISHNAMURTHY, Indian Institute of Science, KARLIS MIKELSONS, Global Science and Technology — Feshbach resonances are often swept through to bind atoms into weakly bound molecules. Here we propose to examine the behavior of systems close to a Feshbach resonance when we modulate the bias magnetic field as a function of time, creating a modulated scattering length. On an optical lattice, this system undergoes rich physical transformations which involve both molecule formation and the hopping of molecules on the lattice and thus goes beyond a single-band Hubbard model description. While experiments have already studied some of this phenomena, especially resonance effects on the binding of molecules, we feel that this system is likely to have interesting physical behavior when on an optical lattice. We propose to probe the behavior with a harmonic modulation of the magnetic field and thus the scattering length across the Feshbach resonance as a generalization of lattice-depth modulation spectroscopy. In the regime in which the single-band Hubbard model is still valid, we provide simulation data for this type of spectroscopy which behaves somewhat differently from conventional modulation spectroscopy (the hopping is not modulated, just the interaction strength).

3:06PM W36.00004 Quantum Melting in a Polariton Lattice, ALEXANDER EDELMAN, PETER LITTLEWOOD, Univ of Chicago — We study a generalized Dicke model of lattice polaritons, with a pair-potential interaction between excited states of the spin component, in the functional integral formalism. Even considering only zero-temperature equilibrium effects with a uniform photon field, there is a rich phase diagram as a function of light-matter coupling, which includes spatially ordered and superfluid phases. Depending sensitively on the form of the potential, the interaction may induce an instability in the sound mode of the polariton condensate, or destroy the condensate altogether. Zero-temperature fluctuations may likewise melt the spatially ordered phases. We consider implications for cold-atom experiments with tunable interactions, as well as interacting exciton-polaritons accessible in the solid state.

3:18PM W36.00005 Quantum fluctuations and gapped Goldstone modes in spinor Bose-Einstein condensates, ARON BEEKMAN, RIKEN Center for Emergent Matter Science — The classical Heisenberg ferromagnet is an exact eigenstate of the quantum Hamiltonian and therefore has no quantum fluctuations. Furthermore it has a reduced number of Goldstone modes, an order parameter that is itself a symmetry generator, is a highest-weight state for the spin algebra, and has no tower of states of vanishing energy. We derive the connection between all these properties and provide general criteria for their presence in other spontaneously-broken symmetry states. The phletora of groundstates in spinor Bose-Einstein condensates is an ideal testing ground for these predictions. In particular the phases with non-maximal polarization (e.g. the F-phase in spin-3 condensates) have an additional gapped mode that is a partner to the quadratically dispersing Goldstone mode, as compared to the maximally polarized, ferromagnetic phase. Furthermore there is a fundamental limit to the coherence time of superpositions in the non-maximally polarized state, which should manifest itself for small-size systems.

3:30PM W36.00006 Emergent dual space-time geometry for free fermions, CHING HUA LEE, XIAO-LIANG QI, Stanford Univ — The theme of holography has attracted great interest among high energy and condensed matter physicists alike. It involves describing a ‘boundary’ system in terms of a ‘bulk’ system in a space one dimension higher, with the emergent direction representing energy scale. We propose a simple exact holographic mapping for lattice systems based on wavelet bases, which naturally entail an emergent dimension representing scale. The system in the new basis is identified as the bulk, whose correlation functions can be interpreted as that of a massive field in curved spacetime. Despite the simplicity of our approach, we obtain in the long wavelength limit geometries that are consistent with those expected from the Ryu-Takayanagi formula, i.e. AdS space for critical zero-temperature systems, a paradigmatic example of the AdS-CFT correspondence. At nonzero temperature, we obtain the BTZ and Lifshitz black holes for linear and nonlinear critical band touchings respectively, as we analytically verify up to the subleading logarithmic correction. Our results remain true in any number of dimensions, under generic local wavelet bases.

3:42PM W36.00007 Supersymmetry in quantum optics and in spin-orbit coupled systems1. MICHAEL TOMKA, Boston University, MIKHAIL PLETYUKHOV, Institute for Theory of Statistical Physics and JARA - Fundamentals of Future Information Technology, RWTH Aachen, VLADIMIR GRITSEV, Institute of Theoretical Physics, University of Amsterdam — Light-matter interaction is naturally described by coupled bosonic and fermionic subsystems. This suggests that a certain Bose-Fermi duality is naturally present in the fundamental quantum mechanical description of photons interacting with atoms. We reveal submanifolds in parameter space of a basic light-matter interacting system where this duality is promoted to a supersymmetry (SUSY) which remains unbroken. We show that SUSY is robust with respect to decoherence and dissipation. In particular, the stationary density matrix at the supersymmetric lines in parameter space has a degenerate subspace. The dimension of this subspace is given by the Witten index that is itself a symmetry generator, is a highest-weight state for the spin algebra, and has no tower of states of vanishing energy. We derive the connection between all these properties and provide general criteria for their presence in other spontaneously-broken symmetry states. The phletora of groundstates in spinor Bose-Einstein condensates is an ideal testing ground for these predictions. In particular the phases with non-maximal polarization (e.g. the F-phase in spin-3 condensates) have an additional gapped mode that is a partner to the quadratically dispersing Goldstone mode, as compared to the maximally polarized, ferromagnetic phase. Furthermore there is a fundamental limit to the coherence time of superpositions in the non-maximally polarized state, which should manifest itself for small-size systems.

1Swiss National Science Foundation

3:54PM W36.00008 Magnetization and Transport Properties for Particles in Spin Textures1, TIMOTHY MCCORMICK, NANDINI TRIVEDI, The Ohio State University — We use exact-diagonalization and Monte Carlo (ED + MC) to calculate the magnetization M(T) and the spin polarization P(T) for a charged particle moving in a variety of ferromagnetic, spiral and chiral spin textures. We derive an effective spin Hamiltonian by integrating out charged degrees of freedom and compare its magnetization with that of the full Hamiltonian. We then calculate transport properties such as the dynamical conductivity (Sigma(omega)) and the anomalous Hall conductivity using the Chern number.

1This work has been supported by grant number NSF-DMR1309461

4:06PM W36.00009 Emergent Magnetic Monopole Charges in a Two Qubit System, TIAGO GRANGEIRO SOUZA BARBOSA LIMA, MICHAEL KOLODRUBETZ, ANATOLI POLKOVNIKOV, Boston Univ — The topology of two coupled qubits has recently been explored using dynamical measurements of their Berry curvature F. Its integral gives the topologically invariant Chern number, which natural maps to the presence of magnetic monopole charges in parameter space. We suggest a method for measuring the magnetic monopole charge density and detail its motion as external parameters are varied. Using Maxwell’s equations with the addition of magnetic monopoles, we obtain the effective charge density and the current density as a function of the parameters. We show how particular choices for parameters give rise to peculiar motion of the monopole charges, which can go from isolated charges to continuous charge distributions like rings and surfaces by properly changing the system’s symmetries through its parameters. Finally, we probe the interesting but as yet unexplored consequences on ∇ × F as said changes are made.

4:18PM W36.00011 Entropy flow in quantum heat engines, MOHAMMAD ANSARI, YULI NAZAROV, Kavli Institute for Nanoscience, Delft University of Technology — We evaluate Shannon and Renyi entropy flows from generic quantum heat engines (QHE) to a weakly-coupled probe environment kept in thermal equilibrium. We show the flows are determined by two quantities: heat flow and fictitious dissipation that manifest the quantum coherence in the engine. Our theory leads to novel physics in quantum heat engines.

3:54PM W36.00008 Magnetization and Transport Properties for Particles in Spin Textures1, TIMOTHY MCCORMICK, NANDINI TRIVEDI, The Ohio State University — We use exact-diagonalization and Monte Carlo (ED + MC) to calculate the magnetization M(T) and the spin polarization P(T) for a charged particle moving in a variety of ferromagnetic, spiral and chiral spin textures. We derive an effective spin Hamiltonian by integrating out charged degrees of freedom and compare its magnetization with that of the full Hamiltonian. We then calculate transport properties such as the dynamical conductivity (Sigma(omega)) and the anomalous Hall conductivity using the Chern number.

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4:06PM W36.00009 Emergent Magnetic Monopole Charges in a Two Qubit System, TIAGO GRANGEIRO SOUZA BARBOSA LIMA, MICHAEL KOLODRUBETZ, ANATOLI POLKOVNIKOV, Boston Univ — The topology of two coupled qubits has recently been explored using dynamical measurements of their Berry curvature F. Its integral gives the topologically invariant Chern number, which natural maps to the presence of magnetic monopole charges in parameter space. We suggest a method for measuring the magnetic monopole charge density and detail its motion as external parameters are varied. Using Maxwell’s equations with the addition of magnetic monopoles, we obtain the effective charge density and the current density as a function of the parameters. We show how particular choices for parameters give rise to peculiar motion of the monopole charges, which can go from isolated charges to continuous charge distributions like rings and surfaces by properly changing the system’s symmetries through its parameters. Finally, we probe the interesting but as yet unexplored consequences on ∇ × F as said changes are made.

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4:30PM W36.00011 Dynamics of Noisy Quantum Systems in the Heisenberg Picture: Application to the Stability of Fractional Charge. ARMIN RAHMANI, University of British Columbia — Based on the Heisenberg-picture analog of the master equation, we develop a method for computing the exact time dependence of noise-averaged observables for (generally interacting) fermionic systems with noisy hopping processes. Our results provide access to a long-time limit, which is not amenable to numerical simulations. As a simple example, we examine the fate of the fractional charge in a noisy dimerized lattice with a domain wall (relevant to cold-atom emulations of polyacetylene). We find that the fractional charge remains robust against noisy hopping processes between different sublattices, while it becomes unstable to fluctuations in hopping on the same sublattice.

1LANL/LDRD, UBC-Max-Planck Fellowship

4:42PM W36.00012 Fermions in a harmonic trap with spin-imbalanced filling. DENIS MORATH, STEFAN A. SOEFFING, SEBASTIAN EGGERT, Univ. of Kaiserslautern — In recent experiments with ultra-cold fermions it was possible to prepare states with imbalanced pseudo-spin fillings, analogous to electrons in quantum dots. This offers the opportunity to make controlled measurements of the effects of interactions, spin filling and temperature on the density of confined fermions. We now consider the situation in a one-dimensional trap theoretically and with numerical quantum simulations (quantum Monte Carlo and DMRG). Already for three particles in a trap there is a surprising alignment of spin up an down particles with a rather dramatic effect of the temperature. Naively an antiferromagnetic correlation between the spin species should be expected for repulsive interactions, i.e. density maxima of spin-up should correlate in space with spin-down minima and vice versa. However, already very low finite temperatures can induce ferromagnetic correlations. Based on the analysis of few particle situations and symmetry considerations we can also explain the behaviour of many particle systems.

Supported by OPTIMAS and the Deutsche Forschungsgemeinschaft via the SFB/TR49

4:54PM W36.00013 Many-Body Transition in a Spin-Orbit Coupled Bose-Einstein Condensate, JEFFREY T.F. POON, XIONG-JUN LIU, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China — In quantum mechanics, a resonant Rabi oscillation can occur between two degenerate single-particle states when such two states are subject to external perturbations. This phenomenon can be qualitatively different in the interacting regime. In this work, we study a spin-orbit coupled Bose-Einstein condensate with degenerate many-body states and examine the transitions between such states. We find that due to the particle-particle interactions the many-body transitions between such degenerate states are completely different from the physics in single-particle systems. Both the numerical and analytic results will be discussed.

5:06PM W36.00014 Landau-Zener transitions in a two-level system that is coupled to a finite-temperature harmonic oscillator. SAHEL ASHHAB, Qatar Environment and Energy Research Institute, Qatar Foundation, Doha, Qatar — The Landau-Zener (LZ) problem is a standard paradigm for studying energy transfer and adiabatic passage protocols. We consider the LZ problem for a two level system when this system interacts with one harmonic oscillator mode that is initially set to a finite-temperature thermal equilibrium state. The oscillator could represent an external mode that is strongly coupled to the system, e.g. an ionic oscillation mode in a molecule, or it could represent a prototypical uncontrolled environment. We analyze the system’s occupation probabilities at the final time in a number of different regimes, varying the system and oscillator frequencies, their coupling strength and the temperature. In particular we find some surprising non-monotonic dependence on the coupling strength and temperature.

5:18PM W36.00015 Effects of nonmagnetic impurities on BCS-BEC crossover in atomic Fermi gases. YANMING CHE, QIJIN CHEN, Zhejiang University — We present a systematic investigation of the effects of nonmagnetic impurities on the $s$-wave BCS-BEC crossover within a pairing fluctuation theory. Both the pairing $T$-matrix and the impurity scattering $T$-matrix are treated self-consistently at the same time, in the context of ultracold atomic Fermi gases. While the system is less sensitive to impurity scattering in the BCS limit, in the strong impurity scattering limit, both the frequency and the gap function are highly renormalized, leading to significant suppression of the superfluid $T_c$. In the BCS regime, the superfluidity may be readily destroyed by the impurity, leading to an effective power law dependence of $T_c$ as a function of pairing strength. In comparison, $T_c$ and (pseudo)gaps in the unitary and BEC regimes are relatively more robust. In either cases, the $s$-wave pairing is less sensitive to impurity than its $d$-wave counterpart. Calculations of superfluid density will also be presented. References: Q.J. Chen and J.R. Schrieffer, Phys. Rev. B 66, 014512 (2002).

Supported by NSF, MOE and MOST of China

Thursday, March 5, 2015 2:30PM - 5:30PM — Session W37 GQI: Focus Session: Semiconductor Qubits - Gated Dots and Impurities II 212A - Charles Tahan, Laboratory for Physical Sciences

2:30PM W37.00001 Theory of the Quantum Dot Hybrid Qubit. MARK FRIESEN, University of Wisconsin-Madison — The quantum dot hybrid qubit, formed from three electrons in two quantum dots, combines the desirable features of charge qubits (fast manipulation) and spin qubits (long coherence times). The hybridized spin and charge states yield a unique energy spectrum with several useful properties, including two different — The quantum dot hybrid qubit, formed from three electrons in two quantum dots, combines the desirable features of charge qubits (fast manipulation) and spin qubits (long coherence times). The hybridized spin and charge states yield a unique energy spectrum with several useful properties, including two different...

3:06PM W37.00002 Rabi oscillations at different tunnel couplings for an ac-gated quantum dot qubit. BRANDUR THORGRIIMSSON, DOHUN KIM, C.B. SIMMONS, DANIEL R. WARD, RYAN H. FOOTE, D.E. SAVAGE, M.G. LAGALLY, MARK FRIESEN, S.N. COPPERSMITH, M.A. ERIKSSON, Univ of Wisconsin, Madison — One way to create a qubit is to use two distinct positions of a single electron as qubit states. Such a system can be achieved by using the left and right positions in a gated double quantum dot. In this system the qubit is strongly coupled to electric fields and has potential for high-speed operations. By tuning specific gate voltages, we can tune the tunnel coupling strength and microwave drive power, and we study strong driving effects such as generation of second harmonics. This work was supported in part by ARO (W911NF-12-0607) and NSF (DMR-1206915 and PHY-1104660). Development and maintenance of the growth facilities used for fabricating samples is supported by DOE (DE-FG02-03ER46028). This research utilized NSF-supported shared facilities at the University of Wisconsin-Madison.

3:06PM W37.00002 Rabi oscillations at different tunnel couplings for an ac-gated quantum dot qubit. — BRANDUR THORGRIIMSSON, DOHUN KIM, C.B. SIMMONS, DANIEL R. WARD, RYAN H. FOOTE, D.E. SAVAGE, M.G. LAGALLY, MARK FRIESEN, S.N. COPPERSMITH, M.A. ERIKSSON, Univ of Wisconsin, Madison — One way to create a qubit is to use two distinct positions of a single electron as qubit states. Such a system can be achieved by using the left and right positions in a gated double quantum dot. In this system the qubit is strongly coupled to electric fields and has potential for high-speed operations. By tuning specific gate voltages, we can tune the tunnel coupling strength and microwave drive power, and we study strong driving effects such as generation of second harmonics. This work was supported in part by ARO (W911NF-12-0607) and NSF (DMR-1206915 and PHY-1104660). Development and maintenance of the growth facilities used for fabricating samples is supported by DOE (DE-FG02-03ER46028). This research utilized NSF-supported shared facilities at the University of Wisconsin-Madison.
3:18PM W37.00003 Single-electron spin resonance in a Si/SiGe double quantum dot with a micromagnet, KENTA TAKEDA, The University of Tokyo, JUN KAMIOKA, Tokyo Institute of Technology, TOSHIKAI OBATA, The University of Tokyo, TOMOHIRO OTSUKA, TAKASHI NAKAJIMA, MATTHIEU DELSECQ, SHINICHI AMADA, JUN YONEDA, CEMS, RIKEN, AKITO NOIRI, RETSU SUZUKI, TAKAYUKI OKAYA, SHUNRI ODA, Tokyo Institute of Technology, SEIGO TAKACHI, University of Tokyo, CEMS, RIKEN, THE UNIVERSITY OF TOKYO TEAM, TOKYO INSTITUTE OF TECHNOLOGY COLLABORATION, CEMS, RIKEN COLLABORATION — Electrons in Si quantum dots are promising candidates for implementing spin qubits because of their long coherence times [1, 2]. We report on our measurement results of addressable electron spin resonance in a Si/SiGe double quantum dot with a micromagnet. We also show that the addressable electron spin resonance is useful to understand two-electron spin and valley states in Si double quantum dot. [1] E. Kawakami et al., Nat. Nanotech. (2014). [2] M. Veldhorst et al., Nat. Nanotech. (2014)

3:30PM W37.00004 Hybrid Spin and Valley Quantum Computing with Single-Triplet Qubits, NIKLAS ROHLING, MAXIMILIAN RUSS, GUIDO BURKARD, Department of Physics, University of Konstanz, Germany — The valley degree of freedom in the electronic band structure of silicon, graphene, and other materials is often considered to be an obstacle for quantum computing (QC) based on electron spins in quantum dots. Here we show that control over the valley state opens new possibilities for quantum information processing. Combining qubits encoded in the singlet-triplet subspace of spin and valley states allows for universal QC using a universal two-qubit gate directly provided by the exchange interaction. We show how spin and valley qubits can be separated in order to allow for single-qubit rotations [1].

3:42PM W37.00005 Single-electron donor-quantum-dot qubit in silicon, PATRICK HARVEY-COLLARD, Université de Sherbrooke, GREGORY A. TEN EYCK, JOEL R. WENDT, TAMMY PLUYM, Sandia National Laboratories, MICHAEL P. LILLY, Center for Integrated Nanotechnologies, Sandia National Laboratories, MALCOLM S. CARROLL, Sandia National Laboratories, MICHEL PIORO-LADRIERE, Université de Sherbrooke — Electron spins bound to phosphorus (P) donors in silicon (Si) are promising qubits due to their high fidelities, but donor-donor coupling is challenging. We propose an alternative two-electron single-triplet quantum-dot (QT) and donor (D) hybrid qubit. A QT is formed at a MOS 28-Si interface and is tunnel-coupled to implanted donors. The proposed two-axis system is defined by the exchange and contact hyperfine interactions. We demonstrate that a few electron QT can be formed and tuned to interact with a donor. We investigate the spin filling of the D-QT system through charge-sensed (CS) magnetotransport and identify spin-up loading consistent with a singlet-triplet splitting of ~100 µeV near a QT-D anti-crossing. We also demonstrate an enhanced CS readout contrast and time window due to the restricted relaxation path of the D through the QT. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

3:54PM W37.00006 Coupling a Si/SiGe quantum dot to an implanted phosphorus donor, RYAN H. FOOTE, DANIEL R. WARD, BRANDUR THORGRIMSSON, University of Wisconsin - Madison, J.R. PRANCE, Lancaster University, Lancaster, UK, ANDRE SARAJIVA, D.E. SAVAGE, MARK FRIESEN, S.N. COPPERSMITH, M.A. ERIKSSON, University of Wisconsin - Madison — We have fabricated quantum dots in a Si/SiGe heterostructure both with and without implanted phosphorus donors. We present the results of transport measurements at dilution refrigerator temperatures through both types of devices. In one device we see evidence of coupling between a dot and a localized state consistent with a donor. We present estimates of the position of the localized state using Coulomb blockade measurements as a function of several different gate voltage configurations. This research supported in part by NSF (DMR-1206915) and ARO (W911NF-12-1-0607). Development and maintenance of the growth facilities used for fabricating samples is supported by DOE (DE-FG02-03ER46028). This research utilized facilities supported by the NSF (DMR-1121288).

4:06PM W37.00007 Few electron quantum-dot coupling to donor implanted electron spins, MARTIN RUDOLPH, PATRICK HARVEY-COLLARD, ERIK NIELSON, JOHN GAMBLE, RICHARD MULLER, TOBY JACOBSON, GREG TEN-EYCK, JOEL WENDT, TAMMY PLUYM, MICHAEL LILLY, MALCOLM CARROLL, Sandia National Laboratory — Donor-based Si qubits are receiving increased interest because of recent demonstrations of high fidelity electron or nuclear spin qubits and their coupling. Quantum dot (QD) mediated interactions between donors are of interest for future coupling of two donors. We present experiment and modeling of a poly silicon/Si MOS QD, charge-sensed by a neighboring many electron QD, capable of coupling to one or two donor implanted electron spins (D) while tuned to the few electron regime. The unique design employs two neighboring gated wire PETS and self-aligned implants, which supports many configurations of implanted donors. We can access the (0,1)⇔(1,0) transition between the D and QD, as well as the resonance condition between the few electron QD and two donors ((0,N,1)⇔(0,N+1,0)⇔(1,N,0)). We characterize capacitances and tunnel rate behavior combined with semi-classical and full configuration interaction simulations to study the energy landscape and kinetics of D-QD transitions. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility. The work was supported by the Sandia National Laboratories Directed Research and Development Program. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

4:18PM W37.00008 Device-Level Models Using Multi-Valley Effective Mass, ANDREW D. BACZEWSKI, Sandia National Laboratories, ADAM FREES, University of Wisconsin-Madison, JOHN KING GAMBLE, XUJIAO GAO, N. TOBIAS JACOBSON, JOHN A. MITCHELL, INÉS MONTAÑO, RICHARD P. MULLER, ERIK NIELSEN, Sandia National Laboratories — Continued progress in quantum electronics depends critically on the availability of robust device-level modeling tools that capture a wide range of physics and effective mass theory (EMT) is one means of building such models. Recent developments in multi-valley EMT show quantitative agreement with more detailed atomistic tight-binding calculations of phosphorus donors in silicon (Gamble, et. al., arXiv:1408.3159). Leveraging existing PDE solvers, we are developing a framework in which this multi-valley EMT is coupled to an integrated device-level description of several experimentally active qubit technologies. Device-level simulations of quantum operations will be discussed, as well as the extraction of process parameters at this level of theory. The authors gratefully acknowledge support from Sandia National Laboratories and Fellowship Program, which is funded by the Laboratory Directed Research and Development (LDRD) Program. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Security Administration under contract DE-AC04-94AL85000.

4:30PM W37.00009 Multi-valley effective mass theory for device-level modeling of open quantum dynamics, N. TOBIAS JACOBSON, ANDREW D. BACZEWSKI, Sandia National Labs, ADAM FREES, University of Wisconsin-Madison, Sandia National Labs, JOHN KING GAMBLE, INÉS MONTANO, JONATHAN E. MOUSSA, RICHARD P. MULLER, ERIK NIELSEN, Sandia National Labs — Simple models for semiconductor-based quantum information processors can provide useful qualitative descriptions of device behavior. However, as experimental implementations have matured, more specific guidance from theory has become necessary, particularly in the form of quantitatively reliable yet computationally efficient modeling. Besides modeling static device properties, improved characterization of noisy gate operations requires a more sophisticated description of device dynamics. Making use of recent developments in multi-valley effective mass theory, we discuss device-level simulations of the open system quantum dynamics of a qubit interacting with phonons and other noise sources.

1Sandia is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.
4:42PM W37.00010 Multi-valley effective mass treatment of donor-dot tunneling in silicon

ADAM FREES, UW-Madison, ANDREW D. BACZEWSKI, JOHN KING GAMBLE, N. TOBIAS JACOBSON, RICHARD P. MULLER, ERIK NIELSEN, Sandia National Laboratories — Many cutting-edge experiments in silicon-based devices for quantum information processing involve the tunneling of an individual electron from a donor atom within the material to the interface of the heterostructure. Understanding how this tunneling process varies among different realistic devices is therefore of great interest. Using a multi-valley effective mass approximation method, we find the tunnel coupling, adiabatic min-gap, and ionizing electric field strength between a phosphorous donor in silicon and a nearby quantum dot at a Si/SiO₂ interface. Additionally, we calculate these quantities for a phosphorous donor in strained silicon and a Si/SiGe interface. We consider how these properties change as a function of relative position between the donor and the dot. The authors gratefully acknowledge support from the Sandia National Laboratories Truman Fellowship Program, which is funded by the Laboratory Directed Research and Development (LDRD) Program. Sandia is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the US Department of Energy’s National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

4:54PM W37.00011 Electron spin coherence of shallow donors in germanium

M.T. BELL, J. Paramanandam, L.B. Ioffe, and M.E. Gershenson.

When the flux qubit is readout by a dc-SQUID, normally people use a coil to bias both the qubit and the dc-SQUID. Here we consider an alternative method in which a single coil is used to bias both the qubit and the dc-SQUID. This method has the advantage of being able to change the flux bias of the qubit very little because of the very small mutual inductance between the qubit and the trap loop. We will discuss the experimental aspects of the FPQ optimization and the possibility of fault-tolerant operations with these qubits.

5:06PM W37.00012 Spin ensembles as sensitive probes of environmental magnetic field noise

ABRAHAM ASFAW, Department of Electrical Engineering, Princeton University, Princeton NJ 08544, USA, GARY WOLFOWICZ, JOHN J. L. MORTON, London Centre for Nanotechnology, University College London, London WC1H OAH, UK, ALEXEI TYRSHSKIN, STEPHEN LYON, Department of Electrical Engineering, Princeton University, Princeton NJ 08544, USA — Environmental magnetic field noise makes quantum control of electron and nuclear spins difficult. Conversely, the sensitivity of spins to small magnetic fields implies that they can be used as sensitive probes of magnetic field fluctuations. We report spin resonance measurements of donors in silicon showing that the phase information in single-shot measurements of spin ensembles combined with quadrature detection can yield useful information about environmental noise. By measuring the accumulated phase statistics with time, we extract the power spectrum of the environmental magnetic field noise. The range of noise frequencies probed in this way is set by the magnetic moment of the spins. We measure the noise power spectrum at high frequencies (100 Hz - 10 kHz) using electron spins and at low frequencies (1 - 100 Hz) using nuclear spins. We also show that a broadband measurement of the noise power spectrum can be obtained by tuning the magnetic moment of electron spins in bismuth donors over a wide range from 0.01 to 1 electron magnetic moment. Our method, which uses the full statistics of the accumulated phase, can be viewed as complementary to existing dynamical decoupling schemes which use filter functions to probe the noise power spectrum.

5:18PM W37.00013 Mechanical tuning of ionized donors in silicon

DAVID P. FRANKE, FLORIAN M. HRUBESCH, MARKUS KUENZL, MATTHEW BELL, Rutgers University and University of Massachusetts, Boston, XIAOYUE JIN, Rutgers University, LEV IOFFE, Rutgers University and University Centre for Nanotechnology, University College London, London WC1H OAH, UK, ALEXEI TYRSHSKIN, STEPHEN LYON, Department of Electrical Engineering, Princeton University, Princeton NJ 08544, USA — Ionized donors in silicon have shown to have extraordinarily long coherence times, exceeding tens of minutes even at room temperature, which, combined with the very advanced state of silicon technology, makes them attractive candidates for the realization of solid state qubits. The corresponding near perfect isolation from their environment, however, renders the individual addressing and coupling of such qubits a major challenge on the way towards a spin quantum computer based on ionized donors. We show that the application of strain to the silicon host crystal leads to shifts of the nuclear spin resonance frequencies of 75As due to the nuclear quadrupole interaction with crystal fields. This shift can be larger than the resonance linewidth for modest strains, as we demonstrate by electrically detected electron nuclear double resonance (ED ENDOR) measurements on arsenic donors in strained silicon. We discuss how quadrupole interactions could allow for the individual addressing of ionized nuclear spins by mechanical tuning of their resonance frequency and, possibly, permit the elastic coupling of nuclear spin qubits to a mechanical resonator.

Thursday, March 5, 2015 2:30PM - 5:30PM —
Session W39 GQI: Focus Session: Superconducting Qubits: Measurement and Novel Architectures

2:30PM W39.00001 Parity Protection in Flux-Pairing Qubits

WENYUAN ZHANG, Rutgers University, MATTHEW BELL, Rutgers University and University of Massachusetts, Boston, XIAOYUE JIN, Rutgers University, LEV IOFFE, Rutgers University and MATTHEW BELL, Rutgers University and University of Massachusetts, Boston, XIAOYUE JIN, Rutgers University, LEV IOFFE, Rutgers University and MATTHEW BELL, Rutgers University and University of Massachusetts, Boston, XIAOYUE JIN, Rutgers University, LEV IOFFE, Rutgers University and MATTHEW BELL, Rutgers University and University of Massachusetts, Boston, XIAOYUE JIN, Rutgers University, LEV IOFFE, Rutgers University and MATTHEW BELL, Rutgers University and University of Massachusetts, Boston, XIAOYUE JIN, Rutgers University, LEV IOFFE, Rutgers University and MATTHEW BELL, Rutgers University and University of Massachusetts, Boston, XIAOYUE JIN, Rutgers University, LEV IOFFE, Rutgers University and MATTHEW BELL, Rutgers University and University of Massachusetts, Boston, XIAOYUE JIN, Rutgers University, LEV IOFFE, Rutgers University and MATTHEW BELL, Rutgers University and University of Massachusetts, Boston, XIAOYUE JIN, Rutgers University, LEV IOFFE, Rutgers University and

2:42PM W39.00002 Adjusting the dc-SQUID working point by a flux trapping loop for readout of gap-tunable flux qubit

XIAOBO ZHU, YULIN WU, HUI DENG, YARUI ZHENG, NAHEED AKHTAR, JIE FAN, DONGNING ZHENG, LI LU, Chinese Academy of Sci (CAS) — When the flux qubit is readout by a dc-SQUID, normally people use a coil to bias both the qubit and the dc-SQUID. However, if the working point of the qubit is located on the bottom or the top of the dc-SQUID’s critical current modulation region, the readout is hardly carried out. We insert a flux trapping loop into the readout dc-SQUID. By trapping different numbers of fluxoids in the loop, the flux bias of the dc-SQUID can be changed accordingly, while the flux bias of the qubit changes very little because of the very small mutual inductance between the qubit and the trap loop. This improvement enables us to carry out the readout in the complicated experiments of gap-tunable flux qubit.
Ramsey experiment performed shortly after the pulse. Comparing the result to that obtained using a square pulse followed by a delay of the same length as the envelope. The pulse differs from a square pulse only by the addition of two segments at the end, whose width and amplitude depend on the resonator linewidth. Here we demonstrate fast, qubit-state-independent resonator reset using a readout pulse with a simple piecewise-constant decay constant is inadequate for multi-qubit operations in which some qubits need to be measured and reused while others remain in superpositions, which would lose coherence during this time. Any residual photons continue to measure and Stark-shift the qubit, preventing high-fidelity gates. Simply waiting several times the resonator coherence time is impractical. We first explain that because of these features, only a limited improvement of measurement fidelity is possible if one uses single-mode squeezed states. We then show that by using two-mode squeezed states in a novel two-cavity geometry, one can achieve a dramatic fidelity improvement (and Heisenberg-limited scaling) using squeezed light for qubit measurement in circuit QED. In contrast to the standard problem, the phase shifts here are not deterministic and can be substantially reduced by encoding the logical qubit in a non-orthogonal basis, but can be substantially reduced by encoding the logical qubit in the eigenvectors. The process of measurement leads to quantum jumps in the eigenbasis. As a result, the excitation of the measured qubit may switch between the two qubits at a rate that depends on the qubit-qubit detuning and coupling, as well as the linewidth of the readout resonator. The switching produces readout misidentification error, which cannot be eliminated with a longer measurement. However, we show that this error can be made negligible by using a readout resonator with a sufficiently narrow linewidth.

We acknowledge support from IARPA under contract W911NF-10-1-0324.

**1** We acknowledge support from IARPA under contract W911NF-10-1-0324.
4:06PM W39.00009 Adjustable Josephson Coupler for Transmon Qubit Measurement, EVAN JEFFREY, Google Inc. — Transmon qubits are measured via a dispersive interaction with a linear resonator. In order to be scalable this measurement must be fast, accurate, and not disrupt the state of the qubit. Speed of particular importance in a scalable architecture with error correction as the measurement accounts for substantial portion of the cycle time and waiting time associated with measurement is a major source of decoherence. We have found that measurement speed and accuracy can be improved by driving the qubit beyond the critical photon number $n_{crit} = \frac{\Delta \gamma}{\Delta}$ by a factor of 2-3 without compromising the QND nature of the measurement. While it is expected that such strong drive will cause qubit state transitions, we find that as long as the readout is sufficiently fast, those transitions are negligible, however they grow rapidly with time, and are not described by a simple rate. Measuring in this regime requires parametric amplifiers with very high saturation power, on the order of -105 dBm in order to avoid losing SNR when increasing the power. It also requires a Purcell filter to allow fast ring-up and ring-down. Adjustable couplers can be used to further increase the measurement performance, by switching the dispersive interaction on and off much faster than the cavity ring-down time. This technique can also be used to investigate the dynamics of the qubit cavity interaction beyond the weak dispersive limit $n_{cavity} < n_{crit}$ not easily accessible to standard dispersive measurement due to the cavity time constant.

4:42PM W39.00010 Quantum analysis of a bandpass Purcell filter for accurate qubit readout, EYOBI A. SETE, University of California, Riverside, JOHN M. MARTINIS, University of California and Google Inc., Santa Barbara, ALEXANDER N. KOROTKOY, University of California, Riverside — In a circuit QED setup the readout fidelity of a superconducting qubit is partially limited by the qubit relaxation through the resonator into a transmission line, which is also known as the Purcell effect. One way to suppress this effect is to employ a filter, which impedes microwave propagation at the qubit frequency. We present a quantum analysis for the bandpass Purcell filter that was recently realized by E. Jeffrey et al. [PRL 112, 190504 (2014)]. Using experimental parameters, we show that the bandpass filter suppresses the qubit relaxation rate by two orders of magnitude while keeping the measurement rate the same. We also show that in the presence of a microwave drive the qubit relaxation rate further decreases with increasing drive strength.

5:06PM W39.00011 Characterizing a Superconducting Resonator with Frequency-Compensated Tunable Coupling, JAMES WENNER, B. CAMPBELL, Z. CHEN, B. CHIARO, A. DUNSWORTH, I.-C. HOI, J. KELLY, A. MEGRANT, C. NEILL, P.J.J. O’MALLEY, C. QUINTANA, T. C. WHITE, University of California, Santa Barbara, R. BARENDTS, Y. CHEN, A. C. FOWLER, E. JEFFREY, J. M. MARTINIS, University of California and Google, Santa Barbara — Deterministic quantum state transfer between devices on different chips requires the ability to transfer quantum states between traveling qubits and fixed logic qubits. Reflections must be minimized to avoid energy loss and phase interference; this requires tunable coupling to an inter-chip line while the two devices are at equal frequencies. To achieve this, we present a 6GHz superconducting coplanar resonator with tunable coupling to a 50 Ohm transmission line. We compensate for the resulting shift in resonator frequency by simultaneously tuning a second SQUID. We further demonstrate the device coherence and the ability both to release a single-frequency shaped pulse into the transmission line and to efficiently capture a shaped pulse, prerequisites for efficient inter-chip deterministic quantum state transfer.

5:40PM W39.00012 Design of a Tunable 3D Microwave Cavity for Use in Coupling to Quantum Superconducting Circuits, JQI and CNAM, Dept. of Physics, University of Maryland — We have designed a tunable 3D cavity system for use with transmon qubits. We use an rf SQUID loop as a variable inductive element that perturbs the cavity modes and produces a shift in the cavity frequency that depends on the flux applied to the loop. Our 3D cavity is made of aluminum and has a lowest mode TE101 frequency of 6.2 GHz. Following a method developed by E. U. Condon, we estimate our cavity to have an effective inductance of 100 nH [1]. Our inductive SQUID loop is made of thermally deposited aluminum on a sapphire substrate, with dimensions 250µm x 250µm, which yields an expected geometric inductance of 0.9 nH. We use a single junction in our inductive loop with a critical current of approximately 1µA. We tune the effective inductance of the loop by using a modulation coil that is well isolated from the cavity at the resonance frequency. [1] Condon, E. U. Reviews of Modern Physics. Volume 14, Number 4 (1942)

5:20PM W39.00013 Scalable architecture for coherent microwave control of weakly anharmonic qubits, DURIE DEURLOO, WOUTER VLOTHUIZEN, TNO (Netherlands Organisation for Applied Scientific Research), Delft, LEO DICARLO, Delft University of Technology, Delft, QUTECH COLLABORATION — As the number of qubits in quantum processors continues to increase in the near future, architectures offering scalability of control signals will be essential. We describe an architecture and prototype for improved scalability in microwave control of weakly anharmonic qubits in quantum processors based on repeated unit cells. We present the scalable architecture and test results on a multi-qubit processor based on circuit quantum electrodynamics.

Thursday, March 5, 2015 2:30PM - 5:30PM — Session W41 DPOLY: Polymer Nanocomposites II — 214A - Shengfeng Cheng, Virginia Polytechnic Institute and State University

2:30PM W41.00001 Liquid crystal self-assembly of zirconium phosphate nanosheet in polymeric matrix, XIAYUN HUANG, XUEZHEN WANG, ZHENGDONG CHENG, Texas A&M University — The controlled assembly of nanomaterials requires them to be well-organized over large area with controlled orientation and density. Although progress has been achieved via Langmuir-Blodgett technique, electric field directed assembly, and flow-assisted alignment, it remains a challenge for the future to control the density and orientation, especially the anisotropic particle, in the polymeric matrix. Here, we investigate the controlled assembly via liquid crystal assembly of discotic α-zirconium phosphate (α-ZrP) aqueous suspension. Liquid crystal is the material with spontaneous orientation order and our group have shown the strong aspect ratio dependency of the anisotropic-nematic transition of discotic α-ZrP nanosheet suspension. These α-ZrP discotic suspension exhibited the stable nematic alignment at low volume fractions. When volume fraction increases, it follows with the phase transition to smectic phase. Moreover, intrinsic high anisotropic nanosheet enables the formation of highly ordered liquid crystal orientation at much reduced concentration and the polymeric matrix brings the extra-functionailities, such as thermal, optical, electrical and mechanical properties. The liquid crystal phase orientation will remains in the polymeric matrix and the polymeric matrix serves as the interlayer spacer. The liquid crystal polymer nanocomposite was fabricated using high-aspect-ratio α-ZrP nanosheet embedded into a polymeric network. Due to the hydrogen bonding interaction of hydroxyl group of α-ZrP and polymeric matrix, liquid crystal nanocomposite has the interesting thermal-optical response.
Polyvinylidene Fluoride – Fe₃O₄ Nanocomposites

JERRY CONTRERAS, IBRAHIM ELAMIN, JASON PARSONS, DORINA M. CHIPARA, JAMES HINTHORNE, KAREN LOZANO, MICREA CHIPARA, The University of Texas Pan American — Fe₃O₄ nanoparticles of about 75 nm from Nanostructured & Amorphous Materials, Inc. have been dispersed into the polyvinylidene fluoride (PVDF) by melt mixing. Nanocomposites with various weight fraction of nanofiller (0%, 0.2 %, 0.6 %, 1.2 %, 2.4 %, 5.8 %, 12 %, 23 %, and 30 %) have been obtained and measured by Wide Angle X-Ray Scattering (WAXS, Bruker Discovery 8 with the Cu Kα radiation), Raman spectroscopy (Bruker Senterra confocal Raman microscope operating at 785 nm), and UV-Vis. Raman spectra indicated that alpha PVDF is the main crystalline component of the polymeric matrix and revealed a fast decay of the polymer lines as the loading with iron oxide is increased. The Raman lines have been successfully fitted by an extended Breit-Wigner Fano lineshape. The effect of the nanofiller on the position, amplitude, and width of Raman lines is analyzed in detail. WAXS investigations confirmed the presence of magnetite. The effect of the loading with nanoparticles on the position, amplitude, and width of WAXS lines of Fe₃O₄ and PVDF are reported.

Synergistic templated self-assembly of cellulose nanocrystals in thin block copolymer films

DANIELLE GROLMAN, The University of Akron — Nanofillers in thin polymer films offer unique advantage to potentially modify the film’s thermal, optical, electrical and mechanical properties due to the high surface area to volume ratio and intrinsic property change at the nanoscale. Nanofilled polymer films have been shown to exhibit unusual film stability to dewetting with a nonmonotonic behavior with nanofiller loading, potentially arising from factors such as competitive phase behavior and filler aggregation, particularly in the high nanofiller concentration limit. In this regard, block copolymer films can act as ideal nanoscale structured templates to selectively sequester and organize nanofillers. In conjunction with incorporated cellulose nanocrystals (CNCS), we seek to understand how individual anisotropic nanofillers can provide synergistic reinforcement to inherently anisotropic nanostructured block copolymer films. A clear enhancement in the Young’s Modulus was observed with increased CNC loading using strain-induced elastic buckling instability for mechanical measurements (SIEBIMM) for thin films. To this end, we examine the nanoscale to microscale morphology of the blend film through AFM, TEM and grazing incidence X-ray diffraction.

Polyisoprene-Block Polystyrene - Graphene Nanocomposites

SIEBIMM for thin films. To this end, we examine the nanoscale to microscale morphology of the blend film through AFM, TEM and grazing incidence X-ray diffraction.

3:06PM W41.00004 Raman and Wide Angle X-Ray Studies on Polystyrene-Block Polyisoprene-Block Polystyrene - Graphene Nanocomposites

DORINA CHIPARA, OSCAR M. GUERRERO, ALEJANDRA GONZALEZ, BRIAN YUST, IBRAHIM ELAMIN, JAMES HINTHORNE, MICREA CHIPARA, The University of Texas Pan American — Nanocomposites have been obtained by loading a block copolymer (Polyisoprene-Block Polystyrene (PS-b-PI-b-PS), containing 17% styrene (purified from Sigma Aldrich) with various amounts of graphene nano platelets (HD Plas Grade 4), purchased from Cheap Tubes Inc., through the solution path: PS-bPI-bPS was dissolved within cyclohexane, then nanofiller was added and the mixture was sonicated for 1 hr. The high power sonication (500 mW) improved the dispersion of the filler within the polymeric matrix. The homogenized solution was poured on glass slides covered by aluminum foil and left to evaporate the solvent. A final thermal treatment of the as obtained nanocomposites at 75 °C, has been performed overnight, in an oven. Nanocomposites containing various weight fraction of fillers ranging between 0% and 40% have been obtained. The as obtained films have been investigated by Wide Angle X-Ray Scattering, using a Bruker Discovery 8 spectrometer, FTIR (Bruker Tensor 27), UV-Vis, and Raman spectroscopy, (using a Bruker Senterra, confocal Raman microscope operating at 785 nm). The dependence of these spectra originating from the polymeric matrix and from the filler on the loading with graphene is discussed.

Computations Related to Nanoparticle Characterization and Nanocomposite Property Estimation

FERNANDO VARGAS-LARA, NIST/Wesleyan, AHMED HASSAN, EDWARD GARBOCZI, JACK F. DOUGLAS, NIST — The macroscopic properties of high-performance bulk polymer composite materials derive from the properties of the microscopic building block component particles, the polymer matrix in which they are placed, and the state of particle dispersion. The rational design of new materials then requires the characterization of the polymer matrix and the individual particles, as well as an understanding of how particle properties change as a function of spatial dispersion and particle size polydispersity and shape fluctuations. To systematically explore this multi-dimensional parameter space, we combine molecular dynamic simulations, numerical path-integrations (ZENO) and finite element calculations (COMSOL). As a specific illustration of this computational path, we calculate the electric and magnetic polarizability tensor of carbon nanotubes and graphene sheets having complex morphologies. Knowing these basic particle properties, one then can estimate electromagnetic properties of nanocomposites made with these particles, i.e., conductivity.

3:30PM W41.00006 Differential Scanning Calorimetry Investigations on Polyvinylidene Fluoride – Fe₃O₄ Nanocomposites

SAMANTHA SALINAS, ROBERT JONES, DORINA M. CHIPARA, MICREA CHIPARA, The University of Texas Pan American — Nanocomposites of polyvinylidene fluoride (PVDF)–magnetite (Fe₃O₄) with various weight fractions of nanofiller (0%, 0.2 %, 0.6 %, 1.2 %, 2.4 %, 5.8 %, 12 %, 23 %, and 30 %) have been obtained via melt mixing by loading PVDF with Fe₃O₄ particles (average size 75 nm from Nanostructured & Amorphous Materials, Inc.). Thermal stability of PVDF-Fe₃O₄ has been investigated by TGA in nitrogen. The increase of the thermal stability of PVDF due to the loading with Fe₃O₄ was quantified by the shift of the temperature at which the (mass) degradation rate is maximum as a function of Fe₃O₄ content. The effect of the nanofiller on the crystallization of PVDF was investigated by isothermal DSC (TA Instruments, Q500). Non-isothermal DSC tests, (at various heating rates ranging from 1 to 25 °C/min) have been used to locate the glass, crystallization, and melting temperatures. The dependence of the glass, crystallization, and melting temperatures on the concentration of nanoparticles is reported and analyzed in detail. The data are critically analyzed within the classical Avrami theory.

3:42PM W41.00007 Characteristics of vinyl-ester and carbon fiber composite dry and wet probe by Positron Annihilation Lifetime Spectroscopy

MAHMOUD MADANI, RICHARD D. GRANATA, Florida Atlantic University— Carbon fiber composites of vinyl-ester resins, Derakane 8084 and 510A, were studied dry and after water exposure. In this study, positron annihilation lifetime spectroscopy (PALS) was used to investigate the free volume fraction and the size of the free volume voids within the polymer matrix. The relative free volume (fractions replace by of positron lifetime intensities) in VE8084 polymer and in VE510A (Space) polymer were 35.2% and 13.8%, respectively. The free volume lifetime and intensities were determined as a function of the polymer thickness and significant differences were observed in both polymers with versus without postcuring. The effects are similar in PEI, where PEI and PE100 materials were also determined by PALS. Water uptake showed a 2% change in intensity of the longer lifetime (1.85 ns) in VE8084 polymer and in VE510A about 1.8%. The longer lifetime intensities in the wet composites were 17.1% in the 8084 polymer and its carbon fiber composite and 7.1% in the 510A polymer and its carbon fiber composite. For composite with 8084 polymer saturated (0.33% water gain) with seawater at 40 or 60 °C, no change in the longer lifetime intensity was observed which indicates no water entered the free volume voids (indicates replace by and ) some differences between composite and neat polymer. For 510A resin the third lifetime intensity dropped from 7.1% to 3.9% indicating 48% of the void volume filled with water in the composite only after saturation with seawater with respect to dry one.
4:06PM W41.00009 Controlling the dispersion and configuration of nanoﬁllers in electrically driven polymer jets with and without air flow1. YEVGEN ZHMAYEV, YONG JOO, JAY PARK, LING FEI, PRABHLEEN KAUR, HONGSHEN LIU, Cornell University — Controlling the dispersion of nanoﬁllers in polymer matrices has a signiﬁcant effect on their properties. Employing circumferentially uniform air ﬂow through the sheath layer of the concentric coaxial nozzle, the gas-assisted electrospinning utilizes both high electric field and controlled air ﬂow which can offer i) enhanced stretching of ﬂuid jet and thus much higher throughput and thinner ﬁbers, and ii) better control of dispersion and conﬁguration of nanoﬁllers in a polymer matrix even at high loadings. The ability to tailor the distribution of various nanoﬁllers (1.85-12.92 vol. % of spherical SiO2 and Si nanoparticles and rod/tube-like carbon nanotubes and carbon nanoribbons) in a polyvinyl alcohol (PVA) jet was demonstrated by varying electric potentials in conventional electrospinning and air ﬂow rates in gas-assisted electrospinning. The distribution of nanoﬁllers in nanoﬁbers was measured by transmission electron microscopy (TEM), and analyzed using an image processing software to obtain concentration proﬁles. By increasing the electric potential in conventional electrospinning from 80 to 125 kV/m, we observed almost a twofold improvement in NP distribution. The further enhancement of nanoparticle dispersion was observed in gas-assisted electrospinning: Our analysis indicated an additional 70 percent improvement with the application of high, but controlled air ﬂow. Lastly, the enhanced performance by the resulting nanoﬁbers with controlled nanoﬁller dispersion will also be addressed in Li-ion battery anode applications.

1 Axiom battery, AZ Electronic Materials

4:18PM W41.00010 Flow Effect on Alignment of MWCNTs in Polymer Nanocomposites. MASHAEL ALGHAMI, Worcester Polytechnic Institute, GEORGI GEORGEY, Assumption College, GERMANO IANNACCHIONE, Worcester Polytechnic Institute — Polymer nanocomposites are grabbing attraction for their light weight, low cost, and enhanced characteristics. In this study, we present fabrication of polyethylene ﬁlms embedded with multiwalled carbon nanotubes (MWCNTs) with anisotropic characteristics. A well dispersion of the MWCNTs in melt polyethylene is controlled through sonication to overcome their natural tendency to aggregate. An elongation process is demonstrated by free ﬂow on temperature-controlled surface in order to create organized long-range alignment of the nanoparticles within the host polymer matrix. The samples harvested off substrate show complete alignment of the CNTs, and the effect of the nanotube alignment on the mechanical and electrical properties of the nanocomposites is also investigated.

4:30PM W41.00011 Polymer Morphology and Crystallinity close to Inorganic Surfaces. KIRI AKI CHRISPOPOULOU, HELLEN PAPANANOU, SPIROS H. ANASTASIADIS, FORTH-IESL and Univ. of Crete, KONSTANTINOS S. ANDRIKOPOULOS, GEORGE A. VOYATZIS, FORTH-ICNA. In polymer science, it is crucial to obtain high-quality polymer blends with high incompatibility, since the immiscibility is a primary reason for the non-uniform dispersion of one component in another. To achieve this, we investigate the morphology, crystallization and chain conformation of a hydrophilic, semi-crystalline polymer, poly(ethylene oxide), PEO, when dissolved in a water-based solvent. Partially sponsored by EU (COST Action MP0902) and by the Greek GSRT through the call for projects "Support Program for Innovative Research Groups - Energy". The preliminary results show that they are extremely promising due to the possibility of creating nanocomposites with desired properties suit certain applications.

4:42PM W41.00012 The path to achieving molecular dispersion in an extremely dense reactive mixture. JIGNESHKUMAR PATEL, ZOU XIANG, SHAW HSU, University of Massachusetts Amherst, ANDREW SCHOCH, Saint-Gobain Research & Development — In any multicomponent reactive system, a uniform and continuous dispersion of reactants is necessary to achieve a complete reaction. In this study, we have examined the role of one additional component to disperse two seemingly unlike reagents, including a highly crystalline hexamethylenetetramine (hexa) and strongly hydrogen bonded phenol formaldehyde resin. By combining information from NMR, infrared spectroscopy and differential scanning calorimetry, we were able to identify the role of the third component in the polymerization reaction, which is required to plasticize the phenol formaldehyde resin in this crosslinking reaction. It is clear that the presence of the third component increased the segmental mobility, disrupted the hydrogen bonded matrix, and freed the hydroxyl units, which further increased the solubility of hexa. Both the endothermic and exothermic transition peaks are observed in the DSC thermogram. This unique system is also applicable to a broad range of reactive systems.

3:54PM W41.00008 Raman Spectroscopy of Poly-Urea Formaldehyde Microcapsules. OMAR ESPINO, DORINA CHIRICHI, MICHELA MARTINEZ, None — The objective of this research project was to add self-healing capabilities to polymeric microcomposites. We used the "classical" method to obtain self-healing polymers with the addition of TiO2 nanoparticles in the self-healing system. Self-healing polymers are obtained by dispersion of ﬁrst generation Grubbs catalysts and microcapsules ﬁlled with monomers (typically DCPD). These kind of "smart materials" are able to survive to high mechanical stress via the ignition of the so called "autonomous self-healing mechanism" which is actually a ring opening metathesis polymerization (ROMP) reaction triggered by mechanical stresses in excess over a threshold limit through the rupture of microcapsules and the release of the monomeric component. As a preliminary step for adding self-healing capabilities in nanocomposites, the synthesis of microcapsules ﬁlled with dicyclopentadiene (DCPD) is vital for the addition of self-healing capabilities to polymeric matrices. We synthesized polyurea-formaldehyde (PUF) microcapsules ﬁlled with monomer (DCPD) using the in-situ polymerization. The synthesis was monitored by Raman spectroscopy, optical microscopy, and pH measurements that has been extensively used as a non-invasive technique in the characterization of polymers and monitoring of organic reactions. The goal of this research was to assess the formation of the microcapsules during synthesis and the presence of the DCPD in the microcapsules. Samples were taken during the synthesis every 30 minutes and analyzed by Raman spectroscopy, and optical microscopy keeping a control over the pH of the solution.

3:54PM W41.00013 Polymer/Pristine Graphene Based Composites: From Emulsions to Strong, Electrically Conducting Foams. STEVEN WOLTORNIST, Univ of Connecticut - Storrs, JAN-MICHAEL CARRILLO, Oak Ridge National Laboratory, THOMAS XU, ANDREY DOBRYNIN, DOUGLAS ADAMSON, Univ of Connecticut - Storrs — The unique electrical, thermal and mechanical properties of graphene make it a perfect candidate for applications in graphene/graphite based polymer composites, yet challenges due to the lack of solubility of pristine graphene/graphite in water, common organic solvents, and polymer solutions and melts have limited its practical utilization. Here we report a scalable and environmentally friendly technique to form water-in-oil type emulsions stabilized by a graphene skin consisting of overlapping pristine graphene sheets that enables the exfoliation of the graphene sheets containing a continuous graphitic skin network that is electrically conducting. At the heart of our technique is the strong attraction between pristine graphene and high energy oil and water interfaces. This allows for the creation of stable water-in-oil type emulsions stabilized by a graphitic skin consisting of overlapping pristine graphene sheets that enables the synthesis of open cell foams containing a continuous graphitic skin network. At the heart of our technique is the strong attraction between pristine graphene and high energy oil and water interfaces. This allows for the creation of stable water-in-oil type emulsions stabilized by a graphitic skin consisting of overlapping pristine graphene sheets that enables the synthesis of open cell foams containing a continuous graphitic skin network. At the heart of our technique is the strong attraction between pristine graphene and high energy oil and water interfaces. This allows for the creation of stable water-in-oil type emulsions stabilized by a graphitic skin consisting of overlapping pristine graphene sheets that enables the synthesis of open cell foams containing a continuous graphitic skin network.
5:06PM W41.00014 Organic-Inorganic Shish-Kebabs: Nanocrystal Kebabs Periodically Assembled on Stretched Flexible Polymer Shish — ZHIQUN LIN, Georgia Inst of Tech, HUI XU, Xiamen University, YUCI XU, Ningbo University, XINCHANG PAN, YANJIE HE, JAEHAN JUNG, Georgia Inst of Tech, HAIPING XIA, Xiamen University — We report an unconventional yet general strategy to craft an exciting variety of 1D necklace-like nanostructures comprising uniform functional nanodisks periodically assembled along a stretched flexible polymer chain by capitalizing on judiciously designed amphiphilic worm-like diblock copolymer as nanoreactors. These nanostructures can be regarded as organic-inorganic shish-kebabs, in which nanodisk kebabs periodically situated on a stretched polymer shish. Simulations based on self-consistent field theory reveal that the formation of organic-inorganic shish-kebabs is guided by the self-assembled elongated star-like diblock copolymer constituents constrained on the highly stretched polymer chain.

5:18PM W41.00015 Strain-Tunable One Dimensional Photonic Crystals Based on Zirconium Dioxide/Slide-Ring Elastomer Nanocomposites for Mechanochromic Sensing — IRENE HOWELL, CHENG LI, NICHOLAS COLELLA, University of Massachusetts-Amherst, KOHZO ITO, University of Tokyo, JAMES WATKINS, University of Massachusetts-Amherst — Here we report on the fabrication and performance of tunable one dimensional photonic crystals (1DPCs) based on zirconium dioxide/Slide-Ring elastomer nanocomposites. 1DPCs, or Bragg mirrors, display a photonic stop band at specified wavelengths based on the design of their alternating high and low refractive index layers. By adjusting the weight percent of nanoparticles in the composite materials, a refractive index contrast of 0.18 can be achieved between filled and unfilled elastomer layers. The novel Slide-Ring matrix material consists of supramolecular polyrotaxane polymers, and maintains elasticity in the composite 1DPCs. Additionally, the high refractive index nanoparticles enable greater refractive index contrast when compared with purely polymer systems. Therefore we are able to demonstrate a 1DPC of just 6 periods, which maintains 40% reflectance over strains up to 42%. Due to their elastic and flexible behavior, these materials can function as colorimetric strain sensors. The applied strain results in a visible color shift from red to blue, demonstrating a tensile mechanochromic ($\Delta \lambda / \lambda_{max}$) sensitivity as high as 6.05 nm%/%.

Thursday, March 5, 2015 2:30PM - 5:30PM — Session W42 DPOLY: Focus Session: Multiscale Modeling of Polymers 214B - Janna Maranas, Pennsylvania State University

2:30PM W42.00001 Coarse graining of polystyrene sulfonate — DVORA PERAHIA, ANUPRIYA AGRAWAL, Clemson University, GARY S. GREST, Sandia National Laboratories — Capturing large length scales in soft matter while retaining atomistic properties is imperative to computational studies. Here we develop a new coarse-grained model for polystyrene sulfonate (PSS) that often serves as a model system because of its narrow molecular weight distribution and defined degree of sulfonation. Four beads are used to represent polymer where the backbone, the phenyl group, and the sulfonated group are each represented by a different bead and the fourth one represents counterion, which is sodium in our case. Initial atomistic simulations of PSS melt with sulfonation levels of 2-10%, with a dielectric constant $\varepsilon = 5$ revealed a “locked” phase where motion of the polymer is limited. Dielectric constant of $\varepsilon = 5$ was used to accelerate the dynamics. Bonded interactions were obtained using Boltzmann inversion on the bonded distributions extracted from atomistic simulation. Non-bonded interaction of polystyrene monomer was taken from our previous work and potential of mean force was used as the initial guess for interaction of the ionic beads. This set of potential was subsequently iterated to get a good match with radial distribution functions. This potential and its transferability across dielectric constants and temperatures will be presented.

2:42PM W42.00002 Morphology and Dynamics of Tapered Diblock Copolymers from fDFT-initialized MD Simulations — LISA M. HALL, YOUNGMI SEO, JONATHAN R. BROWN, The Ohio State University — Tapered block copolymers are similar to AB diblock copolymers, but with a statistical A-B (or B-to-A) (inverse) gradient “taper” between the A and B blocks. Depending on the sequence of monomers along the chain and the segregation strength, the A and B monomers are known to microphase separate into various ordered morphologies. Tapering introduces another parameter, independent of molecular weight or polymer choice, to tune morphology, and has been shown previously to widen the gyroid region of the phase diagram. In this study, we use classical, fluids density functional theory (fDFT) and molecular dynamics (MD) simulations to study the morphology and dynamics of tapered systems. Using fDFT allows us to accurately compare free energies between different potential microphases as a function of interaction parameter and fraction of A. Because of the similarity of the fDFT and MD models, the fDFT results map very closely with the corresponding MD model. We use the fDFT density profiles to generate the initial state of the chains for the simulations. Lamellae, cylinders, and other phases can be generated in this way with approximately correct spacing and density. We apply the streamline simulation setup to analyze the effect of tapering on conformations and dynamics.

2:54PM W42.00003 Properties of Coarse-Grained Polymer Models: Statics, Dynamics, and Crystallinity — GARY GREST, K. MICHAEL SALERNO, Sandia National Laboratories, ANUPRIYA AGRAWAL, DVORA PERAHIA, Clemson University — To capture large length and time scales, coarse-grained (CG) models that combine multiple atoms into one bead have been developed to model polymer melts. In the process microscopic detail is discarded in exchange for computational efficiency. However it is not well-understood how the scale of coarse-graining affects the polymer structure and dynamics. We compare results of atomistic simulations with CG models in which each CG bead represents three, four, or six methylene groups for C$_9$, C$_{12}$, and C$_{15}$H$_{32}$. The CG potential is developed at 500K by iterative Boltzmann inversion. While static properties such as end-to-end distance and radius of gyration are captured by all CG models, the entanglement length deviates from experimental results with increased CG scale. The mean squared displacement of CG models is used to determine scale factors between the atomistic and CG models. During cooling to low temperature, the three and four-carbon models form a semi-crystalline structure while the six-carbon model and a four-carbon model based on the MARTINI force field remain amorphous at all temperatures. These findings show that the level of coarse-graining and CG interactions can strongly affect model temperature transferability.

3:06PM W42.00004 Thermodynamically Consistent Coarse-Graining of Polymers — MARINA GUENZA, University of Oregon — Structural and dynamical properties of macromolecular liquids, melts and mixtures, bridge an extensive range of length- and time-scales. For these systems, the computational limitations of the atomistic description prevent the study of the properties of interest and coarse-grained models remain the only viable approach. In coarse-grained models, structural and thermodynamic consistency across multiple length scales is essential for the predictive role of multi-scale modeling and molecular dynamic simulations that use mesoscale descriptions. This talk presents a coarse-graining approach that conserves structural and thermodynamic quantities independent of the extent of coarse-graining, and describes a model for the reconstruction of the dynamics measured in mesoscale simulations of the coarse-grained system. Some of the general challenges of preserving structural and thermodynamic consistency in coarse-grained models are discussed together with the conditions by which the problem is lessened.

1Grant DE-SC007908
3:42PM W42.00005 Modelling and multiscale simulations of meta aromatic polyurea: microscopic geometry and dielectric properties, RUI DONG, VIVEK RANJAN, North Carolina State Univ, MARCO BUONGIORNO NARDELLI, University of North Texas, JERZY BERNHOLC, North Carolina State Univ — BOPP is the state-of-art material for high-power-density capacitors. However, its efficiency drastically drops at high electric fields. Recently, polymers in the polyurea/polythiourea family have been shown to have much higher energy density and efficiency at high fields than BOPP [1-2]. We perform multiscale simulations to investigate dielectric and structural properties of meta aromatic polyurea (mAAP). Both crystalline and disordered structures have been studied, and much larger ionic contribution to permittivity is found in disordered structures. The specific volume is 10% to 20% larger in the latter, leading to greater structural flexibility. For example, the orientation variations of polar units are 100% larger than in the crystal structure, and the phonon density of states in the low frequency regime is significantly enhanced. At the same time, we find that meta aromatic polyurea has a higher tendency to be disordered than other members in the polyurea family. All these facts lead to a significantly larger permittivity of mAAP.


3:54PM W42.00006 The conditional reversible work method for molecular coarse graining of soft matter, NICO VAN DER VEGT, EMILIANO BRINI, GREGOR DEICHMANN, Technische Universität Darmstadt, COMPUTATIONAL PHYSICAL CHEMISTRY GROUP TEAM — I will discuss a recently introduced systematic coarse-graining method that provides transferable coarse-grained potentials for scale-bridging simulations of soft matter systems. The method [1-3] is based on direct calculation of pair potentials in the gas or liquid phase with thermodynamic integration or free energy perturbation methods and has been coined the Conditional Reversible Work (CRW) method. I will discuss the CRW method in the general context of systematic coarse graining, a recent extension to dynamically-consistent coarse-grained simulations [4], and show some practical examples, including coarse-grained simulations of molecular liquids and polymers.


4:06PM W42.00007 Systematic and Simulation-Free Coarse Graining of Polymeric Systems: A Structure-based Study, DELIAN YANG, QIANG WANG, Colorado State University — We propose a systematic and simulation-free strategy for coarse graining of multicomponent polymeric systems, where we use the Polymer Reference Interaction Site Model theory, instead of many-chain molecular simulations, to calculate the structure and thermodynamic properties of both the original and coarse-grained (CG) models, and quantitatively examine how the effective CG pair potentials and properties of CG systems vary with the coarse-graining level. Our strategy is general and versatile, is much faster than those using many-chain simulations, and practically solves the transferability problem of coarse graining. As an example, here we apply it to structure-based coarse graining of homopolymer melts, which matches the structure correlations of CG segments between the original and CG systems. Our numerical results clearly show that structure-based coarse graining cannot give thermodynamic consistency between the original and CG systems at any coarse-graining level due to the information loss of coarse graining.

4:18PM W42.00008 Systematic and Simulation-Free Coarse Graining of Polymeric Systems: A Relative-Entropy-based Study, QIANG WANG, DELIAN YANG, Department of Chemical and Biological Engineering, Colorado State University — Relative-entropy-based coarse graining minimizes the relative entropy (RE) quantifying the information loss due to coarse graining. [1] When pair potentials are used for coarse-grained (CG) segments, RE-based coarse graining becomes equivalent to structure-based coarse graining if the pair potentials are unconstrained. [1] Here we apply our systematic and simulation-free strategy to RE-based coarse graining of homopolymer melts; that is, we use the Polymer Reference Interaction Site Model (PRISM) theory, instead of many-chain molecular simulations, to calculate the structure and thermodynamic properties of both the original and CG systems, and quantitatively examine how the CG pair potentials and properties of CG systems vary with the coarse-graining level. We consider various analytic functional forms of CG pair potential as suggested by structure-based coarse graining, and minimize RE to obtain the associated parameters. Values of minimized RE are then used to select the appropriate analytic form of CG pair potential, which is much easier to use than the tabulated (numerical) CG pair potential obtained from structure-based coarse graining. This is the first application of RE-based coarse graining to polymers. [1] M. S. Shell, J. Chem. Phys. 129, 144108 (2008).

4:30PM W42.00009 A proposed method for directed self-assembly of graphene nanoribbons, JAMES GERAETS, REIDUN TWARECK, YVETTE HANCHOCK, University of York — There is an opportunity for modeling to inform the experimental synthesis and design of graphene nanoribbons (GNRs). We present here a new coarse-graining algorithm for simulating GNR synthesis by the self-assembly of aromatic carbon precursor molecules. The model uses a Gillespie algorithm to form a network of possible coupling reactions between these molecules, and exploits a novel way of representing their geometries to speed up the simulations. Based on this method, we identify areas in parameter space given by temperature, binding energy, functional groups, and concentration of precursor molecules, which lead to GNRs with desirable properties. We demonstrate use of the model based on two precursors that self-assemble together to form a nanoporous GNR, namely, functionalized tetrabenzanthracene and benzene. We demonstrate that, unlike a pristine GNR, the GNRs formed by these molecules have regular repeating holes, and exhibit a band gap of 1.6eV independent of the ribbon width.

4:42PM W42.00010 Universal aspects of conformations and transverse fluctuations of a two-dimensional semi-flexible chain, HSIAO-PING HSU, Johannes Gutenberg-Universität Mainz, AIQUN HUANG, ANIKET BHATTACHARYA, University of Central Florida, KURT BINDER, Johannes Gutenberg-Universität Mainz — In this talk we compare the results obtained from Monte Carlo (MC) and Brownian dynamics (BD) simulation for the universal properties of a semi-flexible chain. Specifically we compare MC results obtained using pruned-enriched Rosenbluth method (PERM) with those obtained from BD simulation. We find that the scaled plot of root-mean-square (RMS) end-to-end distance $\langle R^2 \rangle / L_p$ and RMS transverse fluctuations $\sqrt{\langle \epsilon^2 \rangle / L_p}$ as a function of $L/L_p$ (where $L$ and $L_p$ are the contour length, and the persistence length respectively) are universal and independent of the definition of the persistence length used in MC and BD schemes. We further investigate to what extent these results agree for a semi-flexible polymer confined in a quasi one dimensional channel.
4:54PM W42.00011 Stretching wormlike chain: interplay between chain stiffness and excluded volume in the long chain limit. XIAOLAN LI, ABHIRAM MURALIDHAR, Chemical Engineering and Materials Science, University of Minnesota, CHARLES SCHROEDER, Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign, KEVIN DORPMAN, Chemical Engineering and Materials Science, University of Minnesota — Nearly 20 years ago, Marko and Siggia (Macromolecules 1995, 8759-8770) proposed an approximate interpolation formula for the force-extension (f-z) behavior of a wormlike chain that has found widespread use in biophysics and polymer physics. We have extended their result to account for excluded volume interactions. Our analysis takes advantage of Pruned-Enriched-Rosenbluth Method (PERM) simulations of wormlike chains of varying monomer anisotropy. Our simulations use up to 80,000 hard beads, allowing us to reach the long chain limit with sub-persistence length resolution. The simulations produce the Pincus scaling $z \sim f^{2/3}$, followed by a crossover to the linear behavior $z \sim f$, and subsequent saturation approaching the fully stretched limit. We also developed an approximate interpolation formula that captures these three regimes. This interpolation formula is in good agreement with PERM simulation results and can be reduced to the Marko-Siggia interpolation formula when the excluded volume effect is eliminated. Practically, our work provides a handy description of force-extension behavior for real wormlike chain, which will be useful for coarse-grained simulations and interpreting experiment results.

5:06PM W42.00012 ABSTRACT WITHDRAWN —

5:18PM W42.00013 Accelerated dynamics of bead-spring polymer chains. GOPINATH SUBRAMANIAN, Univ of Southern Mississippi — We present results from the application of the recently generalized parallel replica method to a system of bead-spring polymer chains. The statistics of chain breakage show that individual chains, after a relatively short dephasing time, display an exponential distribution of breakage times over a wide range of extension ratios, thereby allowing us to exploit the notion of the quasi-stationary distribution and accelerate the dynamical evolution of a representative volume element.

Thursday, March 5, 2015 2:30PM - 5:30PM —
Session W43 DPOLY: Focus Session: Dynamics of Glassy Polymers Under Confinement III
214C - David Simmons, University of Akron

2:30PM W43.00001 Molecular-weight Dependent Tg Depression of Silica-supported Poly(alpha-methyl styrene) Films1, OLPHELIA TSUI, KUN GENG, Boston Univ — The glass transition temperature ($T_g$) of poly(a-methyl styrene) (PaMS) films supported by silica is studied as a function of film thicknesses from 17 to 168 nm at three molecular weights of 1.3, 20 and 420 kg/mol. For the 20 and 420 kg/mol films, the glass transition temperature decreases with decreasing film thickness, consistent with previous results. But for the 1.3 kg/mol films, it becomes independent of the film thickness. We tentatively suggest the $T_g$ depression to be caused by free volume excess at the polymer-air interface and that its influence diminishes at low enough molecular weights because of a chain stiffness effect.

1We acknowledge support of NSF through the projects DMR-1004648 and DMR-1310536.

2:42PM W43.00002 Influence of the chemical structure on the slip boundary condition of liquids. MISCHA KLOS, SEBASTIAN BACKES2, Saarland University, Experimental Physics, D-66123 Saarbrücken, JUAN MANUEL CASTILLO SANCHEZ, MARTIN HORSCH, HANS HASSE, TU Kaiserslautern, Laboratory of Engineering Thermodynamics, D-67663 Kaiserslautern, KARIN JACOBS, Saarland University, Experimental Physics, D-66123 Saarbrücken — On small scales, especially in microfluidic devices, the role of the solid/liquid interface gets more important for the flow dynamics. Our experiments probe slippage via the dewetting of thin polymer films on hydrophobic substrates [1]. As hydrophobic coatings we use amorphous polymers (AF1600, AF2400) and different types of highly ordered self-assembled silane monolayers on top of silicon substrates. On silane surfaces, polystyrene (PS) of low molecular weight exhibit slip lengths up to micrometers [2]. On AF1600, no significant slip is observed. Scattering studies reveal an ordering of the PS side chains at the solid/liquid interface depending on the structure of the substrate [3]. Recent simulations were able to characterize these SAMs [4]. However, the situation changes if PMMA or Polyvinylpyridine (PVP) are used: Dewetting experiments show that slip is less pronounced in PVP and in PMMA films. Obviously, the structure of the side groups plays a significant role. X-ray reflectometry supplements this hypothesis and give further insight to the slippage mechanism at the solid/liquid interface. [1] O. Bäumchen, et.al., J Phys Condens Matter 24 (2012) [2] R. Fetzer, et.al., Europhys Lett 75 (2006) [3] P. Gutfreund, et.al., Phys Rev E 87 (2013) [4] J.M. Castillo Sanchez, et. al. submitted

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2:54PM W43.00003 New paradigm for stabilization of liquid polymer films on solids1, TAD KOGA, NAISHENG JIANG, JIAXUN WANG, XIAOYU DI, JUSTIN CHEUNG, MAYA ENDOH, Stony Brook University — We report that wetting/dewetting behavior of liquid polymer films on solids can be controlled by nanoscale architectures of polymer chains irreversibly adsorbed on the impenetrable surfaces. Monodisperse polystyrene (PS) ultrathin films (20 nm in thickness) with different molecular weights on silicon (Si) substrates with a natural amorphous Si dioxide layer was used as models. The PS thin films were annealed at high temperatures at T>Tg (Tg is the bulk glass transition temperature) for several days, and the surface structures were studied by using optical and atomic force microscopes. At the same time, the annealed PS films were further leached with a good solvent and the residue films (i.e., irreversibly adsorbed layers) were characterized by x-ray reflectivity. The experimental data reveals a strong correlation between the conformations of the adsorbed polymer chains and the stability of the liquid films on top.

1T. K. acknowledges the partial financial support from NSF Grant No. CMMI-1332499.

3:06PM W43.00004 Approach to universal self-similar attractor for the levelling of thin liquid films. ELIE RAPHAEL, MICHAEL BENZAQUEN, UMR CNRS 7083 Gulliver, ESPCI ParisTech, PSL Research University, PAUL FOWLER, Department of Physics and Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, Canada, LAETITIA JUBIN, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, Canada, THOMAS SALEZ, UMR CNRS 7083 Gulliver, ESPCI ParisTech, PSL Research University, KARI DALKOKI-VERESS, Department of Physics and Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, Canada — We compare the capillary levelling of a random surface perturbation on a thin polystyrene film with a theoretical study on the two-dimensional capillary-driven thin film equation. Using atomic force microscopy, we follow the time evolution of samples prepared with different initial perturbations of the free surface. In particular, we show that the surface profiles present long term self-similarity, and furthermore, that they converge to a universal self-similar attractor that only depends on the volume of the perturbation, consistent with the theory. Finally, we look at the convergence time for the different samples and find very good agreement with the analytical predictions.
3:18PM W43.00005 Confinement Effects with Films of Nonlinear Polystyrene, MARK FOSTER, QIMING HE, The University of Akron, SURESH NARAYANAN, Argonne National Laboratory, DAVID WU, Colorado School of Mines — The surface fluctuations of annealed melt films of 6k cyclic polystyrene (CPS), its linear analog, and a long-branched chain were measured using X-ray photon correlation spectroscopy (XPCS) for films of various thicknesses. The surface fluctuations of the 6k linear PS melt films 17 nm and thicker and the 6k cyclic melt films 28 nm and thicker can be described using a hydrodynamic continuum theory (HCT) that assumes the film is characterized only by the bulk viscosity. When a film of CPS is 24 nm or thinner, the behavior can no longer be captured using the HCT with bulk viscosity. The surface fluctuations behave as though the film has an effective viscosity higher than the bulk value. The thickness at which confinement effects are seen for the 6k CPS chains is larger than that for the linear analogs. Confinement effects for long-branched chains appear at even larger thicknesses relative to Rg. Acknowledgements: Use of the Advanced Photon Source at Argonne National Laboratory was supported by the DOE's Office of Science under Contract DE-AC02-06CH11357. This work was supported by NSF Grants CBET-0730692 and CBET-0731319.

3:30PM W43.00006 The Dynamics of a Polymer Confined in Anodic Aluminum Oxide Nanopore, GI XUE, YE SA, Nanjing University — The dynamics of poly(n-butyl methacrylate) confined in porous templates are investigated using DSC and Fluorescence nonradiative energy transfer. Two glass transition temperatures are obtained at a slow cooling rate of which one bulk-like phase reflects core layer while the other at much higher temperature indicates interfacial layer in the confined polymer glass. Because of cylindrical geometry, the glass transition energy barrier of interfacial layer is elevated, and the thereof temperature threshold to form one or two glass transitions is determined through adjusting infiltrating temperatures. In addition, the glass transition behavior is speculated to be mediated by the counterbalance of the size and interfacial effects in the confined space.

3:42PM W43.00007 The effect of surface chemistry on the glass transition of amorphous polycarbonate inside cylindrical nanopores, DARIYA REID, Texas A&M University, Chemical Engineering Department, MARCELA ALVES FREIRE, Universidade Federal de Minas Gerais, Brasil, JODIE LUTKENHAUS, Texas A&M University, Chemical Engineering Department — Nanoporous anodic aluminum oxide (AAO) templates are used to study the effect of confinement on the glass transition of amorphous polycarbonate (PC). In order to further study the effect of surface chemistry on physical behavior, the bare AAO surface is modified using alkyl- and fluoro-silanes of varying length. PC nanowires (200 nm in diameter) are prepared by melt-wetting the polymer into AAO templates under applied pressure. Using modulated differential scanning calorimetry (MDSC) and thermogravimetric analysis (TGA), it is found that the hydrophilic surface of bare AAO contributes to the degradation of the polymer. Modifying the AAO surface using silane chemistry prevents polymer degradation and introduces additional features in MDSC thermograms, which could be due to the interaction of the polymer with the nanopore surface. Using scanning electron microscopy (SEM), changes are observed in the tips of the PC nanowires as the AAO surface transitions from hydrophilic to hydrophobic.

3:54PM W43.00008 Large-scale diffusion of entangled polymers along nanochannels, KAY SAALWACHTER, FRANK LANGE, Martin-Luther-U. Halle-Wittenberg, Germany, MARTIN STEINHART, U. Osnabruck, Germany, PATRICK JUDEINSTEIN, Lab. Leon Brillouin, CNRS-CEA Saclay, France — Confinement-induced changes in polymer mobility are still under active discussion. For weakly interacting polymers, confinement effects for long-branched chains appear at even larger thicknesses relative to Rg. The University of Akron, SURESH NARAYANAN, Argonne National Laboratory, DAVID WU, Colorado School of Mines — The surface fluctuations of the 6k linear PS melt films 17 nm and thicker and the 6k cyclic melt films 28 nm and thicker can be described using a hydrodynamic continuum theory (HCT) that assumes the film is characterized only by the bulk viscosity. When a film of CPS is 24 nm or thinner, the behavior can no longer be captured using the HCT with bulk viscosity. The surface fluctuations behave as though the film has an effective viscosity higher than the bulk value. The thickness at which confinement effects are seen for the 6k CPS chains is larger than that for the linear analogs. Confinement effects for long-branched chains appear at even larger thicknesses relative to Rg. Acknowledgements: Use of the Advanced Photon Source at Argonne National Laboratory was supported by the DOE's Office of Science under Contract DE-AC02-06CH11357. This work was supported by NSF Grants CBET-0730692 and CBET-0731319.

4:06PM W43.00009 Nanoscale pattern fidelity and transfer of hierarchically patterned thermoplastics films, YING CHEN, MANISH KULKARNI, the University of Akron, ALLAN MARSHALL, Omnova Solution Inc., JACK DOUGLAS, National Institute of Standards and Technology, ALAMGIR KARIM, the University of Akron, THE UNIVERSITY OF AKRON TEAM — We demonstrate a versatile and inexpensive method for controlling the surface relief structure of both flexible elastomeric and glassy polymer films over large areas through a two-step imprinting process. First, nanoscale patterns were formed by nanoimprinting polymer films with a pattern on a DVD disk, obtained originally by nanoimprinting from a lithographically etched master pattern on a silicon wafer; micron-scale patterns were then superimposed on the nanoimprinted films by exposing them to ultraviolet radiation in oxygen (UVO) through a TEM grid mask having variable micron-scale patterning. This simple two-stage imprinting method allows for facile fabrication of hierarchically structured elastomer and thermoplastic polymer films. Besides, the thermodynamic properties of dewetting phenomenon of polystyrene film under the confinement of hierarchically patterned PDMS is studied.

4:18PM W43.00010 Elevated single polymer surface diffusion on a film near its glass transition temperature, MARK GEOGHEGAN, MATTHEW MARES, CHRISTOPHER CLARKSON, ZHENYU ZHANG, University of Sheffield, JOHN TORKELSON, Northwestern University — Fluorescence correlation spectroscopy data are presented to show that the diffusion coefficient of poly(ethylene oxide) (PEO) adsorbed onto poly(alkyl methacrylate) (PAMA) and polystyrene films in aqueous solution increases close to (but below) the surface glass transition temperature of the film. This increase disappeared at higher temperatures as the film liquefied, although the diffusion coefficient for the PEO on the polystyrene surface remained greater than the diffusion coefficients for PEO on the PAMA films at temperatures greater than those at which the peak in diffusion occurred. A similar increase was found in the surface tension of all films studied. Experiments on (immiscible) blends of two PAMA homopolymers were performed where two peaks in the diffusion coefficient were observed with increasing temperature. Two peaks were also observed in the surface tension from contact angle experiments, although at temperatures slightly greater than those at which the peak in diffusion was observed. It is concluded that the enhanced surface mobility of the films near the surface glass transition temperature induces conformational changes in the adsorbed PEO molecules resulting in elevated diffusion coefficients.

4:30PM W43.00011 Local Glass Transition Temperature Gradients Near Polymer-Polymer Interfaces, ROMAN BAGLAY, CONNIE ROTH, Department of Physics, Emory University — For decades the glass transition in confined systems has been studied with the hopes of uncovering the governing length scales that impact these dynamics. However, understanding length scales of local gradients in glass transition temperature ($T_g$) near a free surface have been hampered by limitations of how to treat the enhanced mobility at the free surface theoretically. We have previously reported on the local $T_g$ in multilayer structures made from high molecular weight polystyrene (PS) and poly(n-butyl methacrylate) (PnBMA), a weakly immiscible system with a $\sim$ 7 nm interfacial width. Using ultrathin (10-15 nm) pyrene-labeled layers inserted into the multilayer structure at different positions ($z$) from the glassy-rubber interface, we were able to map the local $T_g(z)$ profile across the glassy-rubber interface with temperature-dependent fluorescence intensity measurements. Our work revealed an asymmetric local mobility gradient propagating hundreds of nanometers away from the glassy-rubber interface and we recovered far from the surface. Here we extend these measurements to investigate how the local $T_g(z)$ profile in PS varies when in contact with a variety of immiscible polymers whose $T_g$s vary between +90 K to ~80 K relative to the $T_g$ of PS, so-called hard vs soft confinement.

4:42PM W43.00012 Free Surface and Interfacial Effects on Tg Confinement Behavior of Template Supported Nanotubes, ANTHONY TAN, Northwestern University — Free surface and interfacial effects have a large impact upon the magnitude and direction of $T_g$-confinement behavior for nanoscale materials. In this work, we study the $T_g$ behavior of supported polymers in anodic aluminum oxide templates. The effects of attractive and neutral or non-interacting polymer substrate interactions were investigated. Tailored wall thicknesses were achieved using template melt infiltration by varying the annealing temperature and the molecular weight of the polymers. Nanotube thickness can be related to the polymer conformation and the interactions between the polymer and the substrate. Substantial $T_g$ reductions as a function of wall thickness were observed for supported polystyrene nanotubes and $T_g$ increases for supported poly(methyl methacrylate) or poly(2-vinylpyridine) nanotubes. The $T_g$-confinement behavior of supported nanotubes is found to be similar to the behavior of supported thin films in the presence or absence of interfacial effects.

5:06PM W43.00014 Can a reduction in mass transport occur at invariant segmental time?, SIMONE NAPOLITANO, MICHELE SFERRAZZA, Universite Libre de Bruxelles — The glassy dynamics of polymer melts adsorbed onto solid substrates shows a peculiar confinement effect: a severe reduction in mass transport occurs without a corresponding increase in segmental relaxation time. This phenomenon provides a “negative violation” of the Stokes-Einstein (SE) relation, not observed in bulk melts or confined water. Explaining those findings in analogy to the large drop of thermal expansion reported in polymers under 1D confinement, we considered the presence of an interfacial dead layer where tracer diffusivity assumes negligible values. To verify this hypothesis, we performed an extensive investigation of the diffusion of styrene oligomers, acting as tracers, into matrices of high molecular weight polystyrene, irreversibly adsorbed onto aluminum oxide. We demonstrate that the reduced interfacial diffusion is due to larger residence times of the tracers inside the dead layer, $t_{DL}$. In particular, we show that $t_{DL}$ is directly proportional to the amount of irreversibly adsorbed monomers, a quantity limiting the available space for diffusion. We thus discuss of a dynamic dead layer evolving within the adsorbed layer, and of its role on the dynamics of glassy polymers under confinement and the “negative violation” of the SE relation.

5:18PM W43.00015 Physical Properties of PC-PMMA Multilayers, ARIFUR RAHMAN, ERIC BAER, Case Western Reserve University, ALIN CRISTIAN CHIRA, ROBERT VAJTAJ, PULLICKEL M. AJAYAN, Rice University, JAMES HINTHORNE, IBRAHIM ELAMIN, MIRCEA CHIRA, The University of Texas Pan American, ERIC BAER COLLABORATION, PULLICKEL AJAYAN COLLABORATION, MIRCEA CHIRA COLLABORATION — Multilayers of polycarbonate (PC) and polymethylmethacrylate (PMMA) have been obtained by the layer multiplying coextrusion method. Each sample (1024 layers, of equal thickness, with individual thickness between 10 and 200 nm) has been investigated at room temperature of glassy polymers under confinement and the “negative violation” the SE relation.

5:44PM W43.00016 Residual Stress Relaxation and Stiffness-Confinement Effects in Polymer Films: Characterization by Non-Contact Ellipsometry and Fluorescence Techniques, SHADD ASKAR, JOHN TORKELSON, Northwestern University — The relaxation of residual stresses in spin-coated polymer films is characterized using two optical techniques: ellipsometry and fluorescence. Both techniques show that residual stresses relax over hours at several tens of degrees above the film glass transition temperature ($T_g$). Ellipsometry shows that thickness can increase or decrease during residual stress relaxation depending on thermal history of the film. However, the presence or relaxation of stresses has no measurable effect on $T_g$ as measured by ellipsometry. We have adapted the well-known sensitivity of the pyrene dye fluorescence spectral shape to local environment polarity in order to characterize stress relaxation and to monitor stiffness-confinement effects. The spectral shape of the pyrene fluorescence spectrum shows similar stress relaxation regardless of whether relaxation is accompanied by increases or decreases in film thickness. Fluorescence also indicates that single-layer polystyrene films supported on silica stiffen with decreasing nanoscale thickness. For the first time, stiffness gradients as a function of distance from interfaces are demonstrated using pyrene label fluorescence in conjunction with multilayer films.
2:54PM W44.00003 Scaling of Force Networks for Compressed Particulate Systems1, LENKA KOVALCINOVA, New Jersey Institute of Technology, ARNAUD GOULETTE, Rutgers University, LOU KONDIC, New Jersey Institute of Technology — We consider the distribution of cluster sizes in compressed particulate systems as a function of the force experienced by the particles. The considered systems differ by the distribution of particle sizes and by their frictional properties. To obtain good statistics we consider various systems sizes and large number of realizations. While for some of the considered systems we find consistent scaling exponents describing the behavior of the force clusters, we are also finding that this behavior is not universal. For example, monodisperse frictionless systems that crystallize under compression, show very different scaling properties compared to other systems, particularly as the systems approach jamming transition. The findings are confirmed by explicitly computing fractal dimension of the considered clusters.

1Supported by the NSF Grant No. DMS-083561

3:06PM W44.00004 Steady State Shear Driven Flow of Frictionless Spherocylindrical Particles in Two Dimensions1, DANIEL VAN HOESEN, University of Missouri, THEODORE MARSCHALL, University of Rochester, SCOTT FRANKLIN, Rochester Institute of Technology, STEPHEN TEITEL, University of Rochester — We carry out simulations of a model of frictionless spherocylindrical rods in two dimensions, under uniform steady state shear driven flow. Rods repel elastically when they come into contact, and dissipate energy with respect to a uniformly shared angular velocity, and the nematic and tetragonal orientational order parameters. We find non-monotonic behavior of the orientational order parameters as the packing fraction increases toward the jamming transition. Orientation and translational correlation functions are computed to measure cooperative behavior as the packing fraction increases.

1Supported by NSF grants CBET-1133126 and CBET-1435861 and by NSF award PHY-1156339. Computations carried out at the CIRC at the University of Rochester.

3:18PM W44.00005 Fraction of clogging configurations in granular hopper flow, CHARLES THOMAS, DOUGLAS DURIAN, University of Pennsylvania — The clogging of granular media flowing from a hopper is a quintessential example of a system that spontaneously evolves from a freely flowing state to a jammed state under constant forcing. If suitably arranged, the grains at the opening are stable, initiate a jamming front, and block the flow throughout the bulk. We measure the fraction F of possible grain arrangements that lead to such a system-spanning clog for a range of experimental conditions, varying aperture shape, size, and orientation. We find for circular holes that F is a function only of the aperture size projected in the direction of the average exiting grain velocity. Furthermore, for long narrow slits F is found to be identical to the value expected for a set of independent holes. Finally, we successfully model the form of F versus aperture size by considering the accessible microstates of individual grains near the exit. The data as interpreted through this model suggest that the fraction of individual grain microstates that can lead to a clog is constant for large opening sizes. This conclusion implies that there may be no well-defined critical aperture size above which clogging is impossible.

3:30PM W44.00006 Sub-Jamming Transition in Jammed Binary Sphere Mixtures, ISHAN PRASAD, CHRISTIAN SANTANGELO, GREGORY GRASON, University of Massachusetts Amherst — We study influence of bi-disparity on structural evolution of jammed binary sphere mixtures with increasing small sphere composition, f_s. In binary spheres, maximally dense, random packing is achieved at infinite size ratio and unique composition (f_s \approx 0.2699) where small spheres jam within interstitial volume of jammed large spheres, leading to a kink in total volume fraction, \phi vs. f_s. Using simulations of athermal jammed packings, we explore how this critical feature influences the evolution of random binary sphere packings at finite size ratio, \alpha, ranging from 1 to 10. We report a clear distinction between large and small \alpha behavior, separated by a critical value of \alpha_c \approx 5.8. For \alpha < \alpha_c, structural properties such as volume fraction, rattle fraction and contact statistics are found to crossover smoothly from small to large f_s, while above a critical size asymmetry these properties indicate an abrupt, first-order like transition. We correlate this sharp transition with a "sub-jamming" transition of small-spheres occurring at finite values of f_s, which becomes cooperative only for sufficiently asymmetric mixtures. We propose a heuristic geometric and mechanical argument to understand what determines \alpha_c.

3:42PM W44.00007 A Unified Framework to Understand Shear Induced Rigidity in Athermal Materials, SUMANTRA SARKAR, Brandeis University — Recent studies of athermal systems such as dry grains and dense, non-Brownian suspensions have shown that shear can lead to solidification through the process of shear jamming in grains and discontinuous shear thickening in suspensions. The similarities observed between these two distinct phenomena suggest that the physical processes leading to shear-induced rigidity in athermal materials are universal. We present a unified, non-equilibrium statistical mechanics model for these shear-driven transitions, which exhibits the phenomenology of shear jamming and discontinuous shear thickening in different regions of the predicted phase diagram. Our analysis identifies the crucial physical processes underlying shear-driven rigidity transitions, and clarifies the distinct roles played by shear forces and the density of grains.

4:18PM W44.00008 Effect of Friction on Shear Jamming2, DONG WANG, Duke University, JIE REN, Merck & Co., JOSHUA DIJKSMAN, Wageningen University and Research Centre, JONATHAN BARES, ROBERT BEHRINGER, Duke University — Shear jamming of granular materials was first found for systems of frictional disks, with a static friction coefficient \mu \approx 0.6 (Bi et al. Nature (2011)). Jamming by shear is obtained by starting from a zero-stress state with a packing fraction \phi between \phi_J (isotropic jamming) and a lowest \phi_J for shear jamming. This phenomenon is associated with strong anisotropy in stress and the contact network in the form of force chains, which are stabilized and/or enhanced by the presence of friction. Whether shear jamming occurs for frictionless particles is under debate. The issue we address experimentally is how reducing friction affects shear jamming. We put the Teflon-wrapped photoelastic disks, lowering the friction substantially from previous experiments, in a well-studied 2D shear apparatus (Ren et al. PRL. (2013)), which provides a uniform simple shear. Shear jamming is still observed; however, the difference \phi_J - \phi_J is smaller with lower friction. We also observe larger anisotropies in fragile states compared to experiments with higher friction particles at the same density. In ongoing work we are studying systems using photoelastic disks with fine gears on the edge to generate very large effective friction.

2We acknowledge support from NSF Grant DMR1206351, NSF Grant DMS-1248071, NASA Grant NNX10AU01G and William M. Keck Foundation.

4:30PM W44.00009 Clogging and Jamming Transitions in Granular Matter Flowing Through Obstacles, CYNTHIA OLSON REICHHARDT, CHARLES REICHHARDT, Los Alamos National Laboratory — We consider a two-dimensional system of bidisperse disks driven through a landscape of fixed obstacles. In the limit of a single obstacle, the disks cease moving when the disk density is increased to the jamming density. The threshold density value decreases as the number of obstacles increases, but we also observe a change in the nature of the frozen state. At low obstacle density we find a homogeneous jammed state, but for higher obstacle density we instead find a heterogeneous clogged state containing void areas and possessing a memory of the driving direction. The transition to the clogged state is strongly stochastic and we observe large fluctuations in clogging time both for clogging in the original driving direction and for transverse clogging when the drive is suddenly rotated by 90 degrees. We find evidence for a diverging clogging transition time at a critical disk density well below the jamming density in a clean system.
4:42PM W44.00010 Diffusion in jammed particle packs¹, DAN S. BOLINTINEANU, Sandia National Laboratories, LEONARDO E. SILBERT, University of Southern Illinois, GARY S. GREST, JEREMY B. LECHMAN, Sandia National Laboratories — Diffusive transport in jammed particle packs is of interest for a number of applications, as well as being a potential indicator of structural properties near the jamming point. To this end, we report stochastic simulations of equilibrium diffusion through monodisperse sphere packs near the jamming point in the limit of a perfectly insulating surrounding medium. The time dependence of various diffusion properties is resolved over several orders of magnitude. Two time regimes of expected Fickian diffusion are observed, separated by an intermediate regime of anomalous diffusion. This intermediate regime grows as the particle volume fraction approaches the critical jamming transition. The diffusion behavior is fully controlled by the extent of the contacts between neighboring particles, which in turn depend on proximity to the jamming point. In particular, the mean first passage time associated with the escape of random walkers between neighboring particles is shown to control both the time to recover Fickian diffusion and the long time diffusivity. Scaling laws are established that relate these quantities to the difference between the actual and critical jamming volume fractions.

¹Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s NNSA under Contract DE-AC04-94AL85000.

4:54PM W44.00011 Statistics and Correlations of Conserved Quantities in Mechanically Stable Packings of Frictionless Disks Above Jamming¹, STEPHEN TEITEL, YEGANG WU, Univ of Rochester — We consider mechanically stable packings of soft-core, frictionless, bidisperse disks in two dimensions above the jamming transition. Using an algorithm that generates packings with an isotropic global stress tensor, we compute the distribution of various conserved quantities on compact subclusters of particles, as a function of the total system stress and the cluster size. We consider the stress on the cluster, the Maxwell-Cremona force-tile area, the Voronoi volume, and the numbers of small and big particles in the cluster, and we compute the averages, variances and correlations among these different quantities. We compare two different ensembles of clusters: (i) clusters defined by a fixed radius, and (ii) clusters defined by a fixed number of particles. We find several significant differences between these two ensembles and we comment on the implications of our findings for maximum entropy models of jammed packings.

¹This work was supported by NSF Grant No. DMR-1205800. Computations were carried out at the Center for Integrated Research Computing at the University of Rochester.

5:06PM W44.00012 Shear Jamming in Frictionless Particulate Media¹, THIBAULT BERTRAND, COREY S. O’HERN, Yale University, R.P. BEHRINGER, Duke University, BULBUL CHAKRABORTY, Brandeis University, MARK D. SHATTUCK, City College of the City University of New York — We numerically study two-dimensional packings of frictionless bidisperse disks created using compresive and simple shearing protocols. To create jammed packings by compression, we start N particles from random positions and grow their diameters followed by relaxation of particle overlaps using energy minimization. These compressed packings exist over a range of packing fractions φ. As a result, during compression the system may reach a φ above the minimum value before jamming. If this unjammed packing is then sheared by a strain γt, it can jam. Using a combination of compression and shearing, we can define jamming protocols as trajectories in the (φ, γ) plane that yield jammed packings. In this plane, we can reach a particular point (φn, γn) in many ways. We will focus on two protocols: (1) shearing to γn at φ = 0 followed by compression to φn at γ = γn, and (2) compression to φn at γ = 0 followed by shearing to γn at φ = φn. For protocol 1, we find that the probability of finding a jammed packing at φ and γ, P(φ, γ) = Q(φ) is independent of γ. For protocol 2, we use a simple theory to deduce P(φ, γ) from Q(φ).

¹W. M. Keck Foundation Science and Engineering Grant

5:18PM W44.00013 Jammed elastic shells - a 3D experimental soft frictionless granular system, JISSY JOSE, GERHARD A. BLAB, ALFONSO VAN BLAADEREN, ARNOUT IMHOF, Utrecht University — We present a new experimental system of monodisperse, soft, frictionless, fluorescent labelled elastic shells for the characterization of structure, universal scaling laws and force networks in 3D jammed matter. The interesting fact about these elastic shells is that they can reversibly deform and therefore serve as sensors of local stress in jammed matter. Similar to other soft particles, like emulsion droplets and bubbles in foam, the shells can be packed to volume fractions close to unity, which allows us to characterize the contact force distribution and universal scaling laws as a function of volume fraction, and to compare them with theoretical predictions and numerical simulations. However, our shells, unlike other soft particles, deform rather differently at large stresses. They deform without conserving their inner volume, by forming dimples at contact regions. At each contact one of the shells buckled with a dimple and the other remained spherical, closely resembling overlapping spheres. We conducted 3D quantitative analysis using confocal microscopy and image analysis routines specially developed for these particles. In addition, we analysed the randomness of the process of dimpling, which was found to be volume fraction dependent.

Thursday, March 5, 2015 2:30PM - 5:30PM – Session W45 DPOLY: Structure and Phase Behavior of Charged and Ion Containing Polymers 216AB - Anupriya Agrawal, Clemson University

2:30PM W45.00001 A molecular simulation study on salt response of polyelectrolyte complexes, HANNE ANTILA, Aalto University, Department of Chemistry, PAUL VAN TASSEL, Yale University, Chemical and Environmental Engineering, MARIA SAMMALKORPI, Aalto University, Department of Chemistry — In aqueous solutions, oppositely charged polymers, polyelectrolytes (PEs) form complexes which are known to be sensitive to added salt with responses ranging from shrinking to full destabilization of the complex. As a specific application of PE complexes, the complex formation of DNA with polycations has been demonstrated to be an effective means of transferring genetic material in gene therapy. We use all-atom molecular dynamics and coarse-grained Monte Carlo simulations to investigate the effect of excess salt on DNA-polycation complex stability. The detailed all-atom simulations demonstrate the mechanism of polycation and ion species specific salt-driven dissociation [1] involving charge reversal. More generally, other possible mechanisms of salt driven dissociation exist as well. The coarse grained approach, which describes the PE complex as oppositely charged, rigid rods and ions as hard spheres, provides a more complete understanding of PE interactions in salt, and suggests possible mechanisms leading to expulsion between the oppositely charged polyelectrolytes. [1] H. S. Antila, M. Sammalkorpi, J. Phys. Chem. B, 2014.
2:42PM W45.00002 Coarse-grained Molecular Simulation Studies of Complexation of Sulfobetaine-Lysine Copolymer and DNA for Gene Delivery. AHMADREZA F. GHOBADI, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark Delaware 19716, ARTHI JAYARAMAN, Department of Chemical and Biomolecular Engineering and Department of Materials Science and Engineering, University of Delaware, Newark Delaware 19716 — Gene delivery involves successful transfection of therapeutic DNA by a vector into target cells and protein expression of that genetic material. Viral vectors are effective at gene delivery but elicit harmful immunogenic responses, thus motivating ongoing research on non-viral transfection agents. Cationic polymers are a promising class of non-viral vectors due to their low immunogenic responses and low toxicity, and their ability to bind to the polyanionic DNA backbone to form a polycation-DNA complex (polyplex) that is then internalized in the target cell. While past studies have shown many polycations with differing DNA transfection efficiencies, there is a need for general design guidelines that can relate the molecular features of the polycation to its DNA transfection efficiency. Using atomistic and coarse-grained molecular dynamics simulations we connect polycation design to polycation-DNA binding and experimentally observed transfection efficiency. Specifically in this presentation we will discuss our recent work looking into the effect of incorporating zwitterions into lysine based polycations on the resulting polyplex structure, shape, surface charge density and stability of DNA-polycation complexes.

2:54PM W45.00003 Experiments of salt concentration effects on translocation dynamics of polyelectrolytes passing through alpha-hemolysin pore. BYOUNG-JIN JEON, MURUGAPPAN MUTHUKUMAR, University of Massachusetts — We have investigated physical mechanisms of electric field driven single file translocation of polyelectrolytes through an alpha-hemolysin pore by measuring the translocation time under different voltages, salt concentrations, and pH. Our experiments reveal an intricate coupling among various driving forces in dictating the polycation translocation. For example, we find that the salt concentrations in the donor and the recipient compartments influence the polychain translocation dynamics differently, depending on pH. From a series of systematic experiments, we demonstrate that the salt concentration in the donor compartment influences the polyclain charge and the free energy barrier for entrance and that the salt concentration in the receiver compartment influences the electrostatic interaction between the polyclain and pore. We provide a physical model for the free energy landscape of the translocation process and offer an explanation of the origin of the salt concentration effects on the polycation translocation dynamics for different pH conditions. This study offers an opportunity to understand how different driving forces get coupled in dictating the polycation dynamics under non-equilibrium conditions.

3:06PM W45.00004 Salt Effects on the Structure and Stability of Ionzible Polydots - SANS Study. NARESH OSTI, SIDDHAT WIJESINGHE, MANJULA SENANAYAKE, ANURADHI WICKRAMASINGHE, THUSITHA ETAMPAWALA, DVORA PERAHIA, Clemson University, Clemson, SC 29634 — Confinement of rigid luminescent polymers into nano-dimension forms polydots, long lived nanoparticles, even though the polymer chains are far from their thermodynamically equilibrium conformations. These polydots bare the potential to be tunable by changing the conformation of the polymer, making them promising for new bio-imaging markers and drug delivery vehicles. Here, we investigate ionizable polydots formed by dialkyloxy poly-para-phenyleneethynylene (PPEs). Increasing anion group density causes the shift to the higher pH range. The measurement of local pH near a single P2VP chain indicates that adding counterions can effectively increase the protonation degree on the P2VP chain. Yet the electric potential of the P2VP is found to decrease upon addition of divalent ions and anionic macrorions, suggesting enhanced counterion condensation by multivalent ions. It is also found that inorganic nanocluster macroions of 1 nm in diameter can form dense complexes with P2VP, whose dimension becomes independent of solution pH.

3:18PM W45.00005 Ionic Effect on Conformational Structure of Weak Polyelectrolyte in Dilute Solution: from Monovalent, Multivalent to Macro ions. CHEN QU, Univ of Notre Dame — The electrostatic environment near a charged polymer chain is critical to the structure and function of the polymer in aqueous media. In this work, we compare the effect of small monovalent and divalent ions and multivalent inorganic macrorions on the conformational structure of weak polyelectrolyte, poly(2-vinyl pyridine) (P2VP), in dilute aqueous solutions by single molecule spectroscopy. Divalent counterions at low concentration range show the similar effect as monovalent ones to cause the shift of the critical pH for the coil-to-globule conformational transition of P2VP to the higher pH range. In contrast, divalent counterions at high concentration range and inorganic nano-cluster anions cause the shift of the critical transition pH to the opposite lower pH range. The measurement of local pH near a single P2VP chain indicates that adding counterions can effectively increase the protonation degree on the P2VP chain. Yet the electric potential of the P2VP is found to decrease upon addition of divalent ions and anionic macrorions, suggesting enhanced counterion condensation by multivalent ions. It is also found that inorganic nanocluster macroion of 1 nm in diameter can form dense complexes with P2VP, whose dimension becomes independent of solution pH.

3:30PM W45.00006 Phase Behavior of Charged Nanoparticle-Polyelectrolyte Solution. GUNJA PANDAV, VENKAT GANESAN, University of Texas at Austin — Interactions between charged nanoparticles suspended in a polyelectrolyte solution are studied using single chain in mean field simulations. We consider a model in which the particles and polymers carry a fixed charge in presence of counterions and salt. The effect of nanoparticle size on the polyelectrolyte phase behavior is explored. We also discuss the interactions between nanoparticles arising due to multibody effects and compare it with two-body potentials calculated using a mean-field approach.

3:42PM W45.00007 Effects of mixing ratio, salt concentration and temporal trend on the formation of polyelectrolyte complex. YANPU ZHANG, Department of Chemical Engineering Texas A&M University, EROL YILDIRIM, HANNE ANTILA, MARIA SAMMALKORPI, Department of Chemistry Aalto University, JODIE LUTKENHAUS, Department of Chemical Engineering Texas A&M University, TEXAS A&M UNIVERSITY COLLABORATION, AALTO UNIVERSITY COLLABORATION — Polyelectrolytes complexes (PEC) form by mixing polycation/polyanion solutions together. Promising applications of PECs range from industrial flocculants, coatings, and membranes to advanced materials for solar cells, injectable hydrogels, and chemical sensors. One challenge for PEC processing and application is that their physical properties are often time-dependent. In this work, we report on the influence of polycation/polyanion mixing ratio, salt concentration, and time on the formation of PECs made from poly(diallyldimethylammonium chloride) (PDAC) and poly(styrene sulfonate sodium salt) (PSS). Physical such as turbidity, hydrodynamic size, and zeta potential are investigated as a function of time. We find various critical values that can be used to predict whether a PEC will remain stable in suspension or whether it will gradually aggregate and precipitate. We discuss these findings in relation to the stepwise aggregation model that depicts primary PEC particles gradually forming secondary structures. Finally, we perform detailed coarse-grained molecular dynamics simulations to examine the structure and effective charge distribution of the PECs with their temporal stability at varying mixing ratios and salt concentrations to support the experimental findings.

3:54PM W45.00008 Molecular Connectivity and Correlation Effects in Polymeric Complex Coacervates. MITHUN RADHAKRISHNA, CHARLES SING, University of Illinois at Urbana-Champaign — Complex Coacervation is a liquid-liquid phase separation induced by oppositely charges species and is a complicated process influenced by many factors like the solution pH, temperature, salt concentration, charge size and valency of the salt. Because of this inherent tunability complex coacervates have garnered a significant amount of attention as materials for under water adhesives, drug delivery platforms and self assembled structures. Most theoretical studies to address the complex coacervate materials to date have relied on the use of Poisson-Boltzmann theory (or extensions thereof). While these thermodynamic studies capture the phase behavior of complex coacervates in a qualitative sense, most of these theories neglect some of the important factors such as the effect of polyanion-driven connectivity correlations and excluded volume interactions between the ions in the solution. In the current work we study the effect of these factors on the phase behavior of complex coacervates through molecular simulations coupled to thermodynamic models for phase separation. We demonstrate that these neglected molecular features (connectivity, finite polymer and ion size) profoundly impact the thermodynamics, and by articulating them in theoretical or simulation models, we can start to understand how to design coacervate materials at a molecular level.
Complexes

The cationic species comprised members of the CnMIM (1-alkyl-3-methylimidazolium) family with n ranging from 2 to 10. The anionic component varied from

pure component. In this work, families of ionic liquids were characterized using the Locally Correlated Lattice (LCL) model that was previously used to study

CHEN, RONALD WHITE, JANE LIPSON, Dartmouth Coll — Trends in polymer solution miscibility can be understood by analyzing the properties of each

versatile properties of charged polymers. The charged properties of the polymer backbone and those of the accompanying ions have a large influence on

larger scale (self-assembled) structure and miscibility. With statistical thermodynamic methods, we investigate local ionic structure and the influence of charge

correlations on the phase diagram of polyelectrolyte blends. In particular, we study the effects of added salt on the coexistence lines, and explore the possibilities

of multiple phase coexistence between phases with a different polymer fraction or charge concentration.

14:30PM W45.00011 Image method for Coulomb energy for many-body system of charged dielectric spheres, JIAN QIU, QIN JIE DE PABLO, KARL FREED, University of Chicago — Ion polarization is important for understanding ion solvation and the stability of ion clusters in polymeric materials which typically exhibit a low and spatially inhomogeneous dielectric permittivity. The simplest approach for modeling ion polarization involves treating the ions as charged spheres with an internal dielectric permittivity differing from that of the medium. The surface polarization contribution to the electrostatic energy for a system of such dielectric spheres can be evaluated perturbatively. We derived closed-form expressions for this energy as a function of the positions of an arbitrary number of polarized surfaces. Our approach is a generalization of the image method for conducting spheres. Using this approach, we calculated the polarization corrections to the cohesion energy for ion clusters and for densely packed ionic crystals. The method can be readily adapted for investigating ion polarization effects in both Monte Carlo and molecular dynamics simulations.

4:42PM W45.00012 Phase behavior and multi-body effects in polyelectrolyte - nanoparticles mixtures, VICTOR PRYAMITSYN, VENKAT GANESAN, University of Texas at Austin, JEFFREY ERRINGTON, University of Buffalo — Recently we have developed a SCFT approach which allowed us to compute the effective interactions between charged nanoparticles (CNP) and in a polyelectrolyte (PE) solution. We have adapted such an approach to study the hierarchy of the two-, three- and multi-body interactions between CNP's. We have found that for the strong PE's and absent polarization interactions, the CNP-CNP interactions are essentially pairwise. This result allowed us to use the thermodynamic perturbation theory and the MC simulations to access the phase diagram of PE/CNP mixtures. Such analysis indicates that CNP-PE mixtures exhibit only gas and crystal phases, and that the fluid phase is metastable. The results of MC simulations suggest the suppression of the phase segregation by the formation of highly anisotropic clusters of CNP. The qualitative analysis of the three- and multi-body interaction in comparison with two-body interaction shows that such interaction may enhance the anisotropy of CNP clusters. We have also analyzed of weak PE's and the presence of polarization interaction. In such systems CNP's interactions remain qualitatively similar to the above systems, but the multi-body interactions appears to be significantly enhanced, which makes anisotropic clustering of PE's even more plausible.

4:54PM W45.00013 Ionic Liquids: Trends in Behavior and Miscibility with Polymers, MICHELLE CHEN, RONALD WHITE, JANE LIPSON, Dartmouth Coll — Trends in polymer solution miscibility can be understood by analyzing the properties of each pure component. In this work, families of ionic liquids were characterized using the Locally Correlated Lattice (LCL) model that was previously used to study numerous polymers as well as their solutions and blends. Ionic liquids were divided into families that incorporated size variation into each of the components. The cationic species comprised members of the CnMIM (1-alkyl-3-methylimidazolium) family with n ranging from 2 to 10. The anionic component varied from

BF$_4^-$ to PF$_6^-$ to NT$_2^-$ (bis(trifluoromethylsulfonyl)amide). Each liquid was characterized using the LCL equation of state and properties such as percent free volume and cohesive energy density were calculated. These properties were observed to be correlated with alkyl chain length and anion size within each family. Analyzing these trends points towards a fundamental understanding of ionic liquid miscibility with poly(ethylene oxide), members of the polymethacrylate family, and others.

1Work supported by NSF-DMR

5:06PM W45.00014 Surface Tension and Lamellar Spacing in Polyelectrolyte Blends and Block Copolymers, CHARLES SING, University of Illinois at Urbana-Champaign, MONICA OLVERA DE LA CRUZ, Northwestern University — Heterogeneous polymer systems such as block copolymers (BCPs) are governed primarily by a competition between the surface tension between different chemical species and the entropic stretching of the polymer chains. Charged BCPs represent a class of materials that is currently of great interest to the polymer community due to the promise of charged BCPs as nanostructured membranes for batteries and fuel cells. The inclusion of charge presents a powerful way to tune the structure of BCPs, and we develop our understanding of how to do so by investigating the interfacial properties (surface tension and microstructure size) of polyelectrolyte blends and block copolymers. We use a new method that combines the features of liquid state (LS) theory and self consistent field theory (SCFT) into a multiscale LS-SCFT theory that provides beyond-mean-field predictions of polyelectrolyte systems. We find that charge size, charge correlations, and the fraction of charged monomers plays a crucial role in determining surface tension, and we therefore demonstrate how BCP structure changes upon inclusion of charges. Finally, we will show that these predictions provide the ideal basis for comparison to experiment and subsequent refinement of LS-SCFT theory.

1Research Fellowship of the German Research Foundation (DFG)
5:18PM W45.00015 Molecular Origins of Thermal Transitions in Polyelectrolyte Assemblies .
EROL YILDIRIM, Aalto University, YANPU ZHANG, Texas A&M University, HANNE S. ANTILA, Aalto University, JODIE L. LUTKENHAUS, Texas A&M University, MARIA SAMMALKORPI, Aalto University, AALTO TEAM, TEXAS A&M TEAM — Polyelectrolyte (PE) multilayers and complexes formed from oppositely charged polymers can exhibit extraordinary superhydrophobicity, mechanical strength and responsiveness resulting in applications ranging functional membranes, optics, sensors and drug delivery. Depending on the assembly conditions, PE assemblies may undergo a thermal transition from glassy to soft behavior under heating. Our earlier work using thermal analysis measurements shows a distinct thermal transition for PE layer-by-layer (LbL) systems assembled with added salt but no analogous transition in films assembled without added salt or dry systems [1]. These findings raise interesting questions on the nature of the thermal transition; here, we explore its molecular origins through characterization of the PE aggregates by temperature-controlled all-atom molecular dynamics simulations. We show via molecular simulations the thermal transition results from the existence of an LCST (lower critical solution temperature) in the PE systems: the diffusion behavior, hydrogen bond formation, and bridging capacity of water molecules plasticizing the complex changes at the transition temperature.

We quantify the behavior, map its chemistry specificity through comparison of strongly and weakly charged PE complexes, and connect the findings to our interrelated QCM-D experiments.


Thursday, March 5, 2015 2:30PM - 5:30PM — Session W46 DBIO GSNP: Invited Session: Collective Behavior and Jamming in Multi-Cellular Systems
217A - Jerry Lee, National Cancer Institute

2:30PM W46.00001 Unjamming phase transition in the asthmatic airway epithelium1 .
JEFFREY FREDBERG, Harvard School of Public Health — In asthma, an aberrant injury-repair response of the airway epithelium is pivotal in disease initiation and progression. Although the mechanism remains unclear, classical understanding emphasizes inflammatory events together with delayed epithelial cell differentiation and maturation. Here we reveal a physical mechanism that is not anticipated by that classical picture but dominates dynamics of cells cultured from airway epithelia nonetheless. In the course of maturation of the pseudostratified epithelial layer comprising primary human bronchial epithelial cells from non-asthmatic donors, we show a striking collective cellular behavior in which an immature, hypermobile, unjammed, fluid-like phase undergoes a transition into a mature, quiescent, jammed, solid-like phase. But compressive stresses on the epithelial layer that mimic bronchospasm drive the solid-like phase back to the fluid-like phase. We show, further, that the uncompressed epithelial layer from asthmatic donors exhibit spontaneous collective migration behavior that is similarly striking to that observed in compressed normal cells but results from a delay in the innate tendency of the epithelial layer to transition from an unjammed phase into a jammed phase. Moreover, the unjammed state of asthmatic epithelial cells accompanies intensified adhesive forces transmitted across cell-cell junctions. We introduce a theory of critical scaling that predicts a priori the existence of the observed phase transition. Surprisingly, this theory predicts the transition to be governed by cell shape and cell-cell adhesive forces in a manner that is paradoxical, but is borne out by our direct experimental observations. Together, these findings establish an unexpected but rigorous physical foundation for further classification and investigation of epithelial layer behavior in asthma, and likely in other processes in disease or development in which epithelial dynamics play a prominent role.

1 National Science Foundation (R01HL102373, R01HL107561, P01HL120839)

3:06PM W46.00002 Minimization of Thermodynamic Costs in Cancer Cell Invasion .
ROBERT AUSTIN, Princeton Univ — No abstract available.

PAK KIN WONG, University of Arizona — The fascinating capability of cellular self-organization (often referred as pattern formation) during tissue morphogenesis and regeneration is a central question in developmental biology, regenerative medicine, and complex systems. How do the cells of a tissue know how to organize into functional tissue structures that are much bigger than themselves? How do the individual cells know what they are supposed to do without a central coordinator or a blueprint? Furthermore, relatively little is known about how multicellular systems interpret the mechanical cues in the microenvironment, such as global forces, local cell-cell interactions, and extracellular matrix properties, to collectively drive the morphogenic process that creates complex tissue structures across multiple length scales. In this talk, I will discuss a nanoengineered framework for investigating the mechanoregulation of tissue morphogenesis, such as the capillary morphogenesis and collective cell migration during wound healing.

4:18PM W46.00004 ECM Organization and Cell-Cell Cooperation .
PETER FRIEDL, Radboud University Nijmegen, The Netherlands — Single-cell or collective invasion results from coordination of cell shape, deformability and actin dynamics relative to the tissue environment. In monomorphic 3D invasion models in vitro, an obligate step of collective invasion is the degradation of extracellular matrix (ECM). Thereby, the density of the ECM determines the invasion mode of mesenchymal tumor cells. Whereas fibroblastic, high porosity ECM enables single-cell dissemination, dense matrix induces cell-cell interaction, leader-follower cell behavior and collective migration as an obligate protease-dependent process. Conversely, in vivo monitored by intravital multiphoton second and third harmonic generation microscopy, tissue microchirons provide invasion-promoting tracks that enable collective migration along tracks of least resistance. As main routes, non-destructive contact-guidance is mediated by preformed multi-interface perimuscular, vascular and neural tracks of 1D, 2D and 3D topography. Consistently, spheroids of mesenchymal melanoma or sarcoma tumor cells switched from single-cell to collective invasion modes when confronted with 3D collagen matrices of increasing density, including gain of cell-to-cell junctions, supracellular polarization, suggesting cell jamming imposed by tissue confinement. Targeting of beta1/beta3 integrins induces unexpected plasticity of invasion, including collective and amoeboid single-cell dissemination, followed by enhanced micrometastasis, implicating a role of integrins in cell-cell cooperation and integrin-independent dissemination as effective route to metastasis. In conclusion, cancer invasion is maintained by physicochemical programs that balance cell-intrinsic adhesion and mechanocoupling with encountered physical space and molecular cues.

4:54PM W46.00005 Swarming in the bacterium Pseudomonas aeruginosa .
JOAO XAVIER, Memorial Sloan-Kettering Cancer Center — The fields of systems and synthetic biology have made great progress towards understanding and engineering biological systems while having the living cell as their central focus. However, many biological functions are multicellular and depend not only on interactions, both physical and chemical, between cells. We investigate organizing principles of multicellular systems using a prokaryotic model: swarming in Pseudomonas aeruginosa. Swarming is a collective form of surface motility that enables P. aeruginosa colonies to migrate over surfaces. We investigate the molecular mechanisms that confer robustness to swarming using a multidisciplinary approach that combines mathematical modeling, quantitative experiments, microbial genetics and comparative genomics to identify and characterize organizing principles of bacterial multicellularity. These “design principles” may inspire the development of robust synthetic multicellular systems that utilize emergent collective behaviors of cell populations to perform functions that individual cells cannot.

Thursday, March 5, 2015 2:30PM - 5:30PM — Session W47 DBIO: Membranes: Biological and Synthetic
217B - Kranthi Mandadapu, University of California, Berkeley
2:30PM W47.00001 Permeation of anions through the central pore of human aquaporin 51

TIERRY WAMBO, LIAO CHEN, Department of Physics & Astronomy, University of Texas at San Antonio — Aquaporin 5 (AQP5) plays an essential role in the physiology of saliva, tears and pulmonary secretion. We performed in silico experiments of the L51R mutant of the human Aquaporin 5 (PDB code: 3D95) for which in vitro experimental data became available recently. Molecular Dynamic Simulations performed on the AQP5 tetramer embedded in a lipid bilayer reveal that the central pore of the AQP5 mutant lost the hydrophobicity of the wild type protein and becomes permeable to anions, but not to cations. This conclusion is in agreement with the in vitro experiments of Qin and Baron, 2013. Quantitatively, we compute the potential of mean force (PMF) of chloride and iodide anions along the permeation path through the central pore. We correlate the PMFs with the experimentally measured conductance of various anions, elucidating the atomistic details of ion conduction through AQP5 mutant.

1 NIH (Grant #GM084834) and Texas Advanced Computing Center at UT Austin

2:42PM W47.00002 Discovery of a fundamental force related to a membrane’s order-disorder transition that can govern protein self-assembly in membranes

SHACHI KATIRA, KRANTHI MANDADAPU, University of California, Berkeley, SURIYANARAYANAN VAIKUNTANATHAN, University of Chicago, BEREND SMIT, DAVID CHANDLER, University of California, Berkeley — The clustering of proteins in cell membranes is a controlling factor in biological processes such as cell signaling and membrane fusion. Using large-scale molecular simulations and a theoretical framework inspired by modern theories of the hydrophobic effect, we have uncovered a fundamental physical force for assembly of trans-membrane proteins in lipid bilayers. This force is a mesoscopic manifestation of the transition between ordered (i.e., gel) and disordered (i.e., fluid) phases of lipid bilayers. It is a pre-transition effect, occurring below the order-disorder transition temperature, nucleated by the protein’s disturbance of the ordered phase. This powerful force acts over several nanometers in range. Conditions at which this force occurs and can lead to clustering of proteins in cell membranes will be discussed.

3:06PM W47.00004 Theory for registered and antiregistered phase separation of amphiphilic bilayers

JOHN WILLIAMSON, PETER OLMSTED, Georgetown University — Phase separation in bilayers can be exploited by nature, and engineers, to design-function via membrane domains. The presence of two separate, yet coupled, leaflets forces one to ask whether and how such domains are aligned (registered) across the bilayer. Experiment and simulation yield intriguingly disparate observables. We introduce a theory for phase separation in coupled leaflets, by explicitly coarse-graining a lattice model that includes molecule-level structure and interactions. We show that hydrophobic mismatch leads to a complex competition of inter-leaflet couplings. The theory helps unify prima facie contradictory observations, by showing that domain antiregistration typically occurs as a metastable state, but can be kinetically preferred. The role of kinetics in governing registration/antiregistration is explored, the theory’s predictions confirmed and illustrated with simulations, which show how a bilayer in the “spinodal region” can require nucleation to equilibrate. Our results shed light on a novel statistical mechanical problem of great practical importance, and motivate future work on intra- and inter-leaflet behaviour of bilayers. Reference: JJW and PDO, arXiv:1408.2744.

1 Funded by CAPITALS (EPSRC, GB), and Georgetown University

3:18PM W47.00005 X-ray Scattering Experiments Support Tilt-dependent Membrane Theory

MICHAEL S. JABLIN, JOHN F. NAGLE, Carnegie Mellon University — Recent molecular dynamics simulations have suggested that the traditional model for topographical fluctuations in lipid bilayers should be enriched to consider molecular tilt. We present the first experimental support for a tilt-dependent theory. X-ray scattering from a liquid crystalline stack of oriented fluid phase lipid bilayers was collected and compared to the predictions of tilt-dependent and tilt-independent membrane models. Both models satisfactorily fit the X-ray data dominated by in-plane lengths greater than membrane thickness (> 100 Å), but only the tilt-dependent model accounts for X-ray data primarily attributable to shorter length correlations. By fitting the measured X-ray scattering intensity, both the bending modulus $K_\epsilon = 8.3 \pm 0.6 \times 10^{-20}$ J and the tilt modulus $K_\theta = 95 \pm 3$ mN/m were determined for DOPC bilayers at 30 °C. Our experimental results support the enrichment of the classic Helfrich continuum model to include an internal degree of freedom, the fluctuations of lipid directors from the local normal.

3:30PM W47.00006 Two-Point Microrheology of Phase Separated Domains in Lipid Bilayers3

TRISTAN HORMEL, MATTHEW REYER, RAGHUVEER PARTHASARATHY, University of Oregon — Though the importance of membrane fluidity for cellular function has been well established for decades, methods for measuring lipid bilayer viscosity remain challenging to devise and implement. Recently, approaches based on characterizing the Brownian dynamics of individual tracers such as colloidal particles or lipid domains have provided insights into bilayer viscosity. In general, however, methods based on single-particle trajectories can be biased by distortions induced by the tracers, and furthermore provide a limited view of hydrodynamic response. The technique of two-point microrheology, in which correlations between the Brownian dynamics of pairs of tracers report on the properties of the intervening medium, resolves these issues, but has never been applied to lipid systems. We present the first two-point microrheological study of lipid bilayers, examining the correlated motion of domains in phase-separated lipid vesicles and comparing one- and two-point results. We measure correlation functions in excellent agreement with the forms predicted by two-dimensional hydrodynamic models, which reveal a viscosity that corresponds to the average of the lipid phases rather than the viscosity of the local neighborhood of the tracer.

3 The authors acknowledge support from the National Science Foundation, Award No. 1006171.
3:42PM W47.00007 Use of Impedance Spectroscopy to Probe Changes in Mitochondrial Membrane Potential. ROOPLEKHA C. MITRA, MARTHA Y. SUÁREZ VILLAGRÁN, JAREK WOSIK, WANDA ZAGOZDZON WOSIK, JOHN H. MILLER, JR.1 University of Houston — The synthesis of ATP is driven by proton gradient and electrical potential across the mitochondrial inner membrane. It’s electrical properties correlates with its physiological and pathological status. Electrical impedance spectroscopy is a non-invasive and relatively low cost technique where the impedance measurements monitors the underlying biological processes to determine parameters for biomarker studies. In this work we implement a multi frequency (1kHz – 10MHz) bio electrical impedance to describe the changes in the electrical properties of mitochondria. The experimental strategy involved treating isolated mitochondria with the substrate succinate ([200µM] in vivo to stimulate the activity of succinate dehydrogenase. Subsequent variability is introduced by the addition of different trifluorocarbonylcyanoide-phenylhydrazone (25µM < FCCCP) < 50µM] and dopamine (50µM < DA < 0.5M) concentration. We observe that succinate alone lead to an increase in the mitochondrial membrane potential ΔΨm. Dielectric spectroscopy measurements show a direct correlation between FCCCP concentration and impedance and higher DA concentrations display marked decrease of membrane potential indicating a significantly reduced mitochondrial respiratory control.

1Principal Investigator

3:54PM W47.00008 Proton-Pumping Mechanism in Complex I of Mitochondria Membrane. DAVNEET KAUR, Queens College CUNY — Mitochondria are the powerhouse of animal cells and also many bacteria. Complex I is the first enzyme in the mitochondrial respiratory chain, the process leading to storage of energy in the form of Adenosine Triphosphate (ATP). The structure of the enzyme was recently resolved and its functionality was correlated to the motion of a helical protein structure. However, the actual mechanism of the electron assisted proton-pumping of Complex I has remained mysterious because the electron (e-) and proton (H+) pathways are well separated by a distance of up to 15 nm making the direct interaction of these charges negligible. We model the helix assisted indirect coupling between the electron and proton pathways as a non-uniformly charged piston oscillating between the coupled sites of a 3 site series system. The energy conversion is determined by single e- and H+ transport events. The piston oscillates between that central proton and electron sites and modulates their energy, while the coupling with other sites is weak and negligible. We show that with realistic values of parameters, this structure allows for proton pumping against the potential gradient.

4:06PM W47.00009 ABSTRACT WITHDRAWN –

4:18PM W47.00010 Thinning silicon-based membranes with electron irradiation for solid-state nanopore sensors1, JULIO ALEJANDRO RODRIGUEZ-MANZO, MATTHEW PUSTER, University of Pennsylvania, Department of Physics and Astronomy, ADRIEN NICOLAI, VINCENT MEUNIER, Rensselaer Polytechnic Institute, Department of Physics, Applied Physics, and Astronomy, MARIJA DRNDC, University of Pennsylvania, Department of Physics and Astronomy — We present a controlled electron irradiation-based method to thin free-standing amorphous silicon membranes to less than 2 nm. Thinning is carried out in a scanning transmission electron microscope using a 200 keV electron probe to sputter silicon atoms. The transmitted electrons, scattered elastically and inelastically, are used as feedback signals to monitor and control the thinning process with sub-nanometer precision. Solid-state nanopore single-molecule sensors were fabricated by drilling a nanopore in the thinned membranes with the electron probe. These sensors operate in aqueous electrolyte and register passage of individual molecules by measuring changes in ionic conductance. We show that these solid-state nanopore single-molecule sensors sustain changes in ionic conductance with signal-to-noise ratios close to 100 at 100 kHz for translocations of double-stranded DNA in 1 M KCl electrolyte at room temperature coupled with conductance blockade of 60-95%.

1This work was supported by NIH Grant R21HG004767, and by the NBIC through the NSF NSEC DMR08-32802

4:30PM W47.00011 Nanoscopic modulated phases in dDPPC:DLPC membranes studied with small angle neutron scattering. NATALIE KRZYZANOWSKI, Univ of Illinois - Chicago, SUMIT GARG, Berg LLC, LIONEL PORCAR, Institut Laue-Langevin, Grenoble, France, URSULA PEREZ-SALAS, Univ of Illinois - Chicago — The lipid raft hypothesis states that functional, small (20-90nm) lateral heterogeneities in the cell membrane arise from the preferential association of proteins, sphingolipids, and cholesterol. Studies of model systems in the past decade have shown the formation of two liquid phases, a liquid-ordered and the typical fluid or liquid-disordered phase in ternary mixtures of a saturated lipid, unsaturated lipid, and cholesterol. These model raft systems on both a nanoscopic and macroscopic level have exhibited circular domains, but these are not the past only possible shapes of phase separated domains. Giant vesicles extracted from live cells studied with fluorescence microscopy can exhibit critical behavior, showing distinctly fluctuating and not circular domains. Non-circular domains have also been observed in quaternary component GUVs in the form of modulated or patterned phases. We use small angle neutron scattering (SANS) to study the nanoscopic phase behavior of the well-studied lipid mixture DPPC:DLPC as a function of temperature. We applied an existing ab initio program to reconstruct the membrane without a priori shape fixing. Modulated phases are shown to persist at the nanoscale in small vesicles.

4:42PM W47.00012 Heterogeneous Rotational Diffusion in Lipid Monolayers, NEDA DADASHVAND, LANELL A. WILLIAMS, CHRISTINA M. OTTHON, Wesleyan Univ — We have developed a new time-resolved fluorescence platform which enables us to follow the molecular orientation and dynamics of a lipid monolayer at the air - water interface. The rotational correlation time of the lipid probe NBD-PC is measured using fluorescence anisotropy for two lipid species. We measure the rotational diffusion in a monolayer of DPPC which displays a phase transition at room temperature from the liquid-expanded to the liquid-condensed phase. The constant rotational diffusion of the probe throughout the phase transition reflects the measurement of dynamics in only the liquid-expanded phase. We contrast the dynamic changes during this phase coexistence to the continuous density increase observed in DMPC at room temperature. We observe a non-exponential decay of the probe diffusion consistent with heterogeneity of the orientational dynamics; as the free-volume is reduced the diffusion becomes increasingly heterogeneous.

4:54PM W47.00013 Scaling and Alpha-helix Regulation of Protein Relaxation in a Lipid Bilayer1, K. CHENG, Trinity Univ, LIMING QIU, CREIGHTON BUIE, MARK VAUGHN, Texas Tech University — Protein conformation and orientation in the lipid membrane play a key role in many cellular processes. Here we use molecular dynamics simulation to investigate the relaxation and C-terminus diffusion of a model helical peptide: beta-amyloid (Aβ)1 in a lipid membrane. We observed that after the helical peptide was initially half-embedded in the extracellular leaflet of phosphatidylcholine (PC) or PC/cholesterol (PC/CHOL) membrane, the C-terminus diffused across the membrane and anchored to PC headgroups of the cytofacial lipid leaflet. In some cases, the membrane insertion domain of the Aβ3 was observed to partially unfold. Applying a sigmoidal fit to the process, we found that the characteristic velocity of the C-terminus, as it moved to its anchor site, scaled with $u_{\text{c}}^{-4/3}$, where $u_{\text{c}}$ is the fraction of the original helix that was lost during a helix to coil transition. Comparing this scaling with that of bead-spring models of polymer relaxation suggests that the C-terminus velocity is highly regulated by the peptide helical content, but that it is independent of the amino acid type. The Aβ was stabilized by the attachment of the positive Lys28 side chain to the negative phosphate of PC or 3β oxygen of CHOL in the extracellular lipid leaflet and of the C-terminus to its anchor site in the cytofacial lipid leaflet.

1NIH (GM090897-02)
Redistribution of Cholesterol by Membrane Active Peptides Alamethicin and Melittin

SHUO QIAN, WILLIAM HELLER, Oak Ridge National Lab — Many membrane active peptides are found to disrupt lipid bilayer of membrane in a concentration-dependent manner and form transmembrane pore over threshold concentrations, as depicted in Two-State Model. However, at low concentration, the interaction between peptide and lipid bilayer remains less understood beyond the thinning effect. Here we present small-angle neutron scattering studies of the interaction of two well-known membrane active peptides (melittin and alamethicin) with lipid bilayers made of dymyristoyl phosphatidylcholine (DMPC) and cholesterol (Chol). Through the use of deuterium-labeled DMPC, changes in the distribution of the lipid and cholesterol in unilamellar vesicles were observed for peptide concentrations well below those that drive pore formation. We have found the binding of the peptides have profound impact on the distribution of cholesterol residing inside the lipid bilayer. Those results point the existence of a possible secondary mechanism of action against cellular membranes as metabolic inhibitors that affect cellular machinery by redistributing cholesterol.

Energetics of interactions between protein inclusions in lipid bilayer membranes

PAUL GOLDBART, MICHAEL DIMITRIYEV, Georgia Institute of Technology, ALEX LEVINE, University of California - Los Angeles — Proteins that are situated in cell membranes play vital roles in numerous cell functions. Examples include the enabling of the selective passage of ions or molecules into and out of cells, or the relaying of signals between cell interiors and their external environments. We develop a framework for understanding the energetics of the interactions that can arise between protein inclusions. We focus on the setting of inclusions in lipid bilayers and interactions that stem from the spatial overlap of the distortions induced by the inclusions in the orientational organization of the lipid molecules that constitute the bilayers.

The structure of infectious disease outbreaks across the animal-human interface

CHRISTOPHER R. MYERS, Cornell University, DAVID J. SCHNEIDER, USDA-ARS and Cornell University, SARABJEET SINGH, Cornell University — Zoonotic infectious diseases that spill over from animal to human populations are responsible for some of the most devastating plagues to haunt humanity throughout its history, including the recent Ebola outbreak. Yet despite considerable efforts by epidemiologists to model specific zoonotic infections, much of the basic underlying structure of cross-species outbreaks has not been well-characterized. Motivated by these gaps and by recent efforts to develop classification schemes for characterizing the spectrum of zoonotic diseases, we have solved – using techniques from multitype branching processes and queuing theory – for the structure and statistics of outbreaks resulting from cross-species spillover, characterizing outbreak sizes, probabilities and first-passage times. In the case of human outbreaks driven by epidemics in animal populations, we find a novel multicritical point at which outbreak size scaling is different than in a single population. When human outbreaks are driven by an endemic disease in an animal reservoir, we find variable exponents characterizing outbreak size and duration that depend upon the rate of cross-species spillover.

The spatial and metabolic profiles of microbial populations non-monomonotonically impact the growth of antibiotic resistant mutants

KARISHMA KAUSHIK, NALIN RATNAYEKE, Univ of Texas, Austin, PARAG KATIRA, Univ of Texas, Austin. Present address: Columbia University, New York, VERNITA GORDON, Univ of Texas, Austin — Spatial heterogeneity in the distribution of antibiotic is known to accelerate the development of genetic antibiotic resistance. However, the effect of the structure of the microbial population is less well studied. Microbial population structure is a type of spatial structure defined by composition, cell density, and spatial organization of cell types. As our cell types, we use antibiotic-resistant and antibiotic-susceptible (wild-type) Pseudomonas aeruginosa along with S. aureus and B. cepacia, both co-pathogens with P. aeruginosa. In spatially-mixed systems, composed of wild-type cells and antibiotic-resistant mutants, we find that increasing cell density reduces the probability of antibiotic-resistant mutant survival in the presence of antibiotic. Using spatially-structured systems, we show that inhibition is mediated by a low-molecular weight, universal, alkaline by-product of bacterial catabolism of amino acids. We demonstrate that for organisms capable of growing on either amino acids or sugars, the nutrient environment provides a switch to activate or deactivate inhibition. Finally, we show that small spatial fluctuations in initial population density can shield mutants from the combined effect of antibiotic and the inhibitory factor.

Evolution of Super-Reciprocity in Noisy Iterated Games

AREND HINTZE, CHRISTOPH ADAMI, Michigan State Univ — In the classical Iterated Prisoner’s Dilemma (IPD), direct reciprocity is a form of communication leading to altruistic behavior. However, if players use stochastic strategies, a secondary form of cooperation in which players alternate in receiving the Temptation (T) and Sucker (S) rewards can emerge (super-reciprocity). This reciprocal behavior will become evolutionary dominant if the reward (T) is increased above a certain threshold, but is inherently more risky than primary cooperation since it relies on trust between players in two consecutive iterations of the game. Here, we investigate how different environmental conditions such as mutation rate, environmental noise, and reward T affect the evolution of reciprocity. Super-reciprocal strategies rely on the synchronization of two genes and are thus much more sensitive to environmental changes that affect the accuracy of players prediction of opponents’ future moves. We find that increasing the environmental noise or mutation rate is deleterious to super-reciprocity, while increasing T stabilizes its evolution. Conversely, in environments that are highly predictable and where there is no payoff advantage to engage in reciprocal cooperation, basic cooperation strategies rely on the synchronization of two genes and are thus much more sensitive to environmental changes that affect the accuracy of players prediction of opponents’ future moves. We find that increasing the environmental noise or mutation rate is deleterious to super-reciprocity, while increasing T stabilizes its evolution. Conversely, in environments that are highly predictable and where there is no payoff advantage to engage in reciprocal cooperation, basic cooperation via reciprocal communication remains the strategy of choice.

An optimal energy dissipation strategy of the MinCDE oscillator in regulating symmetric bacterial cell division

GANHUI LAN, George Washington University — Sustained molecular oscillations are ubiquitous in biology. The obtained oscillatory patterns provide vital functions as timekeepers, pacemakers and spacers. Control-theory type models have been introduced to explain how specific oscillatory behaviors stem from protein interaction feedbacks, whereas the energy dissipation through the oscillating processes and its role in the regulatory function remain elusive. Here we developed a general framework to assess oscillator’s regulation performance at different dissipation levels. Using Escherichia coli MinCDE oscillator as model system, we showed that, unlike stationary regulators’ monotonic performance-to-cost relation, excess dissipation at certain steps in the oscillating process damages the oscillator’s regulatory performance. We further discovered that ATP hydrolysis energy has to be strategically assigned to the MinE-aided MinD release and the MinD immobilization steps for optimal performance, and higher energy budget improves the robustness of the oscillator. These results unfold a novel mode that living systems trade energy for regulatory function.

Work supported by the George Washington University Columbian College Facilitating Fund
3:42PM W48.00005 Quantitative evolutionary dynamics of one million barcoded lineages. JAMIE BLUNDELL, Stanford University, SASHA LEVY, SUNY Stony Brook, SANDEEP VENKATARAM, DMITRI PETROV, DANIEL FISHER, GAVIN SHERLOCK, Stanford University — Evolution of large asexual cell populations underlies ≈ 30% of deaths worldwide, including those caused by bacteria, parasites, and cancer. However, the dynamics underlying these evolutionary processes remain poorly understood because they involve many competing beneficial lineages, most of which never rise above extremely low frequencies. To observe these normally hidden evolutionary dynamics, we constructed a sequencing-based ultra high-resolution lineage tracking system that can monitor the relative frequencies of ≈ 500,000 lineages simultaneously. We find that the spectrum of fitness effects of beneficial mutations is far from exponential and not even monotonic. Early adaptation is a predictable consequence of this distribution and is strikingly reproducible, but the initial small-effect mutations are soon outcompeted by rarer large-effect mutations that result in variability between replicates. Our results suggest that early evolutionary dynamics may be deterministic for a period of time before stochastic effects become important. The interplay between deterministic and stochastic effects is controlled in large part by the distribution of mutation rates to each fitness effect, which high-resolution lineage tracking is uniquely suited to measure.

3:54PM W48.00006 Noise-stabilized Turing Patterns in a Synthetic Biofilm1. K. MICHAEL MARTINI, Department of Mathematics and Institute for Genomic Biology, University of Illinois at Urbana-Champaign, DAVID KARGIR, Research and Exploratory Development Department, Johns Hopkins University Applied Physics Laboratory, TING LU, Department of Bioengineering, Department of Physics and Institute for Genomic Biology, University of Illinois at Urbana-Champaign, NIGEL GOLDENFELD, Department of Physics and Institute for Genomic Biology, University of Illinois at Urbana-Champaign, RON WEISS, Department of Biological Engineering, Massachusetts Institute of Technology — Deterministic Turing instabilities have been proposed to be a major source of pattern formation in biology, but have been hard to document rigorously, in part because of the requirement for a large ratio of the inhibitor to activator diffusion coefficient. A recently developed theory of stochastic Turing patterns predicts that stochastic or noise-stabilized Turing patterns occur over a larger region of parameter space and do not require as large a separation of diffusion rates. We apply this theory to a biofilm whose signaling molecules have been forward-engineered to exhibit activation and inhibition. Outside of the range of deterministic Turing patterns, we observe noise-stabilized patterns that exhibit a power spectrum power law tail with exponent $-2.3 \pm .4$ consistent with theory. Our results are the first report of a spatial pattern in gene expression stabilized by copy number fluctuations.

1 K. M. Martini acknowledges partial support from the CPLC #1430124.

4:06PM W48.00007 Limits on energy dissipation qualitatively change kinetic proofreading in single cells1. JAYAJIT DAS, The Research Institute at the Nationwide Children’s Hospital and the Ohio State University — Cell signaling events, composed of biochemical reactions, usually occur in the absence of the detailed balance condition and continuously dissipate energy. Consequently, when energy supply is limited, specific chemical modification steps might not occur due to the lack of energy to support those reactions. How does the absence of such modification steps, that are intrinsically stochastic in nature, affect single cell signaling kinetics? I address this question in the context of a kinetic proofreading scheme used in a simple model of early T cell signaling. I show, using exact analytical calculations and numerical simulations, that the amount of energy dissipation needed to execute a desired discrimination scheme depends on whether the decision is made at the transient state or in the steady state of the kinetics. Using a modified Gillespie algorithm for simulating biochemical reactions in energy limited conditions, I show that restricting energy dissipation leads to poorer discrimination in single cells for weak and low affinity ligands. Furthermore, restricting energy dissipation produced substantially larger intrinsic cell-to-cell variations of proteins with qualitatively different distributions than the system with unlimited supply of energy.

1 NIH

4:18PM W48.00008 Decision theory for immune ligand recognition. PAUL FRANCOIS, McGill University — Variability in the chemical composition of the extra-cellular environment can significantly degrade the ability of cells to detect rare cognate ligands. Using concepts from statistical detection theory, we formalize the generic problem of detection of small concentrations of ligands in a fluctuating background of biochemically similar ligands binding to the same receptors. We discover that in contrast to expectations arising from considerations of signal amplification, inhibitory interactions between receptors can improve detection performance in the presence of substantial environmental variability, providing an adaptive interpretation to the phenomenon of ligand antagonism. Our results suggest that the structure of signalling pathways responsible for chemodetection in fluctuating and heterogeneous environments might be optimized with respect to the statistics and dynamics of environmental composition. Our formalism stresses the importance of characterizing non-specific interactions to understand function in signalling pathways.

4:54PM W48.00009 Phylogetic Tree from the Tangled Nature Model and Its Community Structure1. OSMAN CANKO, FERHAT TASKIN, KAMIL ARGIN, Erciyes University — In the evolutionary biology, taxonomy and origination of species are a widely emphasized subject. An estimation of the evolutionary tree can be done via available DNA sequence data. The calculation of tree are made by well-known and frequently used methods such as maximum likelihood and neighbor-joining. In order to inquire the results of these methods, an evolutionary tree is pursued computationally by a mathematical model, called Tangled Nature. A relatively small genome space is investigated due to computational burden and it is found that actual and predicted tree are in a reasonably good agreement in terms of shape. Moreover, speciation and emerged community structure of food-web are investigated by modularity.

1 This research has been supported by the Scientific and Technological Research Council of Turkey (TUBITAK) under Grant No: 111T735 and by Erciyes University Research Funds under Grant No: FDA-2013-4638.

5:06PM W48.00010 A Stability Investigation of Dynamically Evolved Tangled Nature Model1. FERHAT TASKIN, OSMAN CANKO, KAMIL ARGIN, Erciyes University — An individual-based Tangled Nature model has non-stationary macro-dynamics of evolutionary ecology. System travels among the multi-space minimum through saddle point and stays in a valley, called quasi-steady states (qSS). We have compared the stability of sequential qSS by perturbation. To investigate stability of community, the perturbed and unperturbed systems are compared by their community structure. Our results exhibit that the angle and distance between two center of mass shows a delayed response to perturbation for aged system. We have observed that the system evolves dynamically to the more stable states and shows robustness to external shocks with passing time.

1 This research has been supported by The Scientific and Technological Research Council of Turkey (TUBITAK) under Grant No: 111T735 and by Erciyes University Research Funds under Grant No: FDA-2013-4638.

Thursday, March 5, 2015 2:30PM - 5:06PM – Session W49 GSOFT: Focus Session: Migration of Cells, Droplets, and Particles on Substrates

217D - Kim Weirich, University of Chicago
2:30PM W49.00001 Kinetic Description for Formation and Dissolution of Living Colonies. CHRISTOPH WEBER, VEN TING LIN, Max Planck Institute for the Physics of Complex Systems, NICOLAS BIAIS, Brooklyn College and The Graduate Center, VASILY ZABURDAEV, Max Planck Institute for the Physics of Complex Systems, COLLECTIVE DYNAMICS OF CELLS TEAM, BIOLOGY DEPARTMENT COLLABORATION — Pathogen bacteria, such as N. gonorrhoeae or N. meningitidis form colonies due to encounters of nearby individuals while the effect of cell division is in general negligible. They use long and thin filaments, called pili, which attach to a substrate, retract and thereby pull the cell forward. Even though it is known that these bacteria interact by pili and adhesion, the question of how single cell motility and cell-cell interactions affect the process of colony formation is poorly understood. To bridge this gap we propose a kinetic description that keeps track of the length scales related to the underlying interactions between the cells and with the substrate. We derive the corresponding hydrodynamic equation and find an ordering instability leading to the formation of colonies. However, colonies can also dissolve which is a key survival mechanism in rapidly deteriorating environmental conditions. Recent experimental studies indicate that colonies can dissolve by switching off either the adhesive or pili-mediated interaction. Remarkably, within the same framework we can show that dissolution is possible, however, there is a region in parameter space where it is precluded. Both scenarios can be explained in terms of the underlying microscopic interactions.

2:42PM W49.00002 Coarse-grained model for a motor protein walker on a bead-spring substrate. JUTTA LUETTMER-STRATHMANN, Departments of Physics and Chemistry, NABINA PAUDYAL, MARAL ADELI KOUDEHI, Department of Physics, The University of Akron, Akron, OH 44325-4001 — Motor proteins play an important role in many biological processes. For example, kinesin molecules are responsible for the transport of vesicles in nerve cells and their malfunction has been linked to neurodegenerative diseases. Unfortunately, the complexity of motor proteins and their environment makes it difficult to model the detailed dynamics of molecular motors over long time scales. In this work, we develop a simple coarse-grained model for a motor protein on a bead-spring substrate under tension. In our model, different pair potentials describe interactions between substrate and motor, motor components and substrate components. The movement of motor proteins entails ATP hydrolysis, which is modeled in terms of mechano-chemical states that couple positional and chemical degrees of freedom. We apply the model to the problem of cargo transport and the effect of motor-protein activity on the mechanical response of a single chain molecule.

2:54PM W49.00003 Effect of silane molecular length on initial attachment of bacteria to silanized glass surfaces. ANDREA JAIMES-LIZCANO, SUMEDHA SHARMA, JACINTA CONRAD, University of Houston — Bacteria adhered to surfaces can form biofilms, which foul biomedical implants, industrial equipment and marine vessels, leading to deleterious costs. Designing surfaces to control bacterial adhesion is therefore of great interest for the prevention of biofouling. In this work, we investigate the effect of silane molecular length on the initial attachment of bacteria. We characterize the initial attachment of Escherichia coli to glass surfaces that are coated with silane molecules with the same functional end group but two different carbon chain lengths. Bacteria are deposited from flow in a microfluidic channel at shear rates ranging from 3.1 s$^{-1}$ to 25 s$^{-1}$ and imaged and tracked using confocal microscopy and high-throughput image processing algorithms. The initial rate at which bacteria deposit on the surface is independent of shear rate for the shorter three-carbon chains but depends on shear rate for the longer nine-carbon chains. We found longer bacterial residence times on the shorter silane molecules at the highest shear rate.

3:06PM W49.00004 Dissecting Subcellular Actomyosin Mechanics with Magnetically Actuated Micropost Arrays. YU SHI, Johns Hopkins University, STEVEN HENRY, JOHN CROCKER, University of Pennsylvania, DANIEL REICH, Johns Hopkins University — The cellular actomyosin cytoskeleton is widely regarded as an archetypal example of an active matter system. However, the extent to which the wide range of observed cellular motility behaviors arise from active-matter physics is not well understood. Characterizing an active matter system requires simultaneous measurement of the fluctuation spectrum of the internal force generators and also the local viscoelasticity to separate the distinct effects of the material’s internal stresses from its viscoelastic response to those stresses. By placing cells on top of PDMS micropost arrays with magnetic nanowires embedded in selected posts, we can actuate local regions of the cells by applying AC magnetic fields to dynamically probe the local viscoelasticity, while simultaneously using the posts as “probe particles” for passive micro rheology measurements of the cytoskeletal force fluctuations. The range of active and passive responses observed for different subcellular regions of fibroblast cells will be presented, and the results compared to simple active material models based on known or predicted behavior of molecular motors in viscoelastic networks. Effects of coupling between local cellular regions as measured by correlations in the micropost’s motion will also be described.

3:18PM W49.00005 Confocal Microscopy Indentation for Hydrogel¹. DONGHEE LEE, MD, MAHMUDUR RAMMAN, YOU ZHOU, SANGJIN RYU, University of Nebraska-Lincoln — It is well known that the stiffness of extracellular matrix affects cellular behaviors, and such effects were observed by culturing cells on hydrogel substrates. Thus it is required to measure the elasticity of the hydrogel substrate rigorously and efficiently. Here we propose a confocal microscopy indentation method for hydrogels. We indented fluorescently stained polyacrylamide gel with a sub-mm-sized ball indenter, and imaged the indented gel using confocal microscopy. Having formed a three-dimensional image stack of the gel, we measured the indentation depth based on automated image processing, and then evaluated the elasticity of the gel. We also validated our method using other well established indentation methods.

¹Supported by Bioengineering for Human Health grant from UNL and UNMC

3:30PM W49.00006 Schwann Cells and the Importance of Finite 3D Deformations in Soft Gels². CHRISTIAN FRANCK, EYAL BAR-KOCHBA, Brown University, CRISTINA LOPEZ-FAGUNDO, University of Zurich, LIANE LIVI, DIANE HOFFMAN-KIM, Brown University — Schwann cells (SCs) are specialized glial cells that are critical for the development, regeneration, and maintenance of nerves in the peripheral nervous system (PNS). Recent studies have shown that the mechanical properties of the extracellular matrix can significantly affect cell structure and function. Studying the mechanical interactions between SCs and their microenvironment can aid in understanding their physical and morphological changes as well as their native function. Using a recently developed 3-D large deformation traction force microscopy (3-D-LDTFM) technique, we investigate the mechanosensitivity of SCs across a physiologically relevant substrate stiffness range (0.24 kPa to 4.80 kPa) in vivo. As oppose to other cell types, we find that the SC spreading area and prominent stress fiber formation was relatively insensitive to substrate stiffness. Consistent with these structural findings, the SCs generated large surface tractions on stiff substrates and large material deformations on soft substrates. Across all moduli, we observed a significant contribution from the out-of-plane traction component, locally giving rise to rotational moments similar to those reported for mesenchymal embryonic fibroblasts.

²The authors gratefully acknowledge NIH R01 NS070653 and NSF Graduate Research Fellowship to C.L.F.; NSF CBET 1134166 to D.H.K.; NSF Graduate Research Fellowship to E.B.K as funding sources.

3:42PM W49.00007 ”Please choose a title, something about migration on substrates”. ERIN RERICA, Vanderbilt University — No abstract available.
4:18PM W49.00008 Complex multi-cellular manifolds\textsuperscript{1} . TAPOMOY BHATTACHARJEE, KYLE G. ROWE, Department of Mechanical and Aerospace Engineering, University of Florida, Gainesville, Florida, 32611 USA, SUHANI JAIN, Stanton College Preparatory, Jacksonville, Florida, 32209 USA, STEVEN M. ZEHNDER, RYAN M. NIXON, Department of Mechanical and Aerospace Engineering, University of Florida, Gainesville, Florida, 32611 USA, W. GREGORY SAWYER, Department of Mechanical and Aerospace Engineering, Department of Materials Science and Eng., University of Florida, Gainesville, Florida, 32611 USA, THOMAS E. ANGELINI, Department of Mechanical and Aerospace Eng., Department of Biomedical Eng., Institute for Cell and Regenerative Medicine, University of Florida, USA — Investigation of collective cell behavior is critical for understanding the evolution of tissue regeneration, embryonic morphogenesis, wound healing, and cancer invasion. Collective behavior has been widely studied in 2D cell monolayers, providing great fundamental understanding of multi-cellular motion and mechanics. Living tissues, by contrast, are densely packed with complex 3D structures including curved manifolds and tubular networks. Exploration of collective cell behavior within such complex 3D structures is essential to our understanding of cell monolayers to their motion and mechanics in tissues. In this study, complex structures have been generated by 3D printing living cells into a viscoelastic cell growth medium, creating cellular manifolds with a wide range of mean and Gaussian curvature, such as linear cylinders and branched tubular networks. Preliminary data describing collective cell behavior within these complex manifolds will be presented.

\textsuperscript{1}NSF Grant No. DMR-1352043

4:30PM W49.00009 Long range self-assembly of microcapsules regulated via the represilator signaling network . HENRY SHUM, VICTOR YASHIN, ANNA BALAZS, University of Pittsburgh — Communication to produce collective motion is a biological characteristic realized by few synthetic systems. Inspired by biological regulatory networks, we design a collection of microcapsules that move in response to self-generated chemical signals. Three microcapsules act as localized sources of distinct chemicals that diffuse through surrounding fluid. Production rates are modulated by the “represilator”: each chemical species represses the production of the next in a cycle. Depending on the maximum production rates and capsule separation distances, we show that immobile capsules either exhibit steady or oscillatory chemical production. We then consider movement of the microcapsules over the substrate, induced by gradients in surface energy due to adsorbed chemicals. We numerically simulate this advection-diffusion-reaction system with solid-fluid interactions by combining lattice Boltzmann, immersed boundary and finite difference methods, and thereby, construct systems where the three capsules spontaneously assemble, forming a close-packed triad. Chemical oscillations are shown to be critical to this assembly. By adjusting parameters, the triad can either remain stationary or translate as a cohesive group. Stationary triads can also be made to “turn off” after assembly.

4:42PM W49.00010 Asymmetric oscillation and dynamic clustering of water-in-oil droplets by hydrodynamic interactions . TAKUYA OHMURA, Department of Physics, Kyoto University, KEN-ICHIRO KAMEI, iCeMS, Kyoto University, MASAOTOSHI ICHIKAWA, Department of Physics, Kyoto University, YUSUKE MAEDA, Department of Physics, The Hakubi Center, Kyoto University, JST PRESTO — Ordered motion or patterns are widely observed in many biological systems, far from equilibrium. Microfluidic droplet crystal is one of the ensemble of water-in-oil droplet moving in immiscible fluid in a microchannel is known to exhibit normal vibrational mode due to inter-droplet hydrodynamic interactions. In this study we study dynamic ordering in the ensemble of different-sized droplets in order to investigate the effect of heterogeneity in the droplet crystal. We find asymmetric back-and-forth motion of single small droplet of 20 \( \mu \)m, which is placed within two droplets of 140 \( \mu \)m, is emerged. As a group of small droplets comes in the middle of large droplets, their motion turns dynamic clustering from oscillation. Numerical analysis indicates that hydrodynamic interactions with boundary wall and large droplets break symmetry of flow field and results in closed streamlines sustaining asymmetric oscillation.

4:54PM W49.00011 Tensional Homeostasis in Single Fibroblasts Probed with Traction Force Microscopy . ROSTISLAV BOLYANSKII, HENRY FOOTE, AARON MERTZ, KATHRYN ROSOWSKI, HOLLY LAURIDSEN, VALERIE HORSLER, JAY HUMPHREY, MARTIN SCHWARTZ, ERIC DUFRESNE, None — Many tissue types, including skin and blood vessels, respond to mechanical perturbations as a means to feedback regulate their behavior. While much of the research has focused on the mechanics of cells in monolayers, recent studies have demonstrated that collective cell contractility is also key to pattern formation and functional tissue regeneration. Here we introduce a new approach to measure cell traction forces using the open-source software NIBLASSI to measure cell traction forces using the open-source software NIBLASSI, enabling us to measure cell traction forces using the open-source software NIBLASSI. This approach allows us to measure cell traction forces using the open-source software NIBLASSI, providing new insights into how mechanical perturbations regulate collective cell behavior.

Thursday, March 5, 2015 2:30PM - 5:18PM – Session W50 GSOFT: Liquid Crystals III: Nematic and Twist Bend Phases 218 - Luz Miranda-Martinez, University of Maryland-College Park

2:30PM W50.00001 Direct mapping of local director field of nematic liquid crystals at the nano-scale . YU XIA, FRANCESCA SERRA, SHU YANG, RANDALL KAMien, Univ of Pennsylvania — The director field in liquid crystals (LCs) has been characterized mainly via polarized optical microscopy, fluorescence confocal microscopy, and Raman spectroscopy, all of which are limited by optical wavelengths ~ hundreds of nanometers to several micrometers. Since LC orientation cannot be resolved directly by these methods, theory is needed to interpret the local director field of LC alignment. In this work, we introduce a new approach to directly visualize the local director field of a nematic LC (NLC) at the nano-scale using scanning electron microscopy (SEM). A new type of NLC monomer bearing crosslinkable groups was designed and synthesized. It can be well-oriented at particle surfaces and patterned polymer substrates, including micron-sized silica colloids, porous membranes, micropillar arrays, and 1D channels. After carefully crosslinking, the molecular orientation of NLCs around the particles or within the patterns could be directly visualized by SEM, showing oriented nanofibers representing LC director from the fractured samples. Here, we could precisely resolve not only the local director field by this approach, but the defect structures of NLCs, including hedgehogs and line defects. The direct mapping of LC directors at the nanoscale using this method will improve our understanding of NLC local director field, and thus their manipulation and applications. More importantly, a theoretical interpretation will no longer be a necessity to resolve a new material system in this field.

2:42PM W50.00002 Topological Defects in Liquid Crystals: Studying the Correlation between Defects and Curvature . CHARLES MELTON, University of California Merced — Topological defects have recently been the subject of many studies in soft condensed matter physics. In particular, linking the evolution of topological defects to curvature changes has been a focus, leading possible applications in the areas such as cosmetics, pharmaceuticals, and electronics. In this study, defects in nematic liquid crystal droplets are investigated via laboratory and theoretical techniques. Nematic liquid crystal defects are reproduced via Monte Carlo simulations using a modified 2D XY-Model Hamiltonian. The simulation is performed on a curved surface to replicate a nematic droplet and examine possible defect configurations. To complement this theoretical work, we have trapped nematic droplets inside a dual-beam optical trap. This system allows controllable non-contact droplet deformation on a microscope based platform. Future work will focus on using the trap to stretch nematic droplets, correlating the changing topological defects with theoretical predictions.
2:54PM W50.00003 Ground States of Nematic Tori with radial boundary conditions, KARTHIK NAYANI, School of Material Science and Engineering, Georgia Institute of Technology, PERRY ELLIS, School of Physics, Georgia Institute of Technology, JUNG OK PARK, MOHAN SRINIVASARAO, School of Material Science and Engineering, Georgia Institute of Technology, ALBERTO FERNANDEZ-NIEVES, School of Physics, Georgia Institute of Technology — We report ground states of radially anchored nematic tori. For strong anchoring conditions we observe the often reported escape radial configuration. However, as the aspect ratio of the torus is lowered the escape configuration evolves to a new structure where the additional splay on the liquid crystal imposed by the geometry of the torus is released as bend. At lower anchoring condition the ground state corresponds to a two +1/2 line defect wrapping the torus. However, as the aspect ratio is lowered we again observed a new ground state where a single line wraps the torus twice. We perform Jones calculus simulations to confirm that our director ansatz reflects the experimental findings.

3:06PM W50.00004 Using chemically patterns with different anchoring behavior to control the orientation of nematic liquid crystal, XIAO LI, JULIO ARMAS PEREZ, JOSE ADRIAN MARTINEZ-GONZALEZ, HELOU XIE, JUAN DE PABLO, PAUL NEALEY, University of Chicago — We present experimental and theoretical study of nematic liquid crystal (5CB) confined to a thin cell between homeotropic anchoring top surface and chemically patterned planar/homeotropic anchoring bottom substrates. The chemically patterned substrate with different dimensions and ~ 4 nm depth topography induce the 5CB to align as the pattern direction as non-degenerate behavior, until the width of the straight line pattern is too wide to confine the 5CB to one direction and back to degenerate behavior. By changing the width of the straight line pattern, a brightness change of the intensity is shown by their corresponding crossed polarizer images. This change is mainly due to a discontinuity of the average angle between the molecules and the surface in function of line width, which is in excellent agreement with the Landau-de Gennes theory when the balance between the elastic deformation in the bulk and orientation of molecules close to the surface is simulated for different pattern dimensions. An elastic free energy transition is also observed from the numerical analysis when the strong planar anchoring for presented experiments is changed to weak. This 3D confinement by chemically patterns and small depth topography offers a new way to generate any geometry pattern controllable non-degenerate orientation, achieving switchable optical properties.

3:18PM W50.00005 Planar Anchoring of Achiral Nematic Liquid Crystals in Capillaries — with a Twist1, ZOEY S. DAVIDSON, JOOHWOO JEONG, LOUIS KANG, Department of Physics & Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA, PETER J. COLLINGS, Department of Physics & Astronomy, Swarthmore, Department of Physics & Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA, TOM C. LUBENSKY, A. G. YODH, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA — In the common three-term Frank free energy of a nematic liquid crystal, the ground state configuration will have no deformations and all nematic directors will be parallel. However, certain confining geometries can impose significant deformations on the ground state, even if a zero-deformation configuration can be drawn that satisfies all boundary conditions. By solving the Euler-Lagrange problem of the Frank free energy equation, including the saddle-splay term, with cylindrical confinement and degenerate planar anchoring, we find conditions for a highly deformed ground state that has a double twist like structure. We explore these effects experimentally with both thermotropic and lyotropic liquid crystal materials, finding good agreement with the theoretically predicted configuration. We also observe a rich phenomenology of defect structures in the liquid crystal samples.

3:30PM W50.00006 Dynamics of isothermal phase transition of liquid crystal with zero anchoring1, JINXIN FU, KARTHIK NAYANI, JUNG OK PARK, MOHAN SRINIVASARAO, Georgia Institute of Technology — Liquid crystal (LC) is an ideal system to mimic the cosmological symmetry breaking in the laboratory. The formation of LC string defects in film and bubble has been shown to be analogous to the formation of cosmic strings previously. Here we study the dynamics of LC isothermal transition from isotropic to nematic phase in a three-dimensionally isotropic environment, which enables us to observe the simultaneous symmetry breaking of matter without any external heat transfer or anchoring boundary condition. The isothermal phase transition is realized by the photochemical conversion of the trans-form to the cis-form of an Azobenzene compound that is added into liquid crystal E7. And a medium composed of carbopol and SDS surfactant provides the zero anchoring. The dynamics of the nucleation of LC and defects are studied under microscope with high-speed camera.

2:54PM W50.00008 Substrate induced gliding for a nematic liquid crystal layer1, ENSELA MEMA, LINDA CUMMINGS, LOU KONDIC, New Jersey Institute of Technology — The interaction between nematic liquid crystals (NLC) and polymer substrates is of current industrial interest, due to a desire to manufacture a new generation of flexible Liquid Crystal Displays (LCDs) for use in portable electronic devices. Polymer substrates present challenges because they can interact with the NLC, exhibiting a phenomenon known as gliding; the preferred orientation of the NLC molecules at the interface changes over timescales of minutes to hours. We present two models for gliding, inspired by the physics and chemistry of the interaction between the NLC and polymer substrate. These models, though simple, lead to non-trivial results, including loss of bistability, a finding that may have implications for display devices.

1Supported by NSF Grant No. DMS-1211713
A novel twisted nematic alignment and its effects on the electro-optical dynamics of nanoscale liquid crystalline films

The Spin Hall Effect dynamics of nanoscale liquid crystalline films

which predicts parameter ranges over which finite-sized rafts are stable. Carlo simulations and a mean field theory to explore the phase diagram of a monolayer of bidisperse rodlike molecules as a function of interparticle interactions engineering. Recent experiments conducted on monolayer membranes composed of two species of chiral rodlike molecules leads to the spontaneous formation

SOFT MATTER THEORY GROUP TEAM — In contrast to bulk liquids or crystals clusters of finite size are rare and their assembly usually requires sophisticated

membranes

Crystal

N

in the twist-bend nematic (N_{tb}) liquid crystalline phase of odd numbered flexible dimer molecules is presented. It is found that the N_{tb} phase is strongly shear-thinning. At shear stresses below 1Pa the apparent viscosity of the N_{tb} phase is 1000 times larger than in the nematic phase. At stresses above 10Pa the N_{tb} viscosity drops by two orders of magnitude and the material exhibits Newtonian fluid behavior. The results are consistent with the behavior of a system with pseudo-layer structure with layer spacing determined by the heliconical pitch. From the measurements of dynamic modulus we estimate the compression modulus of the pseudo-layers to be B ~ 2kPa; this value is discussed within the context of a simple theoretical model based upon a coarse-grained elastic free energy.

3 www.jakligroup.com

4:30PM W50.00011 Second Harmonic Light Scattering Study of a Twist-Bend Nematic Liquid Crystal

1, SHOKIR PARDAEV, JAMES GLEESON, Department of Physics, Kent State University, ANTAL JAKLI, Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State University, SAMUEL SPRUNT, Department of Physics, Kent State University — The twist-bend nematic phase exhibited by certain liquid crystalline dimers has been the subject of intensive recent investigation. In this report we present the results of angle-resolved second harmonic (SH) light scattering measurements from a twist-bend (TB) nematic liquid crystal for various combinations of the fundamental and second harmonic polarizations. These measurements reveal a polarization-dependent pretransitional temperature dependence of the SH signal, as well as an evolution of the SH scattering pattern below the transition (in the TB phase). We will discuss our results in terms of other recent experiments, as well as the current theoretical understanding of the nematic to TB transition and the nature of the TB phase. We thank O. Parri at Merck Chemicals Ltd., Southampton, UK for providing the studied material for us.

A @NSF DMR-0904765 and DMR-1307674.

4:42PM W50.00012 Coarse-grained model and light scattering of the twist-bend nematic phase

1, SHAIKH SHAMID, DAVID ALLENDER, JONATHAN SELINGER, Kent State Univ - Kent — We develop a coarse-grained version of the continuum theory for the twist-bend (TB) nematic phase of liquid crystals. In this theoretical approach, we begin with an ideal, undistorted TB phase, which has a heliconical modulation of the director field. We then calculate the elastic free energy cost of a position-dependent local rotation of the director away from the ideal state. We diagonalize this free energy density to find the eigenmodes of the system. Of these eigenmodes, the soft mode can be regarded as a smectic-like distortion of periodic plates in the TB phase; this mode has effective elastic constants for layer compression and curvature. By comparison, the hard mode involves director variations away from the optimum cone angle. This calculation leads to a prediction for light scattering from the TB nematic phase.

A This work was supported by NSF Grant DMR-1409658.

4:54PM W50.00013 Fullerene (C_{60}) nano-colloids in nematic liquid crystal

1, ANGELO VISCO, KEVIN SOBCZAK, RIZWAN MAHMOOD, Slippery Rock University — We report high resolution homodyne light scattering studies to probe director fluctuations in bend/splay mode in bulk nematic liquid crystal and as a function of fullerene (C_{60}) nanoparticles concentration. The preliminary analysis shows that the relaxation time of these fluctuations is fairly constant with in the experimental uncertainty despite the constraints imposed on the director fluctuations due to the insertion of nano colloids. The relaxation time extracted from the data found to be in nano seconds range and the diffusion constant (D) found to be, D = 4.29 \times 10^{-6} \text{cm/sec}.

1 The authors acknowledge the financial support from grants office, Dean, college of Health, Environment & Science and the physics department.

5:06PM W50.00014 Computational and theoretical analysis of chiral rafts in colloidal membranes

1, RAUNAK SAKHARDANDE, MICHAEL HAGAN, APARNA BASKARAN, BULBUL CHAKRABORTY, Brandeis University, BRANDEIS SOFT MATTER THEORY GROUP TEAM — In contrast to bulk liquids or crystals clusters of finite size are rare and their assembly usually requires sophisticated engineering. Recent experiments conducted on monolayer membranes composed of two species of chiral rodlike molecules leads to the spontaneous formation of thermodynamically stable, rafts with a well-defined finite size. To understand the fundamental forces driving this self-limited assembly, we combine Monte Carlo simulations and a mean field theory to explore the phase diagram of a monolayer of bidisperse rodlike molecules as a function of interparticle interactions and chirality. The simulation demonstrates that differences in chirality between the two rod species can stabilize finite-sized rafts. We present a phase diagram which predicts parameter ranges over which finite-sized rafts are stable.

1 This research was supported by Brandeis-MRSEC

Thursday, March 5, 2015 2:30PM - 5:30PM —
Session W51 DCMP: Invited Session: Recent Advances in Spin Transport: Spin Pumping and the Spin Hall Effect

Grand Ballroom C1 - Thomas Silva, NIST-Boulder
2:06PM W51.00001 Spin Hall effect and spin-transfer torque generated by a topological insulator, DANIEL RALPH, Cornell Univ — No abstract available.

3:06PM W51.00002 Electrical detection of current-induced spin polarization due to spin-momentum locking in the topological insulator Bi$_2$Se$_3$, BEREND JONKER, Naval Research Laboratory — Topological insulators (TIs) exhibit topologically protected metallic surface states populated by massless Dirac fermions with spin-momentum locking — the carrier spins lie in-plane, locked at right angle to the carrier momentum. An unpolarized charge current should thus create a net spin polarization whose amplitude and orientation are controlled by the charge current. Here we show direct electrical detection of this bias current induced spin polarization as a voltage measured on a ferromagnetic (FM) metal tunnel barrier surface contact [1]. The magnetization of the contact determines the spin detection axis, and the voltage measured at this contact is proportional to the projection of the TI spin polarization onto this axis. When the charge current is orthogonal to the magnetization of the FM detector contact, the TI spin is parallel (or antiparallel) to the magnetization, and a spin-related signal is detected at the FM contact proportional to the magnitude of the charge current. The voltage measured scales inversely with Bi$_2$Se$_3$ film thickness, and its sign is that expected from spin-momentum locking and opposite that of a Rashba effect [2]. Similar data are obtained for two different FM contact structures, Fe/Al$_2$O$_3$ and Co/MgO/graphene, underscoring the fact that these behaviors are due to bias current induced spin polarization in the TI surface states rather than the bulk, and are independent of the details of the contact. These results demonstrate simple and direct electrical access to the TI Dirac surface state spin system, provide clear evidence for the spin-momentum locking and bias current-induced spin polarization, and enable utilization of these remarkable properties for future technological applications.


This work is supported by core programs at NRL and the Office of Naval Research.

3:42PM W51.00003 Spin pumping and spin-transfer torques in antiferromagnet, QIAN NIU, The University of Texas at Austin — Spin pumping and spin-transfer torques are key elements of coupled dynamics of magnetization and conduction electron spin, which have been widely studied in various ferromagnetic materials. Recent progress in spintronics suggests that a spin current can significantly affect the behavior of an antiferromagnetic material [1], and the electron motion become adiabatic when the staggered field varies sufficiently slowly [2]. However, pumping from antiferromagnets and its relation to current-induced torques is yet unclear. In a recent study [3], we have solved this puzzle analytically by calculating how electrons scatter off a normal metal-antiferromagnetic interface. The pumped spin and staggered spin currents are derived in terms of the staggered field, the magnetization, and their rates of change. We find that for both compensated and uncompensated interfaces, spin pumping is of a similar magnitude as in ferromagnets; the direction of spin pumping is controlled by the polarization of the driving microwave. Via the Onsager reciprocity relations, the current-induced torques are also derived, the salient feature of which is illustrated by a terahertz nano-oscillator.


In collaboration with Ran Cheng, Jiang Xiao, and A. Brataas.

4:18PM W51.00004 Pure Spin Current in a broad range of materials generated by YIG-based spin pumping, FENGYUAN YANG, The Ohio State University — Spintronics relies on the generation, manipulation, and detection of spin current mediated by itinerant charges or magnetic excitations. FMR spin pumping is a powerful technique in understanding pure spin current. Building on our high-quality Y$_3$Fe$_5$O$_{12}$ (YIG) films and the large inverse spin Hall effect (ISHE) signals enabled by these films [1-10], we have characterized spin currents in several classes of materials with different magnetic structures, including: nonmagnetic and ferromagnetic metals, nonmagnetic insulators, and antiferromagnetic (AF) insulators. The spin Hall angles determined for a series of 3d, 4d, and 5d metals show that both atomic number and d-electron count play important roles in spin Hall physics [1, 6]. Strikingly, we achieved robust spin transport from YIG to Pt across AF insulators, which initially enhances the ISHE signals and can transmit spin currents up to 100 nm thickness, demonstrating highly efficient spin transport through an AF insulator carried by magnetic excitations [3].


This work is supported by DOE (Grant # DE-FG02-03ER46054 and # DE-SC0001304) and NSF MRSEC (grant # DMR-124051).

4:54PM W51.00005 The essential role of spin-memory loss at 3d/5d metallic interfaces in spin pumping, HENRI JAFFRES, Unite Mixte de Physique CNRS-Thales — I will present a review of experiments and theory of spin-pumping in Co/(Cu)/Pt 3d/5d metallic systems in the ferromagnetic resonance (FMR) regime of spin injection [1]. By combining i) FMR analyses of the resonance linewidth of the Co spectra in contact with the Pt (or Cu/Pt) reservoir and ii) detection of the inverse spin-hall effect signal vs. Pt thickness, we were able to evidence two different length scales for the spin-current profile generated or absorbed at the interfaces [2]. The first length scale, extracted from FMR analyses and of the order of 2 nm, represents a typical interface length characteristic of a spin memory loss at the Co/Pt and Co/Cu/Pt interfaces. This represents a typical region of spin-current dissipation by which almost 60-70% of the total current generated is lost before conversion in bulk Pt. The second length scale, roughly equal to 3.4 nm, like determined by Inverse Spin Hall Effect (ISHE) transverse voltage measurement, is more characteristic of the spin-diffusion length of the bulk Pt that governs a part of the spin-to-chargetransfer efficiency by ISHE. After careful analyses, we determined a spin-hall angle of 5.6% for Pt and an intrinsic spin hall conductivity of 3200 (Ohm cm)$^{-1}$ for our corresponding Pt resistivity [2]. In the end, I will focus on the physical description of our experiments within a derived Valet-Fert model describing the spin transport/relaxation in a diffusive approach and using relevant boundary conditions for spin-pumping (constant spin accumulation in the ferromagnet). The origin of the spin-memory loss and spin-current discontinuity, also proposed in a very recent work [3], will be explained in terms of atomic intermixing at interfaces or possible Rashba-split states at Co/Pt interfaces.

2:30PM W52.00001 Preparation and measurement of strongly interacting states of photons. MOHAMMAD HAFEZI, Joint Quantum Institute — Photons has been considered as a promising medium to implement quantum simulators. However, most phenomena that are interesting from quantum simulation perspective involve thermalization and a controllable chemical potential, as a key parameter in phase diagrams, which are both absent for photons. More specifically, on the one hand, photonic systems are dissipative which means that the chemical potential is zero, and on the other hand, due to the weakness of inelastic scatterings, photons do not naturally thermalize. I will discuss various externally driven schemes to prepare many-body states of photons in the presence of dissipation. In fact, such driven-dissipative nature of these systems is the crucial reason of their interest. Specifically, I investigate driven fractional quantum Hall and Bose-Hubbard models. Furthermore, I describe how to characterize and measure various many-body features of correlated states of photons.

3:06PM W52.00002 Confining the state of light to a quantum manifold by engineered two-photon loss. ZAKI LEHTHAS, Yale University — Physical systems usually exhibit quantum behavior, such as superpositions and entanglement, only when they are sufficiently decoupled from a lossy environment. Paradoxically, a specially engineered interaction with the environment can become a resource for the generation and protection of quantum states. This notion can be generalized to the confinement of a system into a manifold of quantum states, consisting of all coherent superpositions of multiple stable steady states. We have experimentally confined the state of a harmonic oscillator to the quantum manifold spanned by two coherent states of opposite phases. In particular, we have observed a Schrödinger cat state spontaneously squeeze out of vacuum, before decaying into a classical mixture. This was accomplished by designing a superconducting microwave resonator whose coupling to a cold bath is dominated by photon pair exchange. This experiment opens new avenues in the fields of nonlinear quantum optics and quantum information, where systems with multi-dimensional steady state manifolds can be used as error corrected logical qubits.

3:42PM W52.00003 Blueprint for an analog quantum code fabric. ELIOT KAPIT, The Graduate Center, City University of New York — A physical realization of self correcting quantum code would be profoundly useful for constructing a quantum computer. In this theoretical talk, we provide a partial solution to major challenges preventing self correcting quantum code from being engineered in realistic devices. We consider a variant of Kitaev’s toric code coupled to propagating bosons, which induce a long-ranged interaction between anyonic defects. By coupling the primary quantum system to an engineered dissipation source through resonant energy transfer, we demonstrate a “rate barrier” which leads to a potentially enormous increase in the system’s quantum state lifetime through purely passive quantum error correction, even when coupled to an infinite temperature bath. While our mechanism is not scalable to infinitely large systems, the maximum effective size can be very large, and it is fully compatible with active error correction schemes. Our model uses only on-site and nearest-neighbor interactions, and could be implemented in superconducting qubits.

4:18PM W52.00004 Topology by Dissipation in Atomic Fermion Systems. SEBASTIAN DIEHL, TU Dresden — Controlled dissipation can be used as a resource to drive a many-body system into quantum mechanically ordered states from an arbitrary initial one. We discuss this concept in the context of atomic fermions, highlighting a dissipatively induced pairing mechanism, which is operative in the absence of attractive forces. We show how this targeted cooling can be utilized to cool atomic fermions into topologically non-trivial states in one dimension by quasi-local dissipative operations, and point out a possible physical implementation. This realizes a dissipative analog of the ground state of Kitaev’s quantum wire. In higher dimensions, the analogy to Hamiltonian ground states breaks down due to a fundamental incompatibility of topology and locality. We present a new quasi-local dissipative mechanism for the preparation of Chern insulators, which bypasses these obstacles by making use of the intrinsic open system character of the preparation process, with no Hamiltonian counterpart. This greatly extends the scope of efficiently attainable topological symmetry classes via tailored dissipation.

4:54PM W52.00005 Real-time observation of fluctuations in a driven-dissipative quantum many-body system undergoing a phase transition. TOBIAS DONNER, Institute for Quantum Electronics, ETH Zürich — A Bose-Einstein condensate whose motional degrees of freedom are coupled to a high-finesse optical cavity via a transverse pump beam constitutes a dissipative quantum many-body system with long range interactions. These interactions can induce a structural phase transition from a flat to a density-modulated state. The transverse pump field simultaneously represents a probe of the atomic density via cavity-enhanced Bragg scattering. By spectrally analyzing the light field leaking out of the cavity, we measure non-destructively the dynamic structure factor of the fluctuating atomic density while the system undergoes the phase transition. An observed asymmetry in the dynamic structure factor is attributed to the coupling to dissipative baths. Critical exponents for both sides of the phase transition can be extracted from the data. We further discuss our progress in adding strong short-range interactions to this system, in order to explore Bose-Hubbard physics with cavity-mediated long-range interactions and self-organization in lower dimensions.

Thursday, March 5, 2015 2:30PM - 5:30PM –
Session W53 DCMP: Invited Session: Discoveries in SrTiO3 Grand Ballroom C3 - Chris Leighton, University of Minnesota

2:30PM W53.00001 Multiband superconductivity in n-doped SrTiO3. KAMRAN BEHNIA, ESPCI — The superconducting state of n-doped SrTiO3 occupies a singular place in the history of superconductivity. Besides being the first oxide superconductor, it was one of the earliest “semiconducting superconductors,” the first experimentally-detected multi-gap superconductor and the first case of a superconducting dome. Half a century after its discovery, it remains the most dilute superconductor [1]. We present a systematic study of quantum oscillations and superconducting transition in doped SrTiO3, over a wide range of carrier concentration from 10¹⁷ to 10²⁸ cm⁻³ [2]. Mobile carriers were introduced either by removing oxygen or by substituting Ti by Nb. Superconductivity was found to persist down to an exceptionally low concentration of mobile electrons (n=3.10¹⁷ cm⁻³ and Tc ≈ 3.4 mK). At this concentration range, with the Fermi temperature below 10 K, the narrowness of the relevant energy window severely restricts possible pairing scenarios. We identify two critical doping levels, which are the filling thresholds of the upper conduction bands. This clarifies the limits of single-band, two-band and three-band superconducting regimes. We find that the exceptionally-wide superconducting dome of SrTiO₃ has a structure with two distinct domes, each peaking near a critical doping level. Thermal conductivity measurements uncover the existence of multiple nodeless superconducting gaps at optimal doping [3].

3:06PM W53.00002 Doping and Hall effect in SrTiO$_3$. SUSANNE STEMMER, University of California, Santa Barbara — Electron-doped SrTiO$_3$ has generated renewed interest because of reports of coexisting magnetism and superconductivity, and of superconducting transitions at extremely low carrier densities. In this talk, we will present new insights into doping and its electronic structure obtained using very high quality SrTiO$_3$ films grown by molecular beam epitaxy. We discuss the arrangements and imaging of individual La dopant atoms and clusters using quantitative scanning transmission electron microscopy. We present studies of the temperature dependence of the Hall coefficient, Hall mobility, and of Shubnikov-de Haas oscillations. We will particularly discuss the significance of the regime in which the resistance follows a $T^2$ temperature-dependence over a wide range of temperatures and doping. This work was performed in collaboration with Evgeny Mikheev, Adam Kajdos, Jinwoo Hwang, Jack Zhang, and Jim Allen.

3:42PM W53.00003 Optically-Induced Persistent Magnetization in Oxygen Deficient Strontium Titanate, SCOTT CROOKER, National High Magnetic Field Laboratory — Interest in electrons and spintronics based on complex oxide materials has exploded in recent years, fueled by the ability to grow atomically-precise heterostructures of various oxides [1]. A foundational material in this burgeoning field is strontium titanate, a (nominally) non-magnetic wide-bandgap semiconductor. Owing to its ubiquity in oxide materials science, studies of SrTiO$_3$’s interesting dielectric, lattice, and optical properties represent mature research areas. However, renewed interest in SrTiO$_3$ was recently sparked by observations of unexpected spin and magnetization phenomena at interfaces between SrTiO$_3$ and other nonmagnetic oxides [1]. The formation and distribution of oxygen vacancies ($V_O$) in SrTiO$_3$ are widely thought to play an essential but as-yet-ineffectively understood role in these emergent phenomena. Here we demonstrate a surprising new aspect to the phenomenology of magnetism in SrTiO$_3$ by reporting the observation of an optically-induced and persistent magnetization in slightly oxygen-deficient SrTiO$_{3-\delta}$ bulk crystals, using magnetic circular dichroism spectroscopy and optically-coupled SQUID studies [2]. This magnetism appears below 18K, persists for hours below 10K, and is tunable via the polarization and wavelength of sub-bandgap (400-500 nm) light. As such, magnetic patterns can be “written” into SrTiO$_{3-\delta}$, and subsequently read out, using light alone. This magnetism occurs only in crystals containing $V_O$, and is consistent with a metastable spin polarization of $V_O$-related defect complexes. These data reveal a detailed interplay between magnetism, lattice defects, and light in an archetypal complex oxide material, which may yield new insights into the recent exciting spin physics observed at oxide interfaces.


4:18PM W53.00004 ABSTRACT WITHDRAWN —

4:54PM W53.00005 Spectroscopic findings in SrTiO$_3$ applications: LaAlO$_3$/SrTiO$_3$ and La$_{0.5}$Sr$_{0.3}$MnO$_3$/SrTiO$_3$ heterostructures, JUN-SIK LEE, SSRL, SLAC National Accelerator Laboratory — Recently, a number of transport and magnetization studies have shown signs of exotic functionalities in SrTiO$_3$ based heterostructures, which are totally unexpected properties with no bulk analog in the constituent materials. However, it is still early stage to understand such a functionality, which limits improving SrTiO$_3$ transport and magnetization studies have shown signs of exotic functionalities in SrTiO$_3$ applications: LaAlO$_3$/SrTiO$_3$ and La$_{0.5}$Sr$_{0.3}$MnO$_3$/SrTiO$_3$ heterostructures. These findings establish a striking example of emergent phenomena at oxide interfaces. In this presentation, I will introduce more details of spectroscopic findings on those heterostructures.

Thursday, March 5, 2015 5:30PM - 7:00PM —
Session X1 APS: Science Film: An Aperture into Science Advocacy — Grand Hyatt San Antonio Presidio

5:30PM X1.00001 Science Film: An Aperture into Science Advocacy — The current funding environment for scientific research necessitates a change in how we foster support for the endeavor. Federal spending is not likely to grow unless constituents—APS members—help communicate the value of science to members of Congress and the public in a compelling and individual way. The event explores how popular film with science-based plots can help physicists communicate the value of science to members of Congress and an increasingly diverse electorate.

Friday, March 6, 2015 8:00AM - 11:00AM —
Session Y1 DMP: Focus Session: Graphene - Multilayer and Interfacial Effects — University of Northern Iowa

8:00AM Y1.00001 The decoupling of epitaxial graphene on SiC by hydrogen intercalation: an ab initio study. LYDIA NEMEC, Fritz-Haber-Institut der MPG, Berlin, DE; PATRICK RINKE, Fritz-Haber-Institut der MPG, Berlin, DE; Aalto University, Helsinki, FI; VOLKER BLUM, Duke University, Durham, NC, USA; MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, DE — Large-scale ordered epitaxial graphene can be grown on various substrates, out of which silicon carbide (SiC) is one of the most promising. The exact material properties of graphene depend on the growth conditions and its interaction with the substrate. By hydrogen intercalation of epitaxial graphene on the Si-face of SiC the graphene layer decouples from the substrate forming quasi-free-standing monolayer graphene (QFMLG) [1]. We performed an density functional theory study of QFMLG on the polar 6H-SiC(0001) surface based on a van der Waals corrected semi-local exchange-correlation functional using the all-electron numeric atom-centered basis function code FHI-aims. We find an adsorption height in excellent agreement with X-ray standing wave experiments, a very low buckling of the graphene layer, and a very homogeneous electron density at the interface. All these features improve the electronic properties of QFMLG compared to epitaxial graphene. Using the insight gleaned on the Si-face, we present the structure of a hypothetical QFMLG phase on the C-face of SiC. We find that hydrogen intercalation is a promising option to control the SiC-graphene interface. [1] C. Riedl, et. al, PRL 103, 246804 (2009).
8:12AM Y1.00002 Lithium Intercalation of Few-Layer Graphenes in the 2-Layer Limit , SHU YANG FRANK ZHAO, Dept. of Physics, Harvard University, GISELLE A. ELBAZ, Dept. of Chemistry, Columbia University, DIMITRI K. EFETOV, Dept. of Physics, MIT, JAYAKANTH RAVICHANDRAN, Dept. of Physics, Harvard University, YINSHENG GUO, LOUIS BRUS, XAVIER ROY, Dept. of Chemistry, Columbia University, PHILIP KIM, Dept. of Physics, Harvard University — Few layer graphene (FLG) intercalate compounds form a new generation of graphene derivative systems where carrier densities are expected to reach $6E14$ cm$^{-2}$ per graphene layer, and novel physical phenomena such as superconductivity and magnetism may emerge. Experimental realization of intercalated FLGs have been limited by harsh intercalation processes which are often incompatible with mesoscopic device fabrication techniques. We developed techniques to electrochemically intercalate FLGs down to 2-layers with lithium in-situ in a controlled manner, minimizing sample degradation from parasitic reactions in the electrolyte by passivating sample surfaces using a combination of hBN (over graphene) and photoresist (over metal contacts). By performing simultaneous Raman spectroscopy as the FLGs intercalate, we found that as FLGs reached the 2-layer limit, the Raman signatures of intercalation began to deviate from that of bulk graphite.

8:24AM Y1.00003 Electronic Structure of Single-Crystal Monolayer Graphene on Hydrogen-Terminated Germanium Surface, SUNG JOON AHN, JAE-HYUN LEE, JOUNG REAL AHN, DONGMOK WHANG, Sungkyunkwan Univ — Graphene, atomically flat 2-Dimensional layered nano material, has a lot of interesting characteristics from its unusual electronic structure. Almost properties of graphene are influenced by its crystallinity, therefore the uniform growth of single crystal graphene and layer control over the wafer scale areas remains a challenge in the fields of electronic, photonic and other devices based on graphene. Here, we report the method to make wafer scale single crystal monolayer graphene on hydrogen terminated germanium(110) surface and properties and electronic band structure of the graphene by using the tool of scanning electron microscopy, transmission electron microscopy, Raman spectroscopy, electron transport measurement, electron diffraction and angle-resolved photoemission spectroscopy.

8:36AM Y1.00004 Formation and electronic properties of coherent in-plane 2D heterostructures1, AN-PING LI, Oak Ridge National Lab — Two-dimensional (2D) interfaces between crystalline materials have been shown to generate unusual interfacial electronic states in complex oxides. Recently, a one-dimensional (1D) interface has been suggested in hexagonal boron nitride (hBN) and graphene planar heterostructures, where a polar-on-nonpolar 1D boundary is expected to possess peculiar electronic states associated with edge states of graphene and the polarity of hBN. Here, we report on the formation and electronic properties of such a 1D interface. By implementing the concept of epitaxy to 2D space, we grow monolayer hBN from fresh edges of monolayer graphene with lattice coherence, forming a 1D boundary [L. Liu et al., Science 343, 163 (2014)]. Scanning tunneling microscopy and spectroscopy measurements reveal an abrupt 1D zigzag oriented boundary, with boundary states about 0.6 eV below or above the Fermi level depending on the termination of the hBN at the boundary [J. Park et al., Nature Commun. 5, 5403 (2014)]. The boundary states are extended along the boundary, and exponentially decay into the bulk of graphene and hBN. The origin of boundary states and the effect of the polarity discontinuity at the interface will be discussed.

1This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

9:12AM Y1.00005 Defect-Stabilized Graphene-Based Organometallic Sandwich Structures, PRATIBHA DEV, THOMAS REINECKE, Naval Research Laboratory, Washington, D.C. — Benzene-transition metal-graphene (Bz—M—Gr) sandwich structures are of interest for a range of applications such as catalysis, spintronics and quantum computing. Although they are predicted to form in several theoretical works, it has proven harder to create these complexes experimentally. Using density functional theory, we propose a chemical route to creating stable Bz—M—Gr sandwich structures. Acceptor-type defects, such as carbon vacancies and pyridinic nitrogen substituents in graphene are used to immobilize the metal onto graphene. It has proven harder to create these complexes experimentally. Using density functional theory, we propose a chemical route to creating stable Bz—M—Gr sandwich structures. Acceptor-type defects, such as carbon vacancies and pyridinic nitrogen substituents in graphene are used to immobilize the metal onto graphene. Placement of a benzene ring atop the metal atom further stabilizes the structure against oxidation. Structural, electronic and magnetic properties of the Bz—M—Gr complexes vary for different defects. High cohesive energies and spin polarization energies make defect-stabilized Bz—M—Gr complexes of interest for use as nanomagnets in ambient conditions.

9:24AM Y1.00006 Single-Valley Engineering in Graphene Superlattices, YAFEI REN, XINZHOU DENG, Univ of Sci & Tech of China, CHANGSHENG LI, Hunan Univ of Art & Sci, JIEJ JUNG, Nat Univ of Singapore, CHANGGAN ZENG, ZHENYU ZHANG, Univ of Sci & Tech of China, QIAN NIU, Univ of Texas at Austin; Peking Univ, ZHENHUA QIAO, Univ of Sci & Tech of China — The two inequivalent valleys in graphene preclude the protection against inter-valley scattering offered by an odd-number of Dirac cones characteristic of topological insulator phases. Here we propose a way to engineer a chiral single-valley phase in a honeycomb lattice via folding K and K′ periodic patterning of the carbon isotope. We consider the difference of pure 12C graphene and 13C graphene. Although they are predicted to form in several theoretical works, it has proven harder to create these complexes experimentally. Using density functional theory, we propose a chemical route to creating stable Bz—M—Gr sandwich structures. Acceptor-type defects, such as carbon vacancies and pyridinic nitrogen substituents in graphene are used to immobilize the metal onto graphene. Placement of a benzene ring atop the metal atom further stabilizes the structure against oxidation. Structural, electronic and magnetic properties of the Bz—M—Gr complexes vary for different defects. High cohesive energies and spin polarization energies make defect-stabilized Bz—M—Gr complexes of interest for use as nanomagnets in ambient conditions.

9:36AM Y1.00007 Polycrystalline Graphene with Single Crystal Electronic Structure, EDWARD B. LOCHOCKI, LOLA BROWN, Cornell University, JOSÉ AVILA, SOLEIL Synchrotron, CHEOL-JOO KIM, YUI OGAWA, ROBIN W. HAVENER, DONG-KI KIM, ERIC J. MONKMAN, DANIEL E. SHAI, HAOFEI I. WEI, MARK P. LEVENDORF, Cornell University, MARIA ASENSIO, SOLEIL Synchrotron, JIWOONG PARK, KYLE SHEN, Cornell University — Stacking two-dimensional materials is a promising method for creating and controlling vertical heterostructures with atomic precision. The relative rotation angles between layers can sensitively tune these structures’ electronic and optical properties, so constituent layers with well-defined lattice orientations are critical for any practical application. Here we report the growth of large scale graphene and hexagonal boron nitride on commercial copper foils, where the resulting films display multiple nucleations yet exhibit a uniform orientation. We characterize the copper and graphene lattices on sizes ranging from nanometers to several centimeters using a multitude of probes including dark field transmission electron microscopy and angle-resolved photoemission spectroscopy. These measurements reveal that each individual graphene grain exhibits an identical electronic structure and orientation consistent with single crystalline graphene. Finally, we create stacked bilayer graphene with a homogeneous interlayer rotation angle, demonstrating a versatile approach for scalable fabrication of layered superlattices with accurate structures.

9:48AM Y1.00008 Isotope dependence of the electronic structure in graphene, TAKASHI KORETSUNE, RIKEN CEMS, SUSUMU SAITO, Tokyo Institute of Technology — It has been known that the effect of electron-phonon couplings on the electronic structure of diamond is not negligible and recently, it has been confirmed that the experiments are well reproduced using first-principles calculations. In case of graphene, the renormalization of the Fermi velocity due to the electron-phonon couplings has been predicted. Thus, we theoretically study the possibility of band structure engineering in graphene using the electron-phonon couplings and the isotope effect. First, we consider the difference of pure 12C graphene and 13C graphene. On the basis of density functional theory, it is found that the depth of so-called Dirac point, that is, work function of graphene, shows isotope dependence, indicating that it is possible to shift the depth of the Dirac point locally without using a gate voltage. We also discuss the possibility of band-gap opening by a periodic patterning of the carbon isotope.

1Supported by the MEXT 25104711 and 25107005.
10:24AM Y1.00011 Dirac Cone Metric and the Origin of the Spin Connections in Monolayer Graphene , BO YANG, Institute of High Performance Computing — There have been extensive efforts in modeling the strain and ripples of the monolayer graphen sheet in the form of the effective gauge fields, both from a microscopic point of view and from the quantum field theoretical (QFT) approach used in treating Dirac spinors moving in a curved space (M.A.H. Vozmediano et.al, Phys. Rep. 496, 109, F. Guinea et.al, Nat. Whys. 6, 30). With the QFT approach, it is argued that the metric from either the two-dimensional manifold of graphene sheet or from the in-plane strain field introduces a spin connection that couples to the sublattice pseudospin. Yet the microscopic origins of such an analogy, and the nature of the “spin connection” that couples to the sublattice pseudospin, was not clear. We solve this issue by showing that the modulation of the hopping amplitudes in the honeycomb lattice of the monolayer graphene uniquely defines a metric which corresponds to the geometry of the Dirac cone. This effective metric is different from the real space metric of the crystal lattice, and is entirely the property of the fermi surface. We show how the exact spin connection of this momentum space effective metric field can be calculated from the microscopic tight-binding Hamiltonian, and discuss its experimental implications.

10:36AM Y1.00012 ABSTRACT WITHDRAWN —

10:48AM Y1.00013 Electronic Properties of Graphene in Strong Static Electric Field1, VADYM APALKOV, HAMED KOOCHAKI KELARDEH, MARK STOCKMAN, Georgia State Univ — We study the dynamics of electrons in an ultra-strong static electric field (a few V/Å) and obtain an analytical solution for the Wannier-Stark (WS) states and corresponding energy spectrum of graphene within the two-band tight binding model. Electron states in graphene have a WS ladder structure with energy levels separated by the Bloch frequency, which is proportional to both the electric field and the lattice period of graphene in the direction of electric field. The strength of the band mixing is determined by the magnitude of the interband dipole matrix element, which for graphene has distinct wave vector dependence seen neither in metals nor in insulators. Namely, at the Dirac points, the dipole matrix elements have sharp peaks due to strong interband coupling leading to redistribution of carrier density and very strong mixture of conduction and valence bands whereas, away from the Dirac point, it shows a broad maximum. As a result of such mixing, the energy spectrum of graphene shows anticrossing points, which are characterized by the corresponding anticrossing gaps. It is shown that the anticrossing gaps are proportional to electric field at the corresponding anticrossing points with the calculated values 2.54/I (eV), where I=1,2,... is the order of the anticrossing point. The largest anticrossing gap ≈ 2.54 eV corresponds to the anticrossing point I = 1 at the electric field ≈ 3.59 V/Å. The achieved results will promisingly draw further attentions toward graphene-based Field Effect Transistors (g-FET).

1The Grant was provided by Naval Research Office N00014-13-1-0649.
This technique show that small polarons can indeed be formed in thin layers. Comparisons with polarons in the bulk and with experiments will be discussed.

To prevent this, we modified the charge of the pseudopotentials, thus providing charge compensation that is confined within the layer. Our results obtained with neutralizing charge needs to be included in supercell calculations. The use of a jellium background leads to divergence problems in low-dimensional systems. To study and applying the MX2, the growth of high-quality MX2 thin film with precise control of layers thickness is favorable. Here we report the molecular beam epitaxial growth of WSe2 thin film, with controllable thickness from monolayer to 8 monolayer. By using in-situ angle-resolved photoemission spectroscopy, we experimented revealing the valence band evolution with film thickness. By applying the potassium doping on the surface, we observed the indirect to direct band gap transition in monolayer WSe2, and the distorted band structure. Combining the ex-situ photoluminescence and scanning tunneling spectroscopy, we further presented the giant band gap renormalization and excitonic effects. Our results will enrich the understanding of WSe2, and bring it more application potential in practical devices.

Electronic properties, Band Gap Renormalization, and Doping Effect in Epitaxial WSe2 thin film, YI ZHANG, Stanford University, MIGUEL UGEDA, SU-FEI SHI, UC Berkeley, BO ZHOU, YEONGKWAN KIM, LBNL, YULIN CHEN, University of Oxford, FENG WANG, MICHAEL CROMMIE, UC Berkeley, ZAHID HUSSAIN, LBNL, ZHI-XUN SHEN, Stanford University, SONG-KWAN MO, LBNL — As a class of graphene-like two-dimensional materials, the layered metal dichalcogenides MX2 (M = Mo, W; X = S, Se, Te) have gained significant interest due to the distinct properties in 2D limit. Examples include the indirect to direct band gap transition in monolayer, and giant spin-splitting of the valence band. These properties give MX2 great application potentials in both optoelectronic and spintronics devices. For practically studying and applying the MX2, the growth of high-quality MX2 thin film with precise control of layers thickness is favorable. Here we report the molecular beam epitaxial growth of WSe2 thin film, with controllable thickness from monolayer to 8 monolayer. By using in-situ angle-resolved photoemission spectroscopy, we experimented revealing the valence band evolution with film thickness. By applying the potassium doping on the surface, we observed the indirect to direct band gap transition in monolayer WSe2, and the distorted band structure. Combining the ex-situ photoluminescence and scanning tunneling spectroscopy, we further presented the giant band gap renormalization and excitonic effects. Our results will enrich the understanding of WSe2, and bring it more application potential in practical devices.

Charge Carrier Transport Properties in Layered Structure of Hexagonal Boron Nitride (h-BN) and Thermal Neutron Detection Based on h-BN, TRI DOAN, SAMUEL GRENAUDIER, SASHIKHANTH MAJETY, JING LI, JINGYU LIN, HONGXING JIANG, Texas Tech Univ, NANOPHOTONICS CENTER - TEXAS TECH UNIVERSITY TEAM — Hexagonal boron nitride (h-BN) epilayers have been synthesized by MOCVD. It was found that the carrier mobility in h-BN epilayers is strongly dependent on the stability of such polarons in bulk GaO3 thin film. The measured carrier mobility-lifetime (µτ) product of h-BN thin films grown on sapphire substrate is 2.83 x 10^7 cm^2/Vs for electrons and holes, which is comparable to that of GaN films grown on sapphire. Thermal neutron detectors based on h-BN epilayers were fabricated and the reaction product pulse-height spectra were measured under thermal neutron irradiation produced by 252Cf source. It was shown that h-BN thin film thermal neutron detectors are capable to resolve specific nuclear reaction products with unprecedentedly high energy resolution.

Polarons in thin GaO3 layers, HARTWIN PEELAERS, University of California, Santa Barbara, JOEL B. VARLEY, Lawrence Livermore National Laboratory, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — GaO3 has a large band gap of 4.9 eV, making it transparent in the UV. It can also be doped n-type, enabling applications as a transparent conductor or in power electronics. The optical properties of GaO3 may be affected by the formation of small polarons, i.e., localized holes trapped by a lattice distortion. First-principles calculations have established the stability of such polarons in bulk GaO3 [J. B. Varley et al., Phys. Rev. B 85, 081109(R) (2012)]. Here we investigate hole polarons in nanomembranes of GaO3. We perform first-principles calculations based on density functional theory using a hybrid functional. Since polarons correspond to positive charges, a neutralizing charge needs to be included in supercell calculations. The use of a jelly background leads to divergence problems in low-dimensional systems. To prevent this, we modified the charge of the pseudopotentials, thus providing charge compensation that is confined within the layer. Our results obtained with this technique show that small polarons can indeed be formed in thin layers. Comparisons with polarons in the bulk and with experiments will be discussed.

Monolayer MoSe2/WSe2 heterojunctions at the atomic level, ANA M. SANCHEZ, Department of Physics, University of Warwick — While graphene is the most studied two-dimensional (2D) material, atomically thin layered transition metal dichalcogenides (TMDs) have recently emerged as a new class of 2D nanomaterials. Due to their band structure, monolayers of direct band gap semiconductor TMDs have promise to complement the zero bandgap energy of graphene, offering extensive range of applications in electronics and optics. The dichalcogenide heterojunctions were grown by physical vapor transport. Lateral heteroepitaxy was visible in an optical microscope and the structures showed enhanced photoluminescence. Atomically resolved transmission electron microscopy using a double-corrected ARM200F (80-200kV) revealed that the MoSe2/WSe2 heterojunction is an undistorted honeycomb lattice in which substitution of one transition metal by another occurs across the interface [1]. There were no dislocations or grain boundaries, i.e. an atomically seamless MoSe2/WSe2 semiconductor junction was achieved. Moreover, strain mapping of atomic resolution images demonstrates negligible distortion at the heterojunction, and the analysis of the different atomic species demonstrates that the interface has a finite width similar to 3D heterojunctions. Vertical stacking of MoSe2/WSe2 bilayers was also analyzed using electron microscopy. An analysis of the intensity in annular dark field images shows that Se atoms of the WSe2 layer align with the Mo atoms of the MoSe2 layer in some of these heterojunctions. We expect that the growth of these lateral junctions will open new device functionalities, such as in-plane transistors and diodes integrated within a single atomically thin layer [1,2,3].

1 C. Huang et al. Nat. Mater. 13 (2014) 1096
2 Y. Gong et al. Nat. Mater. 13 (2014) 1135
3 G.S. Duesberg Nat. Mater. 13 (2014) 1075
9:48AM Y2.00008 Energy band structure of bulk and monolayer vanadium pentoxide (V$_2$O$_5$) beyond the quasiparticle self-consistent GW approximation: lattice polarization effects$^1$. CHURNA BHANDARI, WALTER R.L. LAMCRECHT, Department of Physics, Case Western Reserve University, MARK VAN SCHILFGAARDE, King’s College, London — The quasiparticle self-consistent GW method (QSGW) is known to systematically overestimate the band gaps in semiconductors by about 20\% due to the underestimate of screening by the random phase approximation (RPA). We show that for V$_2$O$_5$, a layered oxide material, the overestimate is significantly larger. The smallest direct gap in QSGW is found to be 4.83 eV compared to 2.35 eV experimentally. The evidence for the experimental gap and optical properties are reviewed. We suggest that a major contribution to the self-energy reduction results from the lattice polarization contribution to the dielectric screening. This results from the large LO/TO splittings in this material. We make a simple estimate of the reduction of $\Gamma$ ($\gamma=0, \omega=0$), and obtain a factor $\sim 0.38$, which if assumed to apply for all $\Gamma$ and reduces the gap to 2.60 eV. The remainder of the gap overestimate is tentatively ascribed to shortcomings of the RPA. We also consider the band structure of this material in monolayer form. We find that the GW correction depends strongly on the layer separation (L) as 1/L. The lattice polarization itself depends on distance between the layers because of the dependence of the phonons on the long-range Coulomb interactions and hence reduced screening in a 2D system.

$^1$Supported by DOE, AFSOR, Simons Foundation.

10:00AM Y2.00009 Observation of Piezoelectricity in Free-standing Monolayer Molybdenum Disulfide, HANYU ZHU, YUAN WANG, JUN XIAO, MING LIU, SHAOMIN XIONG, ZI JING WONG, ZILIANG YE, YU YE, XIAOBO YIN, XIANG ZHANG, Univ of California - Berkeley — Piezoelectricity offers precise and robust conversion between electricity and mechanical force, which originates from the broken inversion symmetry of atomic structure. Yet reducing the size of bulk piezoelectric materials to single molecular layer was challenging, since the surface energy can cause piezoelectric structures to be thermodynamically unstable. Here we report experimental evidence of piezoelectricity in free-standing single layer of molybdenum disulfide (MoS$_2$) crystal, with measured piezoelectric coefficient $e_{31} = 2.9 \times 10^{-10}$ C/m. The free-standing measurement of the intrinsic piezoelectricity is free from the substrate effects, such as doping and parasitic charge. We observed oscillation of piezoelectric response in MoS$_2$ in odd and even number of layers due to breaking and recovery of inversion symmetry, respectively, in sharp contrast to bulk piezoelectric materials. Through the angular dependence of electro-mechanical coupling, we uniquely determined the 2D crystal orientation. The piezoelectricity discovered in single molecular membrane promises new applications in low-power logic switch and ultrasensitive sensors scaled down to single atomic unit cell — the ultimate material limit.

10:12AM Y2.00010 Air Stability of Two-Dimensional Transition Metal Dichalcogenides, SAN-TOSH KC, ROBERTO LONGO, RAFIK ADDOU, Univ of Texas, Dallas, DIEGO BARRERA, Univ of Texas, Dallas, Centro de Investigación en Materiales Avanzados, México, JULIA W.P. HSU, ROBERT M. WALLACE, KYEONGJAE CHO, Univ of Texas, Dallas — Layered transition metal dichalcogenides (TMDs) have emerged as a potential alternative channel material for ultra-thin and low power nanoelectronics. Highly tunable and unique electronic properties of TMDs make them promising novel materials for various other applications as well. However, in order to realize the superior performance of TMD based devices, the physical and chemical properties need to be understood, in particular their stability under different chemical environments. A detailed comparative analysis of the air stability (i.e., oxygen interaction) of various TMDs is still lacking. We have examined various TMD stabilities in air and found them different from graphene which is stable in air. The changes in the electronic properties with air exposure were studied using density functional theory (DFT), Kelvin probe, and photoelectron emission in air. The results reveal that transition metal sulfides are kinetically more stable than selenides in air, but all TMDs are thermodynamically unstable against oxidation. Furthermore, it is shown that TMD surface defects function as facile oxidation sites impacting their air stabilities. These findings provide helpful guidance to controlled exfoliation and device fabrication processes.

$^1$This work was supported in part by the Center for Low Energy Systems Technology (LEAST), National Council of Sci. & Tech., Mexico (CONACyT), and Southwest Academy of Nanoelectronics (SWAN).

10:24AM Y2.00011 Air Stable Doping of MoS2 FETs Using TiOx Sol-Gel, AMRITESH RAI, RUDRESH GHOSH, ANUPAM ROY, AMITRAJ VALSARAJ, HEMA CP MOYVA, SANGWOO KANG, EMANUEL TUTUC, LEONARD REGISTER, SANJAY BANER-JEE, Univ of Texas, Austin — Field effect transistors based on ultra-thin transition metal dichalcogenides suffer from high contact resistances due to the Schottky barrier formed between the metal and the semiconducting channel. An effective way to overcome this issue is to dope the semiconducting channel in order to reduce the Schottky barrier width, thereby enabling efficient electron injection via tunneling. Previously used charge transfer doping techniques employed the use of potassium ions and PEI. However, these doping reagents are unstable in air. Here we report the use of an air stable, self-encapsulating, spin on n-type doping technique on MoS2 utilizing TiOx sol-gel. The doping of the channel is confirmed by the broadening of the A1g Raman mode of MoS2. High performance field effect transistors are demonstrated which show three times improvement in the field effect mobility as well as a two-fold increase in the intrinsic mobility of the MoS2 channel. The enhancement of intrinsic mobility can be attributed to the suppression of the A1g phonon modes of MoS2 as well as screening of charged impurities by the TiOx layer. The devices show extended air stability over two to three weeks. The use of TiOx sol-gel can be a promising way to enhance the performance of TMD based transistors.

$^1$This work is funded by NRI SWAN

10:36AM Y2.00012 Scanning tunneling microscopy study of a new charge density wave phase in VSe$_2$ thin films, DUMING ZHANG, JEONGHOON HA, Center for Nanoscale Science and Technology, National Institute of Standards and Technology/Maryland Nano Center, University of Maryland, HONGWOO BAEK, Center for Nanoscale Science and Technology, NIST/Department of Physics and Astronomy, Seoul National University, FABIAN NATTERER, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, YOUNG KUK, Department of Physics and Astronomy, Seoul National University, NIKOLAI ZHITENEV, JOSEPH STROSCIO, Center for Nanoscale Science and Technology, National Institute of Standards and Technology — Ultra-thin two-dimensional materials of transition metal dichalcogenides have recently attracted great interest due to their diverse electronic properties and potential applications. Upon cooling to low temperature, some materials exhibit interesting phenomena of collective electronic states such as superconductivity and charge density waves. While charge density waves in bulk materials of transition metal dichalcogenides have been extensively studied in the past few decades, the understanding of this collective electronic state in materials with reduced dimensionality is still in its infancy. Here, we report in-situ ultra-low temperature scanning tunneling microscopy and spectroscopy measurements on VSe$_2$ thin films synthesized by molecular beam epitaxy. We observed an unconventional charge density wave which does not follow previous reports of hexagonal symmetry of VSe$_2$. Spectroscopy results will be discussed in relation to other characterizations using electrical transport and transmission electron microscopy.
10:48AM Y2.00013 Two-dimensional materials based transparent flexible electronics1, LILI YU, SUNGJAE HA, DINA EL-DAKAM, ELAINE MCVAY, XI LING, ANANTHA CHANDRASKAN, JING KONG, TOMAS PALACIOS, MIT — Two-dimensional (2D) materials have generated great interest recently as a set of tools for electronics, as these materials can push electronics beyond traditional boundaries. These materials and their heterostructures offer excellent mechanical flexibility, optical transparency, and favorable transport properties for realizing electronic, sensing, and optical systems on arbitrary surfaces. These thin, lightweight, bendable, highly rugged and low-power devices may bring dramatic changes in information processing, communications and human-electronic interaction. In this report, for the first time, we demonstrate two complex transparent flexible systems based on molybdenum disulfide (MoS2) grown by chemical vapor method: a transparent active-matrix organic light-emitting diode (AMOLED) display and a MoS2 wireless link for sensor nodes. The 1/2 x 1/2 square inch, 4 x 5 pixels AMOLED structures are built on transparent substrates, containing MoS2 back plane circuit and OLEDs integrated on top of it. The back plane circuit turns on and off the individual pixel with two MoS2 transistors and a capacitor. The device is designed and fabricated based on SPICE simulation to achieve desired DC and transient performance. We have also demonstrated a MoS2 wireless self-powered sensor node. The system consists of an energy harvester, rectifier, sensor node and logic units. AC signals from the environment, such as near-field wireless power transfer, piezoelectric film and RF signal, are harvest, then rectified into DC signal by a MoS2 diode.

Friday, March 6, 2015 8:00AM - 11:00AM –
Session Y4 GERA DMP FIAP: Materials for Electrochemical Energy Storage II Mayor Cockrell Room 004 -

8:00AM Y4.00001 First-principles molecular dynamics simulations of electrochemical reactions using the ESM method, MINORU OTANI, National Institute of Advanced Industrial Science and Technology — It is important to elucidate a microscopic detail of an electrochemical reaction that takes place at the electrode and electrolyte interface to improve the performance of electrochemical energy storage/harvesting devices, such as secondary batteries, capacitors, fuel cells, and photovoltaic cells. Major difficulties for understanding the reaction are how to incorporate and control the bias potential applied to the interface. To solve these difficulties, we have been developing some intuitive methods to simulate the interfacial electrochemical reaction using first-principles molecular dynamics simulations [1-3]. In this talk I will present our methods and show the bias dependent free-energy profile of the desolvation process of a Li-ion battery and other recent results.


8:36AM Y4.00002 Ab-Initio Molecular Dynamics Study of the Concentration Dependent Diffusivity of Lithium Ions in Acetonitrile Electrolyte using the van der Waals Density Functional, KEITH RAY, Lawrence Livermore National Laboratory, ZHENXING WANG, ISAAK DANIELS, University of Kansas, DAVID OLMSTED, University of California, Berkeley, BRIAN LAIRD, University of Kansas, MARK ASTA, University of California. Berkeley — Pseudocapacitors are devices that store electrical energy faradically, but feature fast reactions/intercalations enabling high power applications. Power density may be improved by utilizing electrolytes with fast Li ion diffusion. In this study we utilize ab-initio molecular dynamics to elucidate the solvation structure as well as the vibrational and diffusion dynamics of Li ions in the acetonitrile electrolyte. Acetonitrile is a promising electrolyte for energy storage applications due to its lower viscosity and higher ionic conductivity when compared to other battery electrolytes such as ethylene carbonate and propylene carbonate. Interestingly, the trends in the Li ion concentration dependent diffusivity are calculated to be qualitatively different depending on whether the PBE or vdW-DF density functional is used.

This work was supported as part of the Molecularly Engineered Energy Materials (MEEM), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award DE-SC0001342.

8:48AM Y4.00003 A joint first principles and ATR-IR study of the vibrational properties of interfacial water at Si(100):H-H2O solid-liquid interfaces1, LEI YANG, STEFANIE TECKLENBURG, ANDREAS ERBE, STEFAN WIPPERMANN, Max-Plank-Institute for Iron Research, FRANCOIS GYGI, University of California, Davis, GIULIA GALLI, University of Chicago — Understanding the structural and bonding properties of solid-liquid interfaces is crucial for a wide range of (photo-)electrochemical applications, such as g. e. solar water splitting and electrolysis. In this report, for the first time, we demonstrate two complex transparent flexible systems based on molybdenum disulfide (MoS2) grown by chemical vapor method: a transparent active-matrix organic light-emitting diode (AMOLED) display and a MoS2 wireless link for sensor nodes. The 1/2 x 1/2 square inch, 4 x 5 pixels AMOLED structures are built on transparent substrates, containing MoS2 back plane circuit and OLEDs integrated on top of it. The back plane circuit turns on and off the individual pixel with two MoS2 transistors and a capacitor. The device is designed and fabricated based on SPICE simulation to achieve desired DC and transient performance. We have also demonstrated a MoS2 wireless self-powered sensor node. The system consists of an energy harvester, rectifier, sensor node and logic units. AC signals from the environment, such as near-field wireless power transfer, piezoelectric film and RF signal, are harvest, then rectified into DC signal by a MoS2 diode.

1This work was supported as part of the Molecularly Engineered Energy Materials (MEEM), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award DE-SC0001342.

9:00AM Y4.00004 High ionic conductivity NASICON based materials for Na-ion batteries: a density functional approach, K. M. BUI, NIMS, V. A. DINH, Osaka Univ., S. OKADA, Tsukuba Univ., T. OHNO, NIMS — Sodium ion batteries are now believed to be the best candidate for large-scale applications. Simultaneously, it is required to develop solid-state batteries using solid electrolytes for advancing the safety and reliability of batteries. The most promising solid-state battery is composed of the 3-D NASICON electrode Na2V2(PO4)3 (NVP) and electrolyte Na2Zr2Si2PO12 (NZSP). In this work, we aim to theoretically investigate the structures and the diffusion pathway of Na in these materials. Using density functional theory (DFT) method, we investigated the structures and diffusion mechanism of Na ions in the materials. They are insulators with large band. The polaron formation is found to occur only in NVP. Na ions can diffuse along three preferential diffusion pathways; these are, two intra-layer and one inter-layer pathway that takes place between Na layers via the empty Na site. In accordance with experiments reported before, the materials have high ionic conductivity with the activation barrier of about 760meV and 370meV for NVP and NZSP, respectively.

1The authors wish to thank T. A. Pham for helpful discussions. G. G. and F. G. acknowledge DOE-BES Grant No. DE-SC0008939.

9:00AM Y4.00004 High ionic conductivity NASICON based materials for Na-ion batteries: a density functional approach, K. M. BUI, NIMS, V. A. DINH, Osaka Univ., S. OKADA, Tsukuba Univ., T. OHNO, NIMS — Sodium ion batteries are now believed to be the best candidate for large-scale applications. Simultaneously, it is required to develop solid-state batteries using solid electrolytes for advancing the safety and reliability of batteries. The most promising solid-state battery is composed of the 3-D NASICON electrode Na2V2(PO4)3 (NVP) and electrolyte Na2Zr2Si2PO12 (NZSP). In this work, we aim to theoretically investigate the structures and the diffusion pathway of Na in these materials. Using density functional theory (DFT) method, we investigated the structures and diffusion mechanism of Na ions in the materials. They are insulators with large band. The polaron formation is found to occur only in NVP. Na ions can diffuse along three preferential diffusion pathways; these are, two intra-layer and one inter-layer pathway that takes place between Na layers via the empty Na site. In accordance with experiments reported before, the materials have high ionic conductivity with the activation barrier of about 760meV and 370meV for NVP and NZSP, respectively.

The authors wish to thank T. A. Pham for helpful discussions. G. G. and F. G. acknowledge DOE-BES Grant No. DE-SC0008939.
9:12 AM Y4.00005 Quasielastic neutron backscattering studies of Li-ion dynamics in Li\(_2\)SO\(_4\) substituted lithium modified phosphate glasses, TOM HEITMANN, University of Missouri, GAVIN HESTER, Missouri State University, MADHU TYAGI, National Institute of Standards and Technology, MUNESH RATHORE, ANSHUMAN DALVI, Birla Institute of Technology and Science, Pilani, SAIBAL MITRA, Missouri State University — A solid with high Li ionic conductivity and a simultaneously low electronic conductivity is an attractive candidate for use as an electrolyte in an all solid-state Li ion battery. Solid state electrolytes would not only improve the reliability, safety, and the ability of the battery to be operated in harsher conditions, but also allow to be scaled for heavy duty industrial applications. We have studied a series of glassy electrolyte candidate materials. Using quasi elastic neutron scattering in a pulsed time-of-flight neutron backscattering spectrometer, we have characterized the Li-ion diffusion behavior of these materials. We find that Li-ion transport relaxation times are strongly dependent on the ionic state of the host glasses. Our results suggest that these glasses are promising materials for all solid-state Li-ion batteries. We have also studied the electronic transport behavior of these glasses using resistivity measurements and observed that the glasses with a low electronic conductivity are promising materials for all solid-state Li-ion batteries.

9:24 AM Y4.00006 X-ray Scattering Studies and Dynamics at Charged Graphene Interface1, AHMET UYSAL, SANG SOO LEE, HUA ZHOU, PAUL FENTER, Argonne National Laboratory, PENGFEI ZHANG, SHENG DAI, Oak Ridge National Laboratory — Room temperature ionic liquids (RTILs) are promising electrolytes for energy storage systems, especially for supercapacitors. However, our knowledge of these highly dense ionic plasmas at electrified interfaces is still at its infancy due to the lack of in situ experimental data about their potential-dependent electric double layer (EDL) structures and dynamics. In particular, the behavior of mixed electrolytes (RTIL/RTIL and Solvent/RTIL), which are significantly important for practical applications, have been little studied with structural probes. We use in situ real-time X-ray reflectivity to elucidate the role of different anion-cation combinations and solvents on the interfacial ionic liquid structure and dynamics at epitaxial graphene electrode during cyclic voltammetry and potential steps. Our results give direct information about the EDL structure and response, which helps us to connect the macroscopic system properties to the nanoscale structure.

1This work was supported as part of the Fluid Interface Reactions, Structures and Transport (FIRST) Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

9:36 AM Y4.00007 The Electronic Structures and Diffusion Kinetics of Li, Na, and Mg Inter-calated TiO\(_2\) Anatase and TiO\(_2\) (B), HANDAN YILDIRIM, JEFFREY P. GREELEY, Purdue University School of Chemical Engineering — Large-scale electrochemical storage that would allow wider use of renewable electricity not only requires new and advanced electrode materials for Li ion batteries, but also beyond-Li technologies such as Na and Mg ion batteries. This grand challenge puts forward the necessity for designing efficient electrode materials providing suitable energetics and rapid diffusion kinetics. In this contribution, we evaluate TiO\(_2\) anatase and TiO\(_2\) (B) as attractive candidates for anodes in Li, Na, and Mg batteries due to their low cost, non-toxicity, cycling stability, reasonable capacity, and high operating potential. While the TiO\(_2\) anatase is discussed as promising material for Li storage, structurally, TiO\(_2\) (B) with large interlayer spacing can be considered as a good electro-active material for Na intercalation. We will report the results of the first principles calculations using generalized gradient approximation (GGA) for Li, Na, and Mg intercalation at low concentration. The differences in the electronic and atomic structures obtained using GGA, Hubbard “+U” correction (GGA+U), and Heyd, Scuseria, and Ernzerhof (HSE) hybrid functional will be reported, and the importance of the “+U” correction for modeling the electronic structure of the intercalated TiO\(_2\) will be discussed. The detailed information on the differences in the diffusion mechanisms and barriers will also be reported for each ion in both structures.

9:48 AM Y4.00008 Joint Density-Functional Theory for Atomically Detailed Structure of the Electrode/Electrolyte Interface, KENDRA LETCHWORTH-WEAVER, CHRISTINE UMBRIGHT, RAISHANKAR SUNDARARAMAN, T.A. ARIAS, Department of Physics, Cornell University, Ithaca, NY 14853 — Understanding the complex and inherently multi-scale interface between a charged electrode surface and a fluid electrolyte would inform design of more efficient and less costly electrochemical energy storage and conversion devices. Joint density-functional theory (JDFT) bridges the relevant length-scales by joining a fully ab initio description of the electrode with a highly efficient, yet atomically detailed classical DFT description of the electrolyte structure. First, we introduce a universal functional to couple any quantum-mechanical solute system with a classical DFT for any liquid. This universal coupling functional captures aqueous and non-aqueous solution free energies of small molecules with a mean absolute error of only 1-2 kcal/mol. We also present classical density-functional for ionic species which reproduce the key features of ion-water correlation functions when combined in a mixture with existing functionals for water. Leveraging the above theoretical innovations and our framework to treat charged systems in periodic boundary conditions, we then predict the voltage-dependent structure and energetics of solvated ions at the interface between a graphene electrode and an aqueous electrolyte.

10:00 AM Y4.00009 Ab Initio Electrochemical Capacitance Studies of Super capacitor Materials in Aqueous and Non-Aqueous Electrolytes, CHRISTINE UMBRIGHT, KENDRA LETCHWORTH-WEAVER, T.A. ARIAS, Department of Physics, Cornell University, Ithaca, NY 14853 — Novel electrical energy storage devices are becoming increasingly necessary as technological advances demand higher energy capacity and more efficient methods of charging. Ab initio Joint Density-Functional Theory (JDFT) allows for the simultaneous study of electrodes, electrolytes, and their interactions in a uniform, comprehensive way. In this work, JDFT is utilized to study the energy storage capabilities of supercapacitor materials, such as graphene. The unique electronic structure of graphene results in a high density of states which minimize the capacitance of the electrode. Confinement effects on capacitance are also investigated, as JDFT allows for prediction of ion-structure changes at the interface between a graphene electrode and an aqueous electrolyte.

10:12 AM Y4.00010 Thermodynamics of alloyed nanoparticles for hydrogen evolution reaction including configurational and adsorbate effects1, LIN-LIN WANG, Ames Laboratory, U.S. Department of Energy, Ames, IA 50011, TECK L. TAN, Institute of High Performance Computing, Agency for Science, Technology and Research, Singapore 138632, Singapore, DUANE D. JOHNSON, Ames Laboratory, U.S. Department of Energy, Ames, IA 50011, Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011 — Changes in the chemical configuration of alloyed nanoparticle (NP) catalysts induced by adsorbrates under working conditions are crucial to understand and design NP functionality. We extend the cluster expansion method to predict the configurational thermodynamics of alloyed NPs on equal footing with adsorbate thermodynamics based on density functional theory data. Exemplified with alloyed PdPt NPs having H-coverage up to a full layer, we describe both the configurational and adsorbate thermodynamic behavior simultaneously across the entire range of NP composition and H-coverage to obtain the H-adsorption isotherms and simulated cyclic voltammetry for hydrogen evolution reaction.

1Supported by DOE-BES CSGB (DE-FG02-03ER15476), MSE (DE-AC02-07CH1135) and Ames Lab LDRD. Research was performed at the Ames Laboratory, which is operated for DOE by Iowa State University under contract DE-AC02-07CH11388.
10:24AM Y4.00011 Self-consistent continuum solvation (SCCS): Towards the accurate modeling of electrochemical systems in plane-wave DFT. STEPHEN WEITZNER, ISMAILA DABO, The Pennsylvania State University — Implicit solvent models have been widely used to study quantum systems in solutions. Nevertheless, these models differ greatly in their phenomenological details and in the complexity of their parameterization. While conventional implicit models rely on atomic positions and tabulated atomic radii to construct the solvent shell that surrounds the quantum solute, recent models aim to reduce the number of parameters by building solvation shells directly from computed electronic densities. The self-consistent continuum solvation (SCCS) model, which belongs to the latter class, has been shown to reproduce the solvation energies of a wide range of molecular species in good agreement with experiment, using only two fitted parameters [J. Chem. Phys. 136, 064102 (2012)]. Here, we report on the SCCS model’s performance in describing the electrical properties of quantum electrodes embedded in continuum electrolytes. We show that one additional parameter is needed to capture experimental shifts in the neutral electrode potential as a function of surface composition and structure, and to correctly calibrate computed results to a common electrochemical reference. Utilizing this approach, we establish a novel framework for studying interfacial electrochemical phenomena.

10:36AM Y4.00012 Fast motif-network scheme for extensive exploration of complex crystal structures in silicate cathodes. KAI-MING HO, XIN ZHAO, Iowa State University, SHUNQING WU, Xiamen University, XIAOBAO LV, University of Science and Technology of China, MANH CUONG NGUYEN, CAI-ZHUHANG WANG, Iowa State University, ZI-JING LIN, University of Science and Technology of China, ZI-ZHONG ZHU. Xiamen University — A motif-network search scheme is proposed to study the crystal structures of the dilithium/disodium transition metal orthosilicates A₂M₂O₄. Using this fast and efficient method, the structures of all six combinations with A = Li or Na and M = Mn, Fe or Co were extensively explored in this work. In addition to finding all previously reported experimental structures, we discover many other different crystal structures which are highly degenerate in energy. These tetrahedral-network-based structures can be classified into 1D, 2D and 3D types. A clear trend of the structural preference in different systems is revealed and possible indicators that affect the structure stabilities are introduced. For the case of Na systems which have been much less investigated in the literature relative to the Li systems, we predicted their ground state structures and found evidence for the existence of new structural motifs.


Friday, March 6, 2015 8:00AM - 10:48AM — Session Y5 DMP DCOMP: Focus Session: Fe-based Superconductors — Madores Synthesis and Characterization

8:00AM Y5.00001 Doping evolution of the anisotropic upper critical field in (Ba₁−ₓKₓ)Fe₂As₂.1 MAKARIY TANATAR, YONG LIU, T.A. LOGRASSO, RUSLAN PROZOROV, Ames Laboratory USDOE, Ames, IA 50011, JAN J. JAROSZYNSKI, J.S. BROOKS, National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, USA — The temperature and magnetic-field-dependent in-plane resistivity measurements were used to determine anisotropic upper critical field, Hc2(T), of the hole-doped iron-based superconductor (Ba₁−ₓKₓ)Fe₂As₂ over the whole doping range x=0 to x=1. We find clear saturation of Hc2(T) line on T→0 in magnetic field perpendicular to the c-axis of the samples in the overdoped range of the phase diagram, suggesting strong paramagnetic limiting effects. Measurements reveal clear difference in the shapes of the Hc2(T) lines for under-doped and over-doped compositions with similar Tc. Origin of this difference will be discussed.1 This work was supported by the Department of Energy Office of Science, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

8:12AM Y5.00002 Investigation of Vortex Lattice in Optimally Doped (Ba₁−ₓKₓ)Fe₂As₂ Using SANS. S. DEMIRDIS, Julich Center for Neutron Science (JCNS), Forschungszentrum Julich GmbH, JCNS at MLZ, D-54476, Germany, J.C. VAN DER BEEK, Laboratoire des Solides Irradiaux, Ecole Polytechnique CNRS UMR 7642 & CEA-DSM-IRAMIS, F 91128 PALAISEAU/France, S. MUHLBAUER, Technische Universitat Munchen, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II) D-85748, Garching, Germany. Y. SU, Julich Center for Neutron Science (JCNS), Forschungszentrum Julich GmbH, JCNS at MLZ, D-54476, Garching, Germany, TH. WOLF, Karlsruher Institut für Technologie, Institut für Festkörperphysik, 7602, Karlsruhe, Germany — Small-angle neutron scattering is used to study the vortex lattice (VL) structure, and to correctly calibrate computed results to a common electrochemical reference. Utilizing this approach, we establish a novel framework for studying interfacial electrochemical phenomena.

8:24AM Y5.00003 Magnetic, optical, and transport properties of BaM₃As₂ and Ba₁−ₓKₓM₃As₂. SHELBY ZELLMAN, DANIEL MCNALLY, Stony Brook University, KANGBO HAO, KIRK POST, DIMITRI BASOV, University of California, San Diego, CHRISTOPHER HOMES, Brookhaven National Laboratory, MEIGAN ARONSON, Stony Brook University, Brookhaven National Laboratory, CORRELATED ELECTRONS GROUP TEAM, INFRARED SPECTROSCOPY OF NOVEL ELECTRONIC AND MAGNETIC MATERIALS COLLABORATION, ELECTRON SPECTROSCOPY GROUP COLLABORATION — Square-net Mn-pnictides are strongly correlated antiferromagnetic (AF) insulators that can potentially be transformed into metals using pressure or charge doping. BaM₃As₂ becomes an AF metal when 5% of K is substituted on the Ba site, and we present here an optical study of this insulator-metal transition. Our measurements confirmed that the resistivity r(T) of undoped BaM₃As₂ is insulating, but becomes metallic with as little as 5%K doping. We measured optical transmission in the visible region of BaM₃As₂, finding a direct charge gap of ~ 5500 cm⁻¹, much larger than previously reported, or the activation gaps determined from r(T). Reflectance measurements were performed to determine if a Drude peak forms at the lowest energies in the doped samples. These measurements underscore the importance of electron correlations in BaM₃As₂ as it approaches metallization. We acknowledge the Office of the Assistant Secretary of Defense for Research and Engineering for providing the NSSEFF funds that supported this research and the DOE under contract No. DE-AC02-98CH10886.
8:36AM 8:36AM Y5.00004 The Ni and Co substitutions in iron chalcogenide single crystals1, V.L. BEZUSYY, D.J. GAWRYLUK, A. MALINOWSKI, M. BERKOWSKI, MARTA Z. CIEPLAK, Institute of Physics PAS, Warsaw — We study the ab-plane resistivity and Hall effect in Fe$_{1-x}$M$_x$Te$_2$Se$_{2.5}$ single crystals with M=Co or Ni, and y up to 0.2. The crystals are grown by Bridgman’s method. The low-temperature Hall coefficient $R_H$ changes sign to negative for crystals with y exceeding 0.135 (Co) and 0.06 (Ni), consistent with the electron doping induced by these impurities. However, the $R_H$ remains positive for all samples at high T, suggesting that remnant hole pockets survive the doping, but the holes become localized at low T in heavily doped crystals. Superconducting transition temperature ($T_c$) approaches zero for y exceeding 0.135 (Co) and 0.06 (Ni), while the resistivity at the $T_c$ onset is only weakly affected by Co doping, but it increases strongly for the Ni. These results suggest that in case of Co impurity the $T_c$ suppression may be attributed to electron doping. On the other hand, the Ni substitution, in addition to electron doping, induces strong localization effects at small impurity contents. Using two-band conduction model we argue that the localization of electron carriers is responsible for strong superconductivity suppression by Ni impurity.

$^1$Supported by EC through the FunDMS Advanced Grant of the ERC (FPT Ideas), by the Polish NCS grant 2011/01/B/ST3/00462, and by the French-Polish Program PICS 2012. Performed in the laboratories co-financed by NanoFun Project POIG.02.02.00-00-025/09.

8:48AM 8:48AM Y5.00005 Generic Superconducting Inhomogeneity in Single Crystal Fe(Fe$_{1-x}$Se$_{2.5}$) Probed by Nanostructure-transport , CHUNLEI YUE, JIN HU, XUE LIU, ZHIQIANG MAO, JIANG WEI, Tulane University — We have investigated the nano-scale electronic properties of the iron-based unconventional superconductor Fe(Fe$_{1-x}$Se$_{2.5}$) with optimal Se content $x=0.5$. Using the microexfoliation method and ion milling thinning, we successfully produced Fe(Fe$_{1-x}$Se$_{2.5}$) devices with thickness varying from 90nm down to 12nm. Our transport measurements revealed a suppression of superconductivity coinciding with the loss of normal state metallicity. Through the simulation of the formation of superconducting region in nano-scale thin flakes, we show that our observation is in line with the nano-scale inhomogeneity proposed for this material; therefore it provides a more direct evidence for the nano-scale inhomogeneous superconductivity in Fe(Fe$_{1-x}$Se$_{2.5}$).

9:00AM 9:00AM Y5.00006 Order/disorder of Fe-vacancy and superconductivity in Fe-chalcogenide superconductors$^1$, MAW-KUEN WU, National Donghwa University and Institute of Physics, Academia Sinica — Having the simplest crystal structure among the Fe-based superconductors, the FeSe superconductor is the best candidate for investigating the mechanism of these new superconductors. How the properties of FeSe superconductor evolve from normal state to superconducting state and what is the parent phase of FeSe system are critical issues for resolving its superconducting mechanism. We have studied the properties of FeSe and K-Fe$_x$Se$_{2-x}$ superconductors in various forms, including polycrystal, single crystal, thin film, nanowire, and nanoparticle. We discovered several Fe-deficient Fe$_{1-x}$Se phases, which exhibit Fe-vacancy ordering. The property of these phases evolves from an insulator to a metal gradually as Fe content increases. Our results provide unambiguous support to the picture that superconducting transition in FeSe and related compounds is closely related to the order to disorder transition of the Fe-vacancy.

$^1$Acknowledgment the financial support from MOST and Academia Sinica, Taiwan.

9:36AM 9:36AM Y5.00007 Fermi-liquid like normal state electronic states in Co-doped BaFe$_2$As$_2$ , ERIK VAN HEUMEN, ALONA TYTARENKO, YINCKAI HUANG, ANNE DE VISSER, University of Amsterdam, STEVEN JOHNSTON, University of Tennessee — Elucidating the origin of high temperature superconductivity requires two equally important ingredients: a framework for the normal state electronic dynamics and a pairing interaction. In iron-pnictide high T$_c$ superconductors the electron doped compounds, such as BaFe$_2$-xCo$_x$As$_2$, are predicted to be weakly correlated Fermi liquids [1,2], but clear evidence has thus far been lacking. In this contribution we unveil the true nature of the normal state dynamics by carefully annealing BaFe$_2$-xCo$_x$As$_2$ single crystals. We show that optical spectroscopy experiments on such annealed crystals display a characteristic Fermi liquid scaling of frequency and temperature over a large energy range [3]. A comparison with as-grown single crystals shows that magnetic impurity scattering has thus far masked this behavior. A further analysis shows that a Fermi-liquid like single-particle self-energy can well describe both the mass renormalization and optical scattering rate, leaving little room for additional contributions.


9:48AM 9:48AM Y5.00008 Anomalous Hall effect in epitaxial Ba(Fe1-x Co)x)2As2 pnictide superconducting thin films and superlattices1, NEIL CAMPBELL, MARK RZCHOWSKI, JULIAN IRWIN, Dept of Physics, Univ of Wisconsin, JONG-HOON KANG, CHANG-BEOM EOM, SANCHAN LEE, Dept of MatSci and Engr, Univ of Wisconsin, ADELE RUOSI, Dipt di Fisica, Univ di Napoli Federico II — Iron-based superconductors have been worked with to the point that now growth of various thin films is very-well controlled, allowing in depth study of associated structures. One exciting pathway of study for pnictides is that they show similarities to cuprate superconductors, regarded as an avenue toward high-Tc superconductors. Specifically, these heterostructures allow study of the competition between antiferromagnetism and superconductivity at the interface between the undoped parent compound, and optimally-doped compound. BaFe2-xCoAs2 (Ba122). At room temperature, these pnictides exhibit anomalous Hall effect (AHE). There is strong evidence for the interface dominating AHE, allowing control AHE with type of substrate, surface termination, and superlattice configuration. We characterized samples of thicknesses from 6nm to 300nm, and with up to 12 interfaces. Such samples have been characterized via magnetotransport measurements at temperatures ranging from 5K to 300K, and magnetic fields up to 8T applied normal to the basal plane with Van der Paw and Hall geometries. Additionally, we measured magnetization with vibrating sample magnetometry. These properties will aid novel device development, making pnictides interesting.

$^1$This work was supported by funding from the DOE Office of Basic Energy Sciences under award number DE-FG02-06ER46327.

10:00AM 10:00AM Y5.00009 Electrodynamics of rare-earth-doped CaFe$_2$As$_2$ , ZHEN XING, T.J. HUFFMAN, PENG XU, A.J. HOLLINGSHEAD, D.J. BROOKER, M.M. QAZILBASH, Department of Physics, College of William and Mary, SHANTA SAHA, TYLER DRYE, CONNOR RONCAIOLI, J. PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park — Rare-earth substitution at alkaline-earth sites leads to the suppression of the spin density wave phase transition in CaFe$_2$As$_2$ without the emergence of bulk superconductivity. In this work, we perform pyroelectric infrared reflectance spectroscopy and spectroscopic ellipsometry on Pr-doped and La-doped CaFe$_2$As$_2$ single crystals. In both Ca$_{0.85}$La$_{0.15}$Fe$_2$As$_2$ and Ca$_{0.85}$Pr$_{0.15}$Fe$_2$As$_2$ samples, the spin density wave transition is completely suppressed. The temperature dependence of the ab-plane optical conductivity of the La-doped CaFe$_2$As$_2$ crystal exhibits conventional metallic behavior consistent with the absence of any structural, magnetic, or superconducting instabilities. On the other hand, the Pr-doped CaFe$_2$As$_2$ crystal undergoes a structural transition about 70 K from a tetragonal lattice to a collapsed tetragonal lattice with the same symmetry but reduced volume. In the Pr-doped CaFe$_2$As$_2$ crystal, the ab-plane optical conductivity reveals subtle but distinct spectral changes upon cooling through the structural transition. We provide results on the influence of the structural collapse on the charge dynamics, correlation effects and the electronic configuration.

$^2$This work was supported by NASA / Virginia Space Grant Consortium.
10:12AM Y5.00010 Systematic growth and physical properties of BaFe$_{2−x}$Cr$_x$Ni$_2$As$_2$. DONGLIANG GONG, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, RUI ZHANG, Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA, SHILIANG LI, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, PENGCHENG DAI, Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA, HUIQIAN LUO, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — We have successfully grown the single crystals of BaFe$_{2−x}$Cr$_x$Ni$_2$As$_2$ with a series of Ni and Cr doping levels. Their physical properties were studied by the elastic neutron scattering and transport measurements. It is found that Cr doping is a very efficient way of suppressing the superconductivity in the BaFe$_{2−x}$Ni$_2$As$_2$ system with little change of the $T_S$ and $T_N$. The magnetic and electronic properties without the presence of the superconductivity may be thus investigated at low temperature.

10:24AM Y5.00011 Observation of pseudogaplike feature in LiFeAs by ultrafast optical spectroscopy. KUNGHUAN LIN, KUAN-JEN WANG, CHUNG-ChIEH CHANG, YU-ChIEH WEN, DZUNG-HAN TSAI, YU-RUEI WU, YAO-TSUNG HSIEH, MING-JYE WANG, Academia Sinica, Taiwan, BING LV, PAUL C.-W. CHU, University of Houston, USA, MAU-KUEN WU, National Dong Hwa University, Taiwan — We utilize ultrafast optical spectroscopy to study the quasiparticle relaxation in stoichiometric LiFeAs crystals. According to our temperature-dependent studies, we have observed three electronic phases in LiFeAs. Below the superconducting (SC) temperature $T_c$ (~15 K), the relaxation time of quasiparticles due to the SC gap is far longer than 50 ps in our experimental conditions. In addition to SC gaps, we have also found a gaplike feature in SC state. This gaplike feature is evident up to 40 K, which is above the SC temperature. Because this is similar to pseudogap in cuprate superconductors, we call this new electronic phase as pseudogaplike feature. The quasiparticle relaxation time due to pseudogaplike feature is in the range of 1-2 ps. We suggest the pseudogaplike feature in LiFeAs is induced by magnetic fluctuations.

10:36AM Y5.00012 Temperature Evolution of Spin Fluctuations in FeAs. A. PODLESNYAK, G. EHLERS, Quantum Condensed Matter Division, ORNL, Oak Ridge, TN 37831, USA, S. TÖTH, Laboratory for Neutron Scattering and Imaging, PSI Villigen & Laboratory for Quantum Magnetism, EPFL, Lausanne, Switzerland, K. GOFRYK, A.S. SEFAT, Materials Science and Technology Division, ORNL, Oak Ridge, TN 37831, USA — The discovery of superconductivity (SC) in iron pnictides has opened a new stage in SC research. The superconducting state appears in iron pnictides with doping in metallic parent compounds. This is an important difference to the cuprates, which exhibit SC near a correlated insulating state. Therefore, the nature of the magnetism in the simplest iron pnictide - binary FeAs - is of fundamental importance for understanding the interplay between localized and itinerant magnetism and superconductivity in these materials. We use inelastic neutron scattering to map spin wave excitations in the monoaesndic FeAs at temperatures above and below the antiferromagnetic transition $T_N \sim 70$ K. We find magnetic excitation spectrum near the Néel temperature to be strongly different from the spectrum in the ground state. Near the transition temperature, magnetic fluctuations clearly indicate two-dimensional character in an intrinsically three-dimensional (3D) system. On the other hand, at low temperature, spin waves in FeAs are anisotropic 3D, suggesting a crossover from two-dimensional to three-dimensional character.

Friday, March 6, 2015 8:00AM - 11:00AM —
Session Y6 DCMP DMP: Optical and Electrical Properties of Hybrid Nanostructures

8:00AM Y6.00001 Tuning the charge transfer plasmon in a metallic nanoparticle dimer bridged by a quantum dot. VIKRAM KULKARNI, ALEJANDRO MANJAVACAS, PETER NORDLANDER, Rice University — Localized surface plasmon resonances (LSPR) are a subject of intense experimental and theoretical research interest. LSPR have found applications in catalysis, solar energy, cancer therapy, and surface enhanced Raman spectroscopy (SERS). This is due to the exceptional light capturing and focusing capabilities of plasmonic nanostructures. An LSPR of particular interest is the charge transfer plasmon (CTP). This mode may be excited when two plasmonic nanoparticles are bridged by a quantum dot. The CTP is extraordinarily sensitive to the conductive properties of the junction. Here we perform a theoretical investigation of the CTP when two plasmonic nanoparticles are bridged by a quantum dot. All simulations are done using the time dependent density functional theory (TD-DFT). By modulating the electronic structure of the quantum dot we are able to effectively turn the CTP on and off. Specifically, the CTP emerges only when a quantum dot energy level is resonant with the fermi energy of the plasmonic nanoparticles. We verify that the conductance through the junction is on the order of the quantum unit of conductance. This work is of great interest to the future design of plasmonic and molecular electronic systems.

8:12AM Y6.00002 Highly tunable gold nanorod dimer resonances mediated through conductive junctions. JAKE FONTANA, BANAHALLI RATNA, Naval Research Lab — Tailoring the resonant frequency in plasmonic nanostructures is critical to developing disruptive metamaterial technologies. Here we numerically study the optical properties of gold nanorod dimers connected end-to-end by a thin metallic bridge [1]. We find the resonant frequency along the long axis of the dimer shifts linearly with the nanorod aspect ratio behaving as it was a single nanorod with an aspect ratio nearly an order of magnitude larger. We show by controlling the material and geometry of the connecting bridge the effective dielectric function of the dimer is significantly modulated tuning the resonant frequency over a decade, from 1 to 10 μm. We present an alternative description for the emergence and behavior of the dimer resonance using a straightforward “Drude-like” model and self-assembly experiments creating such structures.


8:24AM Y6.00003 Surface Plasmon Resonance enhancement via oblique thin film deposition on gratings. ZHAOZHU LI, MICHAEL KLOPF, William and Mary College, GEORGE SCHWARTZ, University of Virginia, MATTHEW HEIMBURGER, LEI WANG, KAIDA YANG, ROSA LUKASZEW, William and Mary College — Surface plasmon resonance (SPR) occurs when light shins at a dielectric-metallic interface under certain configurations such that an evanescent polariton can be excited. This surface plasmon polariton travels across the interface exhibiting electric field intensity greatly enhanced with respect to the incident light, evidenced by the observation of a deep angular reflectivity scans at the resonance angle. To excite the SPR, one can use a diffraction grating coupler in order to satisfy the dispersion relationship, noting that within certain grating-groove aspect-ratios, the electric field intensity in the surface polariton can be further enhanced by increasing the grating amplitude. We have applied oblique shadow deposition (OSD) to deposit metallic layers onto gratings to enhance their grating amplitudes and compare them to films deposited at normal incidence. We report on the effects on the SPR of such configurations, by comparing the results of OSD samples with those for normal incident deposited samples.
8:36AM Y6.00004 Plasmon Excitations for a Linear Assembly of Metallic Spheres. BO GAO, LIUBOV ZHEMCHUZHNA, Hunter College, CUNY, ANDRIII IROV, University of New Mexico and Hunter College, CUNY, GODFREY GUMBS, Hunter College, CUNY and Donostia International Physics Center (DIPC), DANHONG HUANG, Air Force Research Laboratory, Space Vehicles Directorate. We present a general formalism for calculating the Coulomb excitations of a linear array of interacting electron gases confined to the outside surfaces of three spherical shells. The response of these incompressible 2D electron gases to an external electromagnetic field results in charge density oscillations whose anisotropicity with respect to the axis of quantization will be discussed. The dependence of the frequency of the plasma oscillations on the radius of the spheres as well as their separation has been a subject of our investigation and detailed results will be presented. We provided complete numerical results for the plasmon excitation of such system and concluded that the plasmon demonstrate quite different behavior from the earlier considered case of a 2DDEG triad - they are not symmetric on the sign of each potential element for z-alignment and the interaction of the two far-removed spheres is no longer negligible.

8:48AM Y6.00005 Aperiodic Aharonov-Bohm oscillations in coherent transport through a periodic array of quantum dots. L.S. PETROSYAN, T.V. SHAHBAZIAN, Jackson State Univ. We study resonant tunneling through a periodic square array of quantum dots sandwiched between modulation-doped quantum wells. If a magnetic field is applied parallel to the quantum dot plane, the tunneling current exhibits a highly complex Aharonov-Bohm oscillation pattern due to interference of multiple pathways traversed by a tunneling electron. Individual pathways associated with conductance beats can be enumerated by sweeping the magnetic field at various tilt angles. Remarkably, Aharonov-Bohm oscillations are aperiodic unless the magnetic field slope relative to quantum dot lattice axes is a rational number.

9:00AM Y6.00006 Hyperbolic polaritons in nanoparticles. ZHIYUAN SUN, Department of Physics, University of California San Diego, 9500 Gilman Drive, La Jolla, California 92093, USA, ANGEL RUBIO, FRANCISCO GUINEA, Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, E-28049 Madrid, Spain, DIMITRI BASOV, MICHAEL FOGLER, Department of Physics, University of California San Diego, 9500 Gilman Drive, La Jolla, California 92093, USA. Hyperbolic optical materials (HM) are characterized by permittivity tensor that has both positive and negative principal values. Collective electromagnetic modes (polaritons) of HM have novel properties promising for various applications including subdiffractional imaging and on-chip optical communication. Hyperbolic response is actively investigated in the context of metamaterials, anisotropic polar insulators, and layered superconductors. We study polaritons in spheroidal HM nanoparticles using Hamiltonian optics. The field equations are mapped to classical dynamics of fictitious particles (wave packets) of an indefinite Hamiltonian. This dynamics is quantized using the Einstein-Brillouin-Keller quantization rule. The eigenmodes are classified as either solid or surface according to whether their transverse momenta are real or imaginary. To model how such hyperbolic polaritons can be probed by near-field experiments, we compute the field distribution induced inside and outside the spheroid by an external point dipole. At certain magic frequencies the field shows striking geometric patterns whose origin is traced to the classical periodic orbits. The theory is applied to natural hyperbolic materials hexagonal boron nitride and superconducting LaSrCuO.

9:12AM Y6.00007 Generation of acoustic terahertz waves in hybrid InGaN/GaN quantum wells. MEG MAHAT, Department of Physics, University of North Texas, Denton, TX 76203, ANTONIA LLOPIS, Department of Electrical and Computer Engineering, Duke University, Durham, NC 27708, TAE YOUL CHOI, Department of Mechanical and Energy Engineering, University of North Texas, Denton, TX 76203, SERGIO PERIARA, CICECO, Universidade de Aveiro, 3810-193 Aveiro, Portugal, IAN WATSON, SUPA, Institute of Photonics, University of Strathclyde, Glasgow, UK, ARUP NEOGI, Department of Physics, University of North Texas, Denton, TX 76203. We have carried out differential transmission measurements on InGaN/ GaN quantum wells with Au nanoparticles inserted inside V-pits with high filling fraction. We have observed acoustic wave packets generated with multiple THz frequencies as 0.12 THz from GaN buffer layer, 0.22 THz from Au-InGaN multiple quantum wells region, 0.07 THz from sapphire substrate, and 0.17 THz mixed signals from the sample. These THz wave packets are observed as a result of generation of coherent acoustic phonons propagating in hybrid Au-InGaN quantum wells. The study of these acoustic THz wave generation is crucial for the imaging of nanostructures.

9:24AM Y6.00008 Magnetic field- and frequency-dependence- of the phase-shift in the linearly-polarized microwave radiation-induced magnetoresistance oscillations in the GaAs/AlGaAs system. HAN-CHUN LIU, TIANYU YE, Department of Physics & Astronomy, Georgia State University, WERNER WEGSHEIDER, ETH-Zurich, Zurich, Switzerland, RAMESH MANI, Department of Physics & Astronomy, Georgia State University. Nonequilibrium transport studies of the radiation-induced magnetoresistance oscillations (RIMOs) have revealed striking photo-excited zero-resistance states in the GaAs/AlGaAs two-dimensional electron system [1]. Further observations show that RIMOs are linear-polarization-angle-sensitive and follow a sinusoidal fitting formula, \( R_{xx}(\theta) = A \pm C \cos^2(2(\theta - \theta_0)) \) where \( R_{xx} \) is the diagonal resistance, \( \theta \) is the polarization angle, and \( \theta_0 \) is the extracted phase shift. At the present, \( \theta_0 \) is known to be magnetic- and frequency-dependent [2]. Here, we perform magnetic mappings at small \( \theta \) intervals, at a number of radiation frequencies, to study the variation of the phase shift with the magnetic field and frequency. The relationship between phase shift and magnetic fields/frequency will be critically examined and reported in this presentation.


9:36AM Y6.00009 Electrochemically grown InSb nanowires: challenges and growth determined properties. ABHAY SINGH, USHA PHILOPOSE, University of North Texas — InSb nanowires have myriads of applications such as electronic, optoelectronic, and magneto resistive devices. Synthesis of InSb nanowires in the pores of anodic alumina oxide (AAO) template by direct current electrodeposition is challenging because it involves several steps including opening of barrier layer at the bottom of AAO pores, dissolving of the AAO template post-nanowire growth, followed by electrochemical deposition of InSb nanowires. We will provide evidence of these challenges. The InSb nanowires had good composition and crystalline quality as will be shown by EDX, X-ray, and Raman spectroscopy. Transport measurements made on a single InSb nanowire and on an array of nanowires will be presented. A single nanowire connected in an FET type configuration was used to determine carrier concentration and mobility. By tuning the growth parameters during electrochemical deposition, it is possible to modulate the nanowire composition. Temperature dependent measurements are used to show the semiconducting behavior of the nanowires.

9:48AM Y6.00010 Superlattice Phenomena in Nanohelices. CHARLES DOWNING, MATTHEW ROBINSON, MIKHAIL PORTNOI, University of Exeter, UNIVERSITY OF EXETER TEAM. Recently artificially-created nanohelices have been demonstrated in various semiconductor systems. We argue that subjecting a nanohelix to an electric field normal to its axis turns it into a superlattice with easily-tunable electronic properties. We investigate such a system, also subjected to a longitudinal electric field along the nanotube axis, and find Bloch oscillations and negative differential conductivity. Taking into account Zener tunneling across the band gap, we find the characteristic N-type dependence of electron drift velocity on the longitudinal field which is commonly used in high-frequency electronics. The merits of using a nanohelix for novel tunable device applications are assessed. We also study dipole transitions across the energy gap, which can be tuned to the THz range by experimentally attainable external fields. There is a drastic change in selection rules for a helix in a transverse field compared to the case of purely chiral structures. For the excitation propagating along the nanohelix axis our results are somewhat similar to those found for a quantum ring pierced by a magnetic flux, with the momentum of a quasiparticle in a helix playing the same role as a flux through a ring. We also discuss possible devices which could utilize these phenomena.
10:00AM Y6.00011 Tunable Quantum Temperature Oscillations in Graphene Nanostructures
JUSTIN BERGFIELD, MARK RATNER, Northwestern University, CHARLES STAFFORD, University of Arizona, MASSIMILIANO DI VENTRA, University of California, San Diego — Thermal scanning probe microscopy techniques are now capable of nanometer spatial resolution and millikelvin temperature accuracy, raising the fundamental question: What is the meaning of temperature for a quantum system operating far from equilibrium? We investigate this question theoretically using a realistic model of a scanning thermal microscope with atomic resolution, operating in the tunneling regime in ultrahigh vacuum. The thermometer acts as an open three-terminal in a thermoelectric circuit. We investigate the temperature distributions in molecular junctions and graphene nanowires under thermal bias, and find that the local temperature in these systems exhibits quantum oscillations; quantum interference mimics the actions of a Maxwell Demon, allowing electrons from the hot electrode to tunnel onto the temperature probe when it is at certain locations near the system, and blocking electrons from the cold electrode, or vice versa.


10:12AM Y6.00012 Mechanism and Limitation of Heat Conduction in Three-Phase Polymer Composites Having Carbon Nanotubes and Inorganic Nanoparticles, HAI DUONG, FENG GONG, National University of Singapore, DIMITRIOS PAPAVASSILIOU, University of Oklahoma — For the first time, an Off-Lattice Monte Carlo method is developed successfully to predict thermal conductivities ($K_{th}$) of three-phase composites having carbon nanotubes (CNTs) and tungsten disulfide ($WS_2$) nanoparticles more accurately and faster than previous methods such as effective medium theories, molecular dynamics, and finite element methods. The $K_{th}$ predicted by our model using a random walk algorithm and taking into account various thermal boundary resistances at each interface and inter-CNT contact has an excellent agreement with experimental data. Our model can comprehensively explain the mechanism of heat conduction in complex composite structures. Effects of $WS_2$ and CNT morphologies (diameter, length, inter-contact, bundle), CNT concentrations, CNT orientations (parallel, random and perpendicular to heat flux) and thermal boundary resistances of CNT-polymer, $WS_2$-polymer, CNT-CNT, CNT-$WS_2$ on heat conduction limitation of the three-phase composites are also investigated systematically. Our model can be also applied to the biological and nanofluidic systems.


10:24AM Y6.00013 One or two dimensional electronic states in gold nanowires on germanium?
NICK DE JONG, EMMANOUIL FRANTZESKAKIS, University of Amsterdam, RENÉ HEIMBUCH, University of Twente, ANDREI VARKHALOV, Paul Scherrer Institute, HAROLD ZANDVLIET, University of Twente, MARK GOLDEN, University of Amsterdam — Inspired by the formulation of Tomonaga-luttinger liquid (TLL) theory in the 1960’s and its prediction of a spectacular breakdown of Fermi liquid theory in 1D, people have been searching for one dimensional electronic systems. With experimental developments like the advent of scanning tunneling microscopy (STM) and the manipulation of matter on the nanometer and sub nanometer scale, this field has become increasingly accessible for the experimentalist. Self-organised metallic chains on semiconductor surfaces are a class of systems which could harbor 1D behavior. In this field, Au nanowires on the Ge(100) surface have been the subject of debate, with reports of 1D bands from both ARPES and STM (1) and 2D bands in the same system displaying no Luttinger like behavior (2). Here we present high resolution ARPES data from both the Au/Ge(100) system and a new nanowire system: Au/Ge(110). By comparing these different systems with each other and with the electronic structure of the bare Ge(110) surface, we try to give a definitive answer on the question of the dimensionality of the electronic structure of Au nanowires on germanium.

1J. Schafer et al., PRL101, 236802 (2008)
2K. Nakatsuji, at al., PRB88, 081406(R) (2009)

1Support from FOM and the EU is gratefully acknowledged.

10:36AM Y6.00014 Observation of Franck-Condon Blockade in Single Molecules Gated by Local Electric Field
AIDI ZHAO, CHUNSHENG ZHOU, WEIYI WANG, Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, GUANGJUN TIAN, Division of Theoretical Chemistry & Biology, KTH Royal Institute of Technology, HUAN SHAN, SHULAI LEI, YINGBO ZHAO, YI LUO, QUNXIANG LI, BING WANG, J.G. HOU, Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China — Electron transport through single molecules is greatly influenced by a discrete spectrum of vibrational modes in strong electron-vibron coupling regime. Theory predicts a current suppression at low biases known as Franck-Condon blockade. However, how Franck-Condon blockade emerges in a real orbital-gated single molecule transistor is still elusive. In this study, by using a low-temperature scanning tunneling microscope, we report the real-space observation of Franck-Condon blockade in single molecules adsorbed on metal surfaces. The frontier molecular orbitals and charge state of the bare Ge(110) surface, we try to give a definitive answer on the question of the dimensionality of the electronic structure of Au nanowires on germanium.

1J. Schafer et al., PRL101, 236802 (2008)
2K. Nakatsuji, at al., PRB88, 081406(R) (2009)

10:48AM Y6.00015 Two-channel Kondo effect and the low-temperature crossover
ANDREW KELLER, LUCAS PEETERS, Stanford University, IRENEUSZ WEYMANN, Adam Mickiewicz University, CĂTALIN PAŞCU MOCA, Budapest University of Technology and Economics, University of Oradea, DIANA MAHALU, VLADIMIR UMANSKY, Weizmann Institute of Science, GERGELEY ZARAND, Budapest University of Technology and Economics, DAVID GOLDHABER-GORDON, Stanford University — The two-channel Kondo (2CK) state, where a spin-1/2 impurity is equally exchange-coupled to two independent reservoirs, is a canonical non-Fermi liquid state. Experimental observations are rare because of its sensitivity to common and hard-to-control perturbations. We implement experimentally a 2CK state in a coupled dot-system (Potok, et al., doi:10.1038/nature05556), and explore the physics of the low-temperature crossover: how magnetic field and gate voltage drive the system towards a Fermi liquid ground state. Our experimental findings are corroborated by detailed numerical renormalization group modeling of our device.

Support from FOM and the EU is gratefully acknowledged.

Friday, March 6, 2015 8:00AM - 10:48AM — Session Y7 — DCMP: Insulators: Transport, Spectroscopies, etc.
006B - Andrei Sushkov, University of Maryland
8:00 AM Y7.00001 Nanoscale Determination of the Mass Enhancement Factor in Lightly-Doped Bulk Insulator PbSe, KANE SCIPIONI, ILIJA ZELJKOVIC, DANIEL WALKUP, Boston College, YOSHINORI OKADA, Tohoku University, WENWEN ZHOU, Boston College, RAMAN SANKAR, National Taiwan University, GUOQING CHANG, National University of Singapore, YUNG JUI WANG, Northeastern University, HSIN LAN, National University of Singapore, ARUN BANSIL, Northeastern University, FANCHENG CHOU, National Taiwan University, ZIQIANG WANG, Boston College, VIDYA MADHAVAN, University of Illinois Urbana-Champaign — Phonons play a significant role in achieving the desired thermoelectric properties of many materials. Recent evidence suggests that electron-phonon coupling plays an important role in specifically the lead and bismuth chalcogenides. Thus, quantifying the interaction between phonons and electrons is of immense importance for understanding of these systems. Nearly all information about electron-phonon coupling is contained in the Eliashberg function of the material, but its precise extraction has in part been limited due to the lack of local experimental probes. By utilizing Landau level spectroscopy, we construct a method to directly extract the Eliashberg function, and demonstrate its applicability to lightly-doped thermoelectric bulk insulator PbSe. In addition to high energy, and access to both occupied and unoccupied electronic states, this novel experimental method could be used to detect variations in the mass enhancement factor (λ) on microscopic length scales, which opens up a unique pathway for investigating the effects of chemical defects, surface doping and strain on λ.

8:12 AM Y7.00002 Dimerization-Induced Fermi Surface Reconstruction in IrTe2, MANJIN EOM, KYOO KIM, Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea, YOUN JUNG JO, Department of Physics, Kyungbok University, Daegu 790-701, Korea, JUNJIE YANG, Laboratory for Pohang Emergent Materials, Pohang University of Science and Technology, Pohang 790-784, Korea, EUN SANG CHOI, National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, USA, BYUNG IL MIN, JAE-HOON PARK, Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Piscataway, New Jersey 08854, USA, JUN SUNG KIM, Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea — We report a de Haas-van Alphen (dHvA) oscillation study on IrTe2 single crystals showing complex dimer formations. By comparing the angle dependence of dHvA oscillations with band structure calculations, we show distinct Fermi surface reconstruction induced by a 1/5-type and a 1/8-type dimerizations. This verifies that an intriguing quasi-two-dimensional conducting plane across the layers is induced by dimerization in both cases. A phase transition from the 1/5-type to the 1/8-type dimerizations reveals that local instabilities associated with intra- and inter-dimer couplings are the main driving force for complex dimer formations in IrTe2.

8:24 AM Y7.00003 Enhanced terahertz emission from a femtosecond-laser-ablated photoconductor1, ATHANASIOS MARGIOLAKIS, Okinawa Inst of Sci & Tech, ZHEN-YU ZHAO, Department of Physics Shanghai Normal University, PETER HALE, JULIEN MADEO, MICHAEL MAN, Okinawa Inst of Sci & Tech, QUAN-ZHONG ZHAO, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, WEI PENG, Institute of Microsystem and Information Technology, Chinese Academy of Sciences, KESHAV DANI, Okinawa Inst of Sci & Tech — Terahertz (THz) emission properties from bow-tie antennas fabricated on a femtosecond-laser-ablated, semi-insulating gallium arsenide (SI-GaAs) photoconductor are investigated. The ablated material demonstrates increased photoabsorption resulting in increased photocurrent leading to a more efficient optical to THz efficiency. We use THz time-domain spectroscopy (THz-TDS) in order to compare the relative efficiency of the two fabricated devices. The influence of the excitation power and applied bias on the antennas electrodes for both ablated and non-ablated substrates is studied, highlighting the better performances of the ablated devices. A 60% enhancement in THz emission amplitude is observed in the frequency range 0.5 – 4 THz of the ablated SI-GaAs antenna, compared to untreated SI-GaAs. Our experimental results are in agreement with Drude-Lorentz numerical simulations using previously reported absorption and photocurrent properties of femtosecond laser ablated SI-GaAs based photoconductors. This material treatment provides a new way to achieve THz-TDS systems based on SI-GaAs antennas with an improved signal-to-noise ratio.

1National Natural Science Foundation of China (61307130, 11374316)

8:36 AM Y7.00004 Optical and Photo-stimulated EPR Studies on Intrinsic and Mn-doped Zinc Germinates Phosphors, XIAOJUN WANG, Department of Physics, Georgia Southern University, Statesboro, GA 30460, USA, ZHIYI HE, Optoelectronic Institute, Guilin University of Electronic Technology, Guilin, Guanxi, China 541004, LI MA, Department of Physics, George Southern University, Statesboro, GA 30460, USA — Intrinsic zinc germinates (Zn2GeO4) and Mn-doped Zn2GeO4 phosphors have been prepared using solid state reaction and their photoluminescence and phosphorescence studied. Phosphorescence from both the Mn2+ ions and host defects in Zn2GeO4 has observed upon UV excitation, while the Mn3+ ions present a longer persistent time than the defects. The charging process has also been studied and different behaviors of Mn2+ and defects observed. Electron paramagnetic resonance (EPR) and photo (UV)-stimulated EPR spectra have been collected for both host defects and Mn dopants from 20 K to room temperature. UV-induced EPR signal and the decay processes have been analyzed and provided a better understanding of the trapping mechanism for the phosphorescence. EPR signal from Mn2+ has been found decreasing after the UV excitation, indicating that the population of Mn2+ ions decreases in the trapping state and the valence change from Mn2+ to Mn3+ when hole trapping occurred.

8:48 AM Y7.00005 Large thermal Hall effect in a frustrated pyrochlore magnet1, MAX HIRSCHBERGER, Department of Physics, Princeton University, JASON KRIZAN, ROBERT J. CAVA, Department of Chemistry, Princeton University, N. PHUAN ONG, Department of Physics, Princeton University — In frustrated magnetism, the nature of the ground state and its elementary excitations are a matter of considerable debate. We present a detailed study of the full thermal conductivity tensor of a frustrated spin-ice pyrochlore Tb2Ti2O7. The off-diagonal response is large in this insulating material, despite the absence of itinerant electrons experiencing the Lorentz force. Our experiments over the temperature range of 0.8 – 200 K and in fields up to 14 T reveal a remarkable phenomenology: A sizeable field-linear Hall effect is observed below 100 K, and its slope with respect to magnetic field increases strongly as we cool the sample. We observe significant curvature in the field dependence of the Hall effect below 15 K. At the lowest temperatures, both of the initial slope and the initial slope constant in temperature, behavior reminiscent of ferromagnetic heat conduction in dirty metals. Experimental methods and verification of the intrinsic nature of the effect will be discussed.

1R.J.C. and N.P.O. are supported by a MURI grant (ARO W911NF-12-1-0461) and by the US National Science Foundation (grant number DMR 0819860).

9:00 AM Y7.00006 Time-dependent Elastic Deformation in Crystal: Insights from Metric Description and Berry Phase Effect, LIANG DONG, QIAN NIU, University of Texas at Austin — It is well known that elastic deformation in crystal can be described in the language of a metric. However, how the metric couples to the one-electron Hamiltonian in a deformed crystal is not very clear. By coordinate transformation from a Cartesian frame to lattice frame where all coordinates of ions are fixed, the metric emerges naturally both in the kinetic energy and potential energy of an electron. Besides, the velocity field of ions is also manifested in the Hamiltonian, which resembles the role of a vector potential. When the deformation slowly varies both in space and time, the wave-packet method can be used to study the Berry phase effect of deformation. This method applies to finite-strain cases and is accurate up to the first order of strain gradient. Different deformation effects are discussed, such as piezoelectricity, flexoelectricity and curving effect of a two-dimensional material.
9:12AM Y7.00007 Theoretical Studies of the Optical Properties of Eu doped Barium Mixed Halides: From X-ray Storage Phosphor to Bright Scintillator, SLIM CHOUROU, GREGORY BIZARRI, Lawrence Berkeley National Laboratory, ANDREW CANNING, Lawrence Berkeley National Laboratory and University of California, Davis — The Eu doped Ba mixed halide family BaBrX (X=F,Cl,Br,I) changes from being a widely used X-ray Storage Phosphor (BaBrF-Eu) to one of the brightest known new gamma ray detector scintillators (BaBrI-Eu). To help understand these contrasting optical properties and guide in the design of new and improved scintillator detectors, in collaboration with experimental groups, we have performed first principles theoretical studies of these materials. In particular we have studied their electron and hole trapping mechanisms and how that can explain their very different optical properties.

9:24AM Y7.00008 Single-particle dispersion in tetragonal CuO1, CLEMENS ADOLPHS, Univ of British Columbia, MONA BERCUI, Univ of British Columbia, Quantum Matter Institute — We study the single-hole dispersion in a layer of tetragonal CuO using a variational approach in which fluctuations between the copper spins are neglected. This approach has recently been applied to the single-particle dispersion in a CuO2 layer, where it successfully reproduces the experimentally observed dispersion. Since the CuO lattice can be viewed as two interspersed CuO2 lattices with weak intra-layer coupling, we expect this approach to be valid for CuO as well. The intra-layer coupling leads to an interesting spectral feature at \( k = (\pi/2, \pi/2) \), where it turns the minimum found in the CuO2 dispersion into a saddle point. This is a result of the intra-layer coupling lifting the degeneracy between quasiparticles occupying different sublattices.

1Financial support from NSERC and the UBC Four Year Doctoral Fellowship program are acknowledged.

9:36AM Y7.00009 Electric polarization and the photogalvanic effect in solids with a topological band structure1, BENJAMIN M. FREGOSO, Univ of California - Berkeley — It is known that solids without inversion symmetry can exhibit photogalvanic effects and intrinsic electric polarization, e.g., ferroelectrics. Understanding the relation between the strength of the induced current and the electric polarization has proven challenging. We report on model calculations with topologically non-trivial band structure aimed at quantifying these contributions.

1Partial support form Conacyt.

9:48AM Y7.00010 Room Temperature Ferroelectricity in Ultrathin SnTe Films1, KAI CHANG, Tsinghua University, JUNWEI LIU, Massachusetts Institute of Technology, HAICHENG LIN, KUN ZHAO, YONG ZHONG, SHUAI-HUA JI, KE HE, LILI WANG, XUCUN MA, Tsinghua University, LIANG FU, Massachusetts Institute of Technology, XI CHEN, QI-KUN XUE, Tsinghua University — The ultrathin SnTe films with several unit cell thickness grown on graphitized SiC(0001) surface have been studied by the scanning tunneling microscopy and spectroscopy (STM/S). The domain structures, local lattice distortion and the electronic band bending at film edges induced by the in-plane spontaneous polarization along (110) have been revealed at atomic scale. The experiments at variant temperature show that the Curie temperature \( T_c \) of the one unit cell thick (two atomic layers) SnTe film is as high as 280K, much higher than that of the bulk counterpart (~100K); and the 2-4 unit cell thick films even indicate robust ferroelectricity at room temperature. This \( T_c \) enhancement is attributed to the stress-free interface, larger electronic band gap and greatly reduced Sn vacancy concentration in the ultrathin films. The lateral domain size varies from several tens to several hundreds of nanometers, and the spontaneous polarization direction could be modified by STM tip. Those properties of ultrathin SnTe films show the potential application on ferroelectric devices.

1The work was financially supported by Ministry of Science and Technology of China, National Science Foundation and Ministry of Education of China.

10:00AM Y7.00011 A comparison of homogeneous and inhomogeneous absorption broadening in Nd doped Gadolinium Gallium Garnet1, CHRISTOPHER FERRI, SAYANTANI GHOSH, Department of Physics, University of California, Merced — We perform a temperature dependent optical absorption study of the \( ^{4}I_{9/2} \rightarrow ^{4}F_{3/2} (Z_{\text{c}} \rightarrow R_{\text{n}}) \) transition of the Neodymium dopant in Neodymium(III) doped Gadolinium Gallium Garnet. Absorption spectra are acquired for these transitions as a function of temperature from 12K to 300K. The absorption peaks are subsequently fit with Voigt profiles to measure the homogeneous and inhomogeneous broadening for each transition. We find that for the \( Z_{\text{c}} \rightarrow R_{\text{n}} \) transition the homogeneous and inhomogeneous broadening are of the same order. Below 80K, for the \( Z_{\text{c}} \rightarrow R_{\text{n}} \) transition, the homogeneous broadening is below the resolution of our spectrometer (1.85 cm\(^{-1}\)) resulting in a lower bound of \( \sim 18 \) ps for the excited state lifetime which is likely much slower. Furthermore, because of the resolution limit, the ratio of inhomogeneous broadening to homogeneous broadening for this transition has a lower bound of \( \sim 6 \).

1This work was funded by NSF grant DMR-1056860.

10:12AM Y7.00012 Thermal boundary conductance of hydrophilic and hydrophobic ionic liquids1, TAKAFUMI OYAKE, MASANORI SAKATA, SUSUMU YADA, The University of Tokyo, JUNICHIRO SHIOMI, The University of Tokyo, PRESTO Japan Science and Technology — A solid/liquid interface plays a critical role for understanding mechanisms of biological and physical science. Moreover, carrier density of the surface is dramatically enhanced by electric double layer with ionic liquid, salt in the liquid state. Here, we have measured the thermal boundary conductance (TBC) across an interface of gold thin film and ionic liquid by using time-domain thermoreflectance technique. Following the prior researches, we have identified the TBC of two interfaces. One is gold and hydrophilic ionic liquid, N,N-Diethyl-N-methyl-N-(2-methoxyethyl) ammonium tetrafluoroborate (DEME-BF4), which is a hydrophilic ionic liquid, and the other is N,N-Diethyl-N-methyl-N-(2-methoxyethyl) ammonium bis(trifluoromethanesulfonyl) imide (DEME-TFSI), which is a hydrophobic ionic liquid. We found that the TBC between gold and DEME-TFSI (19 MWm\(^{-2}\) K\(^{-1}\) ) is surprisingly lower than the interface between gold and DEME-BF4 (45 MWm\(^{-2}\) K\(^{-1}\) ). With these data, the importance of the wetting angle and ion concentration for the thermal transport at the solid/ionic liquid interface is discussed.

1Part of this work is financially supported by Japan Society for the Promotion of Science (JSPS) and Japan Science and Technology Agency. The author is financially supported by JSPS Fellowship.

10:24AM Y7.00013 Lattice dynamics of negative thermal expansion in ScF3, JASON HANCOCK, SAHAN HANDAKANDA, University of Connecticut, AYMAN SAID, BOGDAN LEU, Argonne National Laboratory, VLADIMIR VORONOY, Kirenskii Institute of Physics, Siberia — We present inelastic scattering spectroscopy of single-crystalline samples of negative thermal expansion material ScF3 to investigate the dispersion of lattice excitations in this unusual system. The spectra reveal important mechanistic information regarding the negative thermal expansion and show that a large class of fluorides can accommodate unconventional lattice dynamics. The connections to nonlinear and distinctly quantum phenomena will be discussed.

Acknowledgements: NSF DMR1310456

1. Acknowledgements: NSF DMR1310456

Friday, March 6, 2015 8:00AM - 11:00AM

Session Y8 DCMP: Ultrathin and Layered Materials 006C - Yuan Huang, Brookhaven National Laboratory

8:00AM Y8.00001 Sliding friction of adsorbed films on fullerene substrates with tunable conductivity1, SAMUEL KENNY, JACQUELINE KRIM, North Carolina State Univ — Friction at the nanoscale is known to encompass phononic, electrostatic, conduction electronic and magnetic effects [1], with electronic contributions being less well characterized than phononic contributions. Experiments measuring friction and diffusion of adsorbed gases on superconductors, for example, have revealed a decrease in resistance of the film concomitant with a decrease in sliding friction, but the electrical properties were difficult to fine tune.[2] Since their discovery nearly thirty years ago, C_{60} and related compounds have been widely studied in the context of photovoltaic research and related photoconductive properties. As such, they constitute ideal systems for studies of sliding friction on substrates with variable electrical resistivity.[3] We report here our quartz crystal microbalance studies of the frictional properties of adsorbate molecules sliding on fullerene films irradiated by visible laser light so as to tune the electrical resistivity of the substrate. [1] J. Krim, Advances in Physics, 61 (2012) pp. 155-323. [2] M. Highland et al., PRL (2006). [3] A. Hamed et al., PRB 47 (1993) pp. 10873-10880.

1. Acknowledgements: NSF DMR1310456

8:12AM Y8.00002 Water Interaction with Pristine and Nanopatterned Graphite Surfaces, DINKO CHAKAROV, Chalmers University of Technology — We used number of surface sensitive techniques to study and compare the interaction of water with pristine surface of highly oriented pyrolytic graphite and model nanostructured surfaces fabricated by hole-mask colloidal lithography and oxygen plasma etching. Surface morphology and concentration of defects play important role and determine the amount of water bound in two- and three-dimensional hydrogen-bonded networks and thus the structure of ice films. Similarly, the amount and concentration of inter sheet openings control the rate of water intercalation into graphite structures. The new findings are of particular interest for development of graphene exfoliation methods and for better understanding of graphene functionalization.

8:24AM Y8.00003 Quantum tunneling effects of 2-dimensional materials and their application for fast response of deep UV detectors1, PETER XIANPING FENG, Univ of Puerto Rico, ALI ALDALBAHI, Department of Chemistry, Collage of Science, King Saud University, Riyadh 11451, Saudi Arabia — We report on our approach to low substrate temperature, digital control, fast (~1 minute) synthesis of 2D single crystalline BNNSs. We focus our experiments on studies of various effects (temperature, tunneling, breakdown, polarization, subtract, thickness) on electrical and electronic properties, as well as on sensitivity, response and recovery times, repeatability, lifetime of BNNSs-based deep UV detectors. Raman scattering spectroscopy, X-ray diffraction (XRD), scanning electron microscope (SEM), Transmission electron microscopy (TEM) and electrometer were used to characterize the BNNSs. SEM and TEM measurements clearly indicate that each sample/membrane consists of a large amount of ultra-thin, high-quality BNNSs with distribution over entire surfaces of substrates (3×3 cm^2). Electrical characterization reveals the effects of temperature on the electrical conductivity of transparent BNNSs highly depend on the directions of observations in the 2D case but vanished from the 3D bulk materials or thick films.

1. This work is financially supported by Army research office/DoD grant (62826-RT-REP), as well as visiting professor program/KSU at KSA. Aldalbahi acknowledges the financial support by King Saud University

8:36AM Y8.00004 Observation of Single and Degenerated Charge Ordering in IrTe_{2} , HYO SUNG KIM, TAE-HWAN KIM, CALDES, IBS, POSTECH, Korea, SOORAN KIM, KYOO KIM, BYUNG IL MIN, CMTL, POSTECH, Korea, YONG-HEUM CHO, JUN JIE YANG, POSTECH, Korea, SANG-WOOK CHEONG, POSTECH, Korea, Rutgers, USA, HAN WOONG YEOM, CALDES, IBS, POSTECH, Korea, STM/STS TEAM, DFT CALCULATION COLLABORATION, SAMPLE SYNTHESIZE COLLABORATION — We investigate the intriguing broken symmetry low-temperature phases of IrTe_{2} using high-resolution scanning tunneling microscopy and spectroscopy. We experimentally separate the structural and electronic modulations of the stripe phase reported previously. This result clearly indicate the charge ordering in the surface Te layer, which is consistent with the expectation of the t_{z} dimerization and charge ordering model but unambiguously denies the charge-density-wave-and-soliton model. In addition, we observe a metastable honeycomb charge-ordered phase. This phase is thought to be a 3\sqrt{3} state of the stripe phase in analogy with the 2\sqrt{3} (3\sqrt{3}) state description of the checkerboard charge order (the skymion spin order).

8:48AM Y8.00005 Surface X-Ray Scattering Studies of TiSe_{2} Thin Films Grown on Se-Terminated GaAs(111)B, XINYUE FANG, Department of Physics, University of Illinois at Urbana-Champaign, HAWOONG HONG, YANG LIU, Advanced Photon Source, Argonne National Lab, SHIH-CHANG WENG, T.-C. CHIANG, Department of Physics, University of Illinois at Urbana-Champaign — Titanium Diselenide (TiSe_{2}) is a prototypical charge density wave (CDW) compound which transforms into a commensurate (2×2×2) superstructure upon cooling to below about 200 K. This transition is marked by substantial changes in the transport properties. Although this system has been studied extensively, the underlying physical mechanism for the structural distortion is still under debate. Studying thin films of TiSe_{2} provides a means to tune the electronic interactions through reduced dimension, and the effects on the CDW transition could provide valuable information about the mechanism. We have successfully grown TiSe_{2} epitaxial films on Se-terminated GaAs(111)B substrates via MBE. The optimum growth condition has been determined, and the CDW order parameter has been measured as a function of temperature for different film thicknesses.
We have provided reasonable atomic models of \( \sqrt{3} \times \sqrt{3} \) Ag surface. At sufficiently high silicon coverage, we observe the precipitation of crystalline, sp\(^2\)-bonded Si(111) domains. These domains are capped with a \( \sqrt{3} \) honeycomb-like phase that is indistinguishable from the silver-induced \( \sqrt{3} \) honeycomb-chained-trimer reconstruction on bulk Si(111). Further \textit{ex-situ} characterization with Raman spectroscopy, atomic force microscopy, cross-sectional transmission electron microscopy, and X-ray photoelectron spectroscopy reveals that these sheets are ultrathin sheets of bulk-like, (111) oriented, sp\(^2\) silicon. Even at the 2D limit, scanning tunneling spectroscopy shows that these silicon nanosheets exhibit semiconducting electronic characteristics.

9:24AM Y8.00008 Growth of Si thin film on 6H-SiC(0001)

HSIN-JU WU, M. TIEN HOANG, YUNTAO LI, PHILLIP N. FIRST, School of Physics, Georgia Institute of Technology — Graphene is much studied for its unusual electronic properties. Other carbon group elements such as silicon (Si) and germanium (Ge) are also predicted to have stable 2D phases for which the electronic structure and properties could be even more interesting. Silicon carbide, already an excellent insulating substrate for epitaxial graphene, could potentially play a similar role for Si. Commonalities in the substrate and processing may lead to the integration of carbon and silicon technologies. Here, we use surface analysis techniques (LEED, AES, STM) to investigate the formation of 2D Si on SiC(0001), under low pressures of silane or silicon. Similar methods allow control of surface graphene growth by compensating Si desorption from SiC. Among several Si-rich reconstructions, we find a single stable hexagonal phase, at a coverage close to twice the Si density predicted for silicene, and with a unit cell consistent with a commensurate layer of silicon or silicene. For a graphitized SiC starting surface, silane is shown to produce a grafted SiC starting surface, silane is shown to etch graphene, reforming SiC.

9:36AM Y8.00009 Layering-induced Superlubricity: Gold on Graphite

ANITA VANOSSE, CNR-IOM Democritos National Simulation Center, Via Bonomea 265, 34136 Trieste, Italy, ROBERTO GUERRA, ERIO TOSATTI, International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy, NANOFRICTION GROUP SISSA TEAM — By means of realistic MD simulations, we explore the static friction trend as a function of the true contact area and the model dimensionality for 2D gold nanoislands and 3D gold nanoclusters deposited on graphite, interesting tribological systems whose slow and fast dynamics have been previously investigated [1]. For increasing island size, because of the relative gold-graphite lattice mismatch, the interface stress energy has the chance to pile up by forming frustrated unmatched (i.e., incommensurate) regions and to develop a continuous solitonic pathway, foreshadowing a possible condition for the occurrence of ultra-low-friction regimes. The significant reduction of the depinning threshold, towards superlubricity, with the system dimensionality can be ascribed to a layering-induced effective stiffness of the interface, favoring the natural Au-C lattice incommensurability.


9:48AM Y8.00010 Electrostatic Manipulation of Graphene On Graphite

CARLOS UNTIEDT, CARMEN RUBIO-VERDU, GIOVANNI SAENZ-ARCE, JESÚS MARTÍNEZ-ASENCIO, DAVID C. MILAN, Universidad de Alicante, Spain, MOHAMED MOAIED, JUAN J. PALACIOS, Universidad Autónoma de Madrid, MARIA JOSE CATURLA, Universidad de Alicante, Spain — We report the use of a Scanning Tunneling Microscope (STM) under ambient and vacuum conditions to study the controlled exfoliation of the last layer of a graphite surface when an electrostatic force is applied from a STM tip. In this work we have focused on the study of two parameters: the applied voltage needed to compensate the graphite interlayer attractive force and the one needed to break atomic bonds to produce folded structures. Additionally, we have studied the influence of edge structure in the breaking geometry. Independently of the edge orientation the graphite layer is found to tear through the zig-zag direction and the lifted layer shows a zig-zag folding direction. Molecular Dynamics simulations and DFT calculations have been performed to understand our results, showing a strong correlation with the experiments.
10:12AM Y8.00012 Effects of Surface Roughness and Electron-Phonon Interaction on Electron Transport of Ultrathin Epitaxial Copper Films¹, YUKTA TIMALISNA, ANDREW HORNING, ROBERT SPIVEY, KIM LEWIS, GWO-CHING WANG, TOH-MING LUI, Center for Materials, Devices & Integrated Systems, and Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute — We report effects of surface roughness and electron-phonon interaction on transport properties of electrons in ultrathin epitaxial copper films of thickness ranging from 5 nm to 500 nm grown on Si(100) substrates. The transport of electrons in the film was examined by measuring the temperature dependent resistivity in the temperature range of 5 K to 300 K. We demonstrate that the temperature independent component of resistivity can be described by the root-mean-square-surface roughness and lateral correlation length with no adjustable parameter, using a recent quasi-classical model developed by Chatterjee and Meyerovich [1]. However, the temperature dependent component of the resistivity can be described using the Bloch-Grüneisen formula with a thickness dependent electron-phonon coupling constant and a thickness dependent Debye temperature. We show that the increase of the electron-phonon coupling constant with the decrease of film thickness gives rise to an enhancement of the temperature dependent component of the resistivity.


¹This work is supported in part by New York State Foundation of Science, Technology and Innovation through Focus Center-New York.

10:24AM Y8.00013 Interplay between Electromagnetic and Coulomb Coupling, DANHONG HUANG, US Air Force Research Laboratory, GODFREY GUMBS, Hunter College of the City University of New York, ALEXEI MARADUDIN, University of California at Irvine, BO GAO, Hunter College of the City University of New York — Both the transverse electromagnetic and longitudinal coulomb couplings of the surface-plasmon mode to the collective excitation of Dirac electrons are investigated. The unique features of coupled quantum-plasmon modes are demonstrated. The predicted dispersion relations of these quantum-plasmon modes should be experimentally observable. For a double-layer graphene structure, the interplay between the interlayer Coulomb forces and the electromagnetic coupling to each layer is calculated. The effective polarizability matrix for coupled double-layer graphene and a semi-infinite conductor is obtained for constructing an effective-medium theory, which includes correlation effects from the Coulomb interaction between electrons in graphene and the conductor as well as the electromagnetic field between them.

10:36AM Y8.00014 Semiconductor- to Metallic-like Behavior in Bi Thin Films Deposited on (100) KCl Substrate, THANH NHAN BUI, IMCN/NAPS, JEAN-PIERRE RASKIN, ICTEAM/ELEN, BENOIT HACKENS, IMCN/NAPS — Bi thin films, with a thickness of 100 nm, are deposited by electron-beam evaporation on a freshly cleaved (100) KCl substrate. The deposition temperature ranges from room temperature up to 170 °C. Scanning electron microscopy reveals that films deposited at room temperature present a maze-like microstructure on its surface typical of the rhombohedral (110) texture as confirmed by X-ray diffraction. By heating the substrate to a temperature above 80 °C during the deposition, another microstructure appears characterized by concentric triangular shapes corresponding to the trigonal texture. Temperature dependence of the resistivity from room temperature down to 10K shows a semiconductor-like behavior for films deposited at room temperature and a metallic-like behavior for films deposited above 80 °C. From low temperature magnetoresistance measurements (at 10K and up to 6 T), we extract the electronic transport parameters (mobility and charge carrier concentration). These data, together with the average grain size, help us provide an explanation for the transition between both behaviors.

10:48AM Y8.00015 Synthesis of Ultra-Thin Single Crystal MgO/Ag/MgO Multilayer for Controlled Photocathode Emissive Properties, DANIEL VELAZQUEZ, RACHEL SEIBERT, ZIKRI YUSOF, JEFF TERRY, LINDA SPENTZOURIS, Illinois Institute of Technology — Developments of new accelerator technologies such as free-electron lasers and high-energy accelerators, among others, continuously set requirements for particle sources to produce higher beam flux. The emissive properties of these photocathodes directly influence the accelerator beam flux and thus the performance of the accelerator as a whole. The objective of this project is to test the possibility of engineering the photomissive properties of materials for potential use as photocathodes. For this purpose we use a Density Functional Theory calculations by collaborator Karoly Nemeth et al. [Phys. Rev. Lett. 104, 046801, 2010], which predict a thickness dependent change in the band structure that results in a change in the work function and dispersion of occupied states at the Fermi level. Multilayered MgO/Ag/MgO in the crystallographic orientations (001) and (111) were grown on Ag/MgO(001) and Ag/Si[111], respectively using pulsed laser deposition (PLD). A series of surface probing techniques were used to characterize physical, chemical and photomissive properties of the films.

Friday, March 6, 2015 8:00AM - 11:12AM –
Session Y9 DMP: Focus Session: Honeycomb and Pyrochlore Lattices
006D - Ribhu Kaul, University of Kentucky

8:00AM Y9.00001 Electronic structure of the harmonic-honeycomb iridates α, β, γ-Li₂IrO₃, ROSER VALENTI, YING LI, HARALD O. JESCHKE, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany — Using ab-initio density functional theory we investigate the electronic and magnetic properties of the harmonic-honeycomb iridates α, β, γ-Li₂IrO₃ with honeycomb, hyperhoneycomb and stripohoneycomb crystal structures, respectively. We describe the distinct features of each class of systems in terms of possible Ir-based molecular-orbitals and the implications on the magnetism in these materials. We further relate the electronic structure to proposals of generalized Kitaev-Heisenberg models.

³This work is supported by the Deutsche Forschungsgemeinschaft under Grant No. FG 1346

8:12AM Y9.00002 Magnetic Excitations in α-RuCl₃, STEPHEN NAGLER, ARNAB BANERJEE, QCMD, Oak Ridge National Laboratory, CRAIG BRIDGES, CSD, Oak Ridge National Laboratory, JIAQIANG YAN, MSTD, Oak Ridge National Laboratory, DAVID MANDRUS, Dep. of Mat. Sci. and Eng., U. Tennessee, MATTTHW STONE, ADAM ACZEL, QCMD, Oak Ridge National Laboratory, LING LI, Dep. of Mat. Sci. and Eng., U. Tennessee, JIANQUAN XU, Dep. of Physics, U. Tennessee, MARK, LUMSDEN, QCMD, Oak Ridge National Laboratory, JOHANNES KNÖLLE, RODERICH MOESSNER, Max-Planck-Institut, Dresden, ALAN TENNANT, NSciD, Oak Ridge National Laboratory — The layered material α-RuCl₃ is composed of stacks of weakly coupled honeycomb lattices of octahedrally coordinated Ru³⁺ ions. The Ru ion ground state has 5 d electrons in the low spin state, with spin-orbit coupling very strong compared to other terms in the single ion Hamiltonian. The material is therefore an excellent candidate for investigating possible Heisenberg-Kitaev physics. In addition, this compound is very amenable to investigation by neutron scattering to explore the magnetic ground state and excitations in detail. Here we discuss new time-of-flight inelastic neutron scattering data on α-RuCl₃. A high energy excitation near 200 meV is identified as a transition from the single ion J=1/2 ground state to the J=3/2 excited state, yielding a direct measurement of the spin orbit coupling energy. Higher resolution measurements reveal two collective modes at much lower energy scales. The results are compared with the theoretical expectations for excitations in the Heisenberg - Kitaev model on a honeycomb lattice, and show that Kitaev interactions are important.

³Research at SNS supported by the DOE BES Scientific User Facilities Division
8:24 AM Y9.00003 Lattice-Tuned Magnetism of Ru\textsuperscript{4+}(4d\textsuperscript{4}) Ions in Single-Crystals of the Layered Honeycomb Ruthenates: Li\textsubscript{2}RuO\textsubscript{3} and Na\textsubscript{2}RuO\textsubscript{3}\textsuperscript{1,2}, JINCHEN WANG, Renmin Univ of China, JASMINKA TERZIC, TONGFEI QI, University of Kentucky, FENG YE, Oak Ridge National Laboratory, SHUJUAN YUAN, SAICHARAN ASWARTHAM, University of Kentucky, SERGEO STREITSOV, Ural Federal University, DANIEL KHOMSKII, Universitaet zu Koeln, RIBHNU KAIL, GANG CAO, University of Kentucky — We synthesize and study single crystals of the layered honeycomb lattice Mott insulators Na\textsubscript{2}RuO\textsubscript{3} and Li\textsubscript{2}RuO\textsubscript{3} with magnetic Ru\textsuperscript{4+}(4d\textsuperscript{4}) ions. The newly found Na\textsubscript{2}RuO\textsubscript{3} features a nearly ideal honeycomb lattice and orders antiferromagnetically at 30 K. Single-crystals of Li\textsubscript{2}RuO\textsubscript{3} adopt a honeycomb lattice with either C2/m or more distorted P2\textsubscript{1}/m below 300 K, depending on detailed synthesis conditions. We find that Li\textsubscript{2}RuO\textsubscript{3} in both structures hosts a well-defined magnetic state, in contrast to the singlet ground state found in polycrystalline Li\textsubscript{2}RuO\textsubscript{3}. A phase diagram generated based on our results uncovers a new, direct correlation between the magnetic ground state and basal-plane distortions in the honeycomb ruthenates.

\textsuperscript{1}This work was supported by NSF via Grant DMR 1265162.

8:36 AM Y9.00004 Majorana metals in spin-orbit entangled quantum matter, SIMON TREBST, University of Cologne — The largely accidental balance of electronic correlations, spin-orbit entanglement, and crystal field effects of 5d transition metal oxides results in a remarkably broad variety of metallic and insulating states. In this talk, we will discuss the physics of spin-orbit entangled j=1/2 Mott insulators whose microscopic description gives rise to three-dimensional variants of the Kitaev model. The analytical tractability of this model allows to study the fractionalization of these moments into Majorana fermions (and a Z2 gauge field) and their emergent collective behavior. We show that the Majorana fermions generically form metallic states which precisely character intimately depends on the underlying lattice structure. Examples range from the well known Dirac semimetal of the two-dimensional Kitaev honeycomb model to three-dimensional metals, in which the gapless modes either form a Fermi line or a Fermi surface akin to a conventional metal [1]. We further discuss our recent finding of a Weyl spin liquid — a state with topologically protected Weyl nodes in the bulk and associated Fermi arcs on the surface [2]. Finally, we comment on the thermodynamic and transport signatures of these various Majorana metals.

Joint work with M. Hermanns and K. O’Brien.


9:12 AM Y9.00005 Gap Measurement of Na\textsubscript{2}IrO\textsubscript{3} with a Scanning Tunneling Microscope\textsuperscript{3}, ARMIN ANSARY, University of Kentucky, JOHN NICHOLS, Oak Ridge National Laboratory, GANG CAO, KWOK-WAI NG, University of Kentucky — 5d transition metal oxides such as iridates have recently stimulated substantial interest. Many exciting new phases can be found in this class of materials because of the comparable strength between spin-orbit coupling and the Coulomb interaction. In particular, we have studied high quality single crystal Na\textsubscript{2}IrO\textsubscript{3} with a scanning tunneling microscope (STM). Na\textsubscript{2}IrO\textsubscript{3} has a layered structure with a honeycomb lattice. The gap is measured to be about 400 meV according to the dI/dV curve, which is consistent with optical measurements. We will show topographic images and discuss the evolution of the density of states and the behavior of the gap from room temperature down to 100 K.

\textsuperscript{3}This work was supported by the National Science Foundation under grant DMR-1265162.

9:24 AM Y9.00006 Spin-orbit correlated magnetic order in honeycomb \(\alpha\)-RuCl\textsubscript{3}, VIJAY SHANKAR VENKATARAMAN, HEUNG-SIK KIM, HAE-YOUNG KEE, University of Toronto — There has been a lot of recent interest in the combined effects of spin-orbit coupling (SOC) and electronic correlations in transition metal compounds. RuCl\textsubscript{3} with layered honeycomb structure was proposed as a candidate material, where SOC boosts the electronic interaction, leading to an insulating phase. However, the role of SOC is not clear in materials with 4d-orbitals, since SOC strength is weaker than 5d-orbitals. Here we study electronic band structures of honeycomb RuCl\textsubscript{3} using ab-initio and tight binding methods, and estimate its SOC strength. We find that SOC in RuCl\textsubscript{3} is not strong enough to justify an effective j_{ eff} = 1/2 single band unlike the iridates. However, when electronic interactions are introduced, a magnetic order develops, and upper- and lower-Hubbard bands are characterized by j_{ eff} = 1/2 and 3/2, respectively. Within a mean field theory with multi-orbital bands, we find that a zig-zag magnetic order is a ground state. Experimental implications are also discussed.

9:36 AM Y9.00007 Structure and magnetic ground states of spin-orbit coupled compound alpha-RuCl\textsubscript{3}\textsuperscript{1}, ARNAB BANERJEE, Quantum Condensed Matter Division, ORNL, USA, CRAIG BRIDGES, Chemical Sciences Division, ORNL, USA, JIAQIANG YAN, Material Sciences Division, ORNL, USA, DAVID MANDRUS, Department of Physics, University of Tennessee, Knoxville, USA, MATTHEW STONE, ADAM ACZEL, Quantum Condensed Matter Division, ORNL, USA, LING LI, YUEN YIU, Department of Physics, University of Tennessee, Knoxville, USA, MARK LUMSDEN, BRYAN CHAKOUMAKOS, Quantum Condensed Matter Division, ORNL, USA, ALAN TENNANT, Neutron Sciences Directorate, ORNL, USA, STEPHEN NAGLER, Quantum Condensed Matter Division, ORNL, USA — The layered material alpha-RuCl\textsubscript{3} is composed of stacks of weakly coupled honeycomb lattices of octahedrally coordinated Ru\textsuperscript{3+} ions. The Ru ion ground state has 5 d electrons in the low spin state, with spin-orbit coupling very strong compared to other terms in the single ion Hamiltonian. The material is therefore an excellent candidate for investigating possible Heisenberg-Kitaev physics. In addition, this compound is very amenable to investigation by neutron scattering to explore the magnetic ground state and excitations in detail. In this talk, we discuss the synthesis of phase-pure alpha-RuCl\textsubscript{3} and the characterization of the magnetization, susceptibility, and heat-capacity. We also report neutron diffraction on both powder and single crystal alpha-RuCl\textsubscript{3}, identifying the low temperature magnetic order observed in the material. The results, when compared to theoretical calculations, shed light on the relative importance of Kitaev and Heisenberg terms in the Hamiltonian.

\textsuperscript{1}The research is supported by the DOE BES Scientific User Facility Division

9:48 AM Y9.00008 Quantum phase transition and anomalous Hall effect in a pyrochlore Kondo lattice, SARAH GREEF, WENXIN DING, QIMIAO SI, Rice University — Motivated by recent experimental evidence for a possible chiral spin liquid phase in the metallic pyrochlore heavy fermion iridates \(\text{Pr}_2\text{Ir}_2\text{O}_7\) [Phys.Rev.Lett. 96, 087204 (2006), Phys.Rev.Lett 98, 057203 (2007), Nature 463, 210 (2010)] as well as quantum critical behavior in this system [Nat. Mater. 13, 356 (2014)], we study the effect of Kondo coupling on various spin liquid states of the Heisenberg model on pyrochlore lattices, including states exhibiting time-reversal-symmetry-breaking. Using a slave fermion representation for the f-moments which are coupled to conduction electrons, we study the large-N limit to determine the ground state energies of various feasible states and map out the zero-temperature phase diagram. We calculate the anomalous Hall response across the quantum phase transition from the Kondo destroyed phase to the Kondo screened phase. Finally we discuss the implications of our results for the properties of \(\text{Pr}_2\text{Ir}_2\text{O}_7\).
10:00AM Y9.00009 Ab Initio Simulations of the Structure and Energetics of Harmonic Honeycomb Iridates 1. TESS SMIDT, QIMIN YAN, JEFFREY NEATON, Univ of California - Berkeley — Edge-sharing iridates present an exciting opportunity to study the competition of Mott insulator physics and strong spin-orbit coupling. Harmonic honeycomb iridates are a recently discovered homologous series of stoichiometrically identical structures that host anisotropic magnetism and exotic spin ordering. We use density functional theory and lattice kinetic Monte Carlo to investigate structural, energetic, and entropic trends in determining the equilibrium ground states of harmonic honeycomb iridates. We predict the formation energies and geometry of as-yet unsynthesized series members and propose why some structures are more prevalent than others.

1This work is supported by NSF and DOE; computations provided by DOE NERSC.

10:12AM Y9.00010 Rotated Heisenberg model 1. FADI SUN, JINWU YE, Mississippi State University, WU-MING LIU, Institute of Physics Chinese Academy of Sciences — We show that Rotated Heisenberg (RH) model is a new class of quantum spin models to describe magnetic materials with strong spin-orbit couplings (SOC). We introduce Wilson loops to characterize frustrations and gauge equivalent class. For a special equivalent class, we identify a new spin-orbital entangled commensurate ground state. It supports a novel gapped elementary excitation named as in-commensurate magnons which have two gap minima continuously tuned by the SOC strength. At low temperatures, the in-commensurate magnons lead to dramatic effects in all physical quantities such as density of states, specific heat, magnetization and various spin correlation functions. At high temperatures, the specific heat and transverse spin structure factors depend on the SOC strength explicitly. We argue that one gauge may be realized in current experiments and other gauges may also be realized in near future experiments. Various experimental detections are discussed.

1This work is supported by NSF-DMR-1161497, NSF-11174210.

10:24AM Y9.00011 Collective modes in two- and three-dimensional electron systems with Rashba spin-orbit coupling 1. SAURABH MAITI, University of Florida, Gainesville and National High Magnetic Field Lab, Tallahassee, VLADIMIR ZYUZIN, DMITRII MASLOV, University of Florida, Gainesville — In addition to charge plasmons, a 2D electron system with Rashba-type spin-orbit coupling (SOC) also supports three collective modes in the spin sector: the chiral-spin modes. We study the dispersions of the charge and spin modes and their coupling to each other within a generalized RPA for arbitrarily strong SOC, and both in 2D and 3D systems. We find that the charge plasmons are coupled to only one of the three chiral-spin modes. In 3D, the chiral-spin modes are strongly damped by particle-hole excitations and disappear for weak electron-electron interaction. Landau damping of the chiral-spin modes in 3D is directly related to the fact that, in contrast to 2D, there is no gap for particle-hole excitations between spin-split subbands. The gapless continuum is also responsible for Landau damping of the charge plasmon in 3D - a qualitatively new feature of the SOC system. The in-plane transverse chiral-spin mode shows up as dispersing peak in the optical conductivity at finite wave number which can be measured in the presence of diffraction gratings. We also discuss possible experimental manifestations of chiral-spin modes in semiconductor quantum wells such InGaAs/AlGaAs and 3D giant Rashba materials of the BiTel family.

1This work was supported by the National Science Foundation via grant NSF DMR-1308972.

10:36AM Y9.00012 Anderson Impurity in Dirac and Weyl semimetals 1. JINHUA SUN, DONG-HUI XU, FU-CHUN ZHANG, YI ZHOU, Department of Physics, Zhejiang University, Hangzhou, China — We utilize variational method to study the Kondo screening of an Anderson impurity in three-dimensional Dirac and Weyl semimetals. We find that the spin correlation between the magnetic impurity and conduction electrons in both the systems are strongly anisotropic due to the spin-orbit coupling, and the spin-spin correlations are of power-law decay in both systems. The differences between Dirac and Weyl semimetals are also investigated.

10:48AM Y9.00013 Magnetic-field control of topological charge-transport properties in Nd$_3$Ir$_2$O$_7$ 1. KENTARO UEDA, Department of Applied Physics and Quantum-Phase Electronics Center (QPEC), University of Tokyo, BOHM-JUNG YANG, RIKEN Center for Emergent Matter Science (CEMS), JUN FUJOKA, Department of Applied Physics and Quantum-Phase Electronics Center (QPEC), University of Tokyo, JUNICHI SHIOGAI, ATSUSHI TSUKAZAKI, Institute for Materials Research, Tohoku University, NAOTO NAGAOSA, YOSHINORI TOKURA, Department of Applied Physics and Quantum-Phase Electronics Center (QPEC). University of Tokyo — Nd$_3$Ir$_2$O$_7$ is a novel quantum phase with topological properties where the linear-dispersive band with a surface Fermi arc state is realized in a three-dimensional bulk. Pyrochlore-type R$_2$Ir$_2$O$_7$ is one of the promising candidates for realization of the Weyl semimetal. In this system, the magnetic ordering pattern is predicted to play a key role for characterizing its electronic band structure. We report the magnetic-transport properties in Nd$_3$Ir$_2$O$_7$ single crystals for several magnetic field directions. We reveal that all-in-all-out type magnetic domain walls, at which the conductive mode inherent to the surface state of Weyl semimetal may be preserved, are finely controlled by an applied field along [111] direction showing unique hysteresis in resistivity. With applied field along [001] direction, the Nd-4f moment forms 2-in-2-out configuration that turns the isolating state into the anomalous metallic one near the Weyl (semi-)metal phase. A mean-field calculation consistent with topological properties where the linear-dispersive band with a surface Fermi arc state is realized in a three-dimensional bulk.

1This work was supported by the National Science Foundation via grant NSF DMR-1308972.

11:00AM Y9.00014 Intrinsic Damping of Collective Spin Modes in a Two-Dimensional Fermi Liquid with Spin-Orbit Interaction 1. DMITRII MASLOV, University of Florida, Gainesville, SAURABH MAITI, University of Florida, Gainesville and National High Magnetic Field Lab., Tallahassee — We address the issue damping of spin collective modes in systems with spin orbit coupling in 2D. We show that these modes exist for arbitrary nature of spin-orbit coupling and are intrinsically damped even in the long wavelength limit. This damping is driven by electron-electron interactions and is unique to spin orbit coupled systems. Its origin is linked to an imperfect cancellation of the self energy and vertex contributions of the interaction. In the Fermi-liquid language, this is an effect arising from residual interaction between quasiparticles. This damping mechanism exists already at T=0 and without impurities and/or phonons. We also discuss the consequences of this damping for the experiment.

1This work was supported by the National Science Foundation via grant NSF DMR-1308972.

Friday, March 6, 2015 8:00AM - 10:36AM
Session Y10 DCMP: Topological Insulators: Band Structures Theory 007A - Philip Brydon, University of Maryland
8:00AM Y10.00001 The Viscoelastic Response of Topological Tight Binding Models. HASSAN SHAPOURIAN, TAYLOR L. HUGHES, SHINSEI RYU, Univ of Illinois - Urbana — The topological response to external perturbations is an effective probe to characterize different topological phases of matter. The Hall viscosity is an example of such a response which has been the subject of a great interest recently. So far, most of studies have focused on the continuum field theories. Here, we investigate this response for the tight binding (lattice) models. The presence of lattice breaks the continuous translational symmetry to a discrete symmetry and this causes two complications: it introduces a new length scale associated with lattice constant and makes the momentum a compact variable. We develop two different methods of how to implement a lattice deformation: (1) the lattice distortion is equal to one half of (1−ϕ)/2 (ϕ is the hopping parameter) micropipet view is adopted and the lattice deformation appears in the gradient expansion of the hopping matrix elements. Consequently, we compute the Hall viscosity through the linear response (Kubo) formula. We examine these methods for three models: the Hofstadter model, the Chern insulator, and the surface of a 3D topological insulator. Our results in certain regimes of parameters, where the continuum limit is relevant, are in agreement with the field theory calculations.

8:12AM Y10.00002 Direct Manifestation of the Band Topology via the Zak Shift of the Wannier-Stark Ladder. WOO-ROM LEE, KWON PARK, Korea Inst for Advanced Study — Topological phases of matter have been topics of intense interest in modern condensed matter physics. Numerous efforts have been devoted to investigating various exotic properties of materials with non-trivial band topology. The dissipationless transport via gapless helical edge or surface states is one of the defining properties of such materials, which, however, has been very difficult to realize in experiment due to various backscattering sources induced in the sample boundaries. In this work, we show that there is a fundamental connection between the non-trivial topology of the band structure and the Zak shift of the Wannier-Stark ladder emerging under a static electric field. As an application of this connection, we propose a novel spectroscopic method to directly manifest the band topology by counting the winding number of the Zak phase across the first Brillouin zone, which is shown to be robust against electron-impurity scattering.

8:24AM Y10.00003 Strong orientation dependence of electronic properties of Antimony Selenide (Sb$_2$Se$_3$) nanostructures. RAJASEKARAKUMAR VADAPOO, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015, USA, SRIDEVI KRISHNAN, Institute of Materials Science, University of Connecticut, CT 06269, USA, HULUSI YILMAZ, Dept. Of Engineering, Zaman University, Phnom Penh, Cambodia, CARLOS MARIN, Institute for Functional Nanomaterials and Department of General Engineering, University of Puerto Rico, Mayaguez, PR 00681, USA — Antimony Selenide has applications in thermoelectric, photovoltaic and optical storage. Recently, it was demonstrated that bulk material under high pressure becomes a topological insulator and further undergoes insulator to metal to superconducting transitions. The Sb$_2$Se$_3$ nanostructures reported so far exhibit direct bandgaps, whereas the bulk has an indirect gap. Considering different crystallographic orientations of synthesized nanostructures and the anisotropic nature of its structure, we have studied the influence of orientation on their electronic behavior. Using first principle methods, we explore the stability of nanowires in different orientations and its influence on electronic structure. We find confinement effects for the narrower nanostructures, whereas the [001] orientation showed a reduced bandgap. This anomalous behavior is discussed considering that bandgap reduction could be attributed to recent experimental findings of an insulator-metal transition, which is related to topological quantum transition. The surface reconstructions show similarities to the distortion of polyhedras occurring in bulk Sb$_2$Se$_3$ under high pressure, which are related to the insulator-metal transition and superconductivity at 8.0 K.

8:36AM Y10.00004 Topological characterization and dynamics of a fermionic fractional Chern insulator. FRANK POLLMANN, ADOLFO GRUSHIN, JOHANNES MOTRUK, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, MICHAEL ZALETEL, Stanford University, US — Using the density matrix renormalization group (DMRG) method on a cylinder geometry, we characterize the fractional Chern insulator (FCI) state in the Haldane honeycomb lattice model at ν = 1/3 filling of the lowest band and check its stability. We investigate the chiral and topological properties of this state through (i) its Hall conductivity, (ii) the topological entanglement entropy, (iii) the U(1) charge spectral flow of the many body entanglement spectrum, and (iv) the charge of the anyons. As the interaction strength is lowered, we observe a direct transition from the FCI into a metallic phase and find indications for the transition to be of first order. Since our approach does not rely on any band or subspace projection, we are able to prove the stability of the fractional state in the presence of interactions exceeding the band gap, as has been suggested in the literature. Additionally, we investigate the characteristic dynamics of the FCI phase using time dependent DMRG.

8:48AM Y10.00005 Disorder and inversion symmetry breaking effect in Chern insulators. LUCIAN COVACI, University of Antwerp, JOSE GARCIA, TATIANA RAPPORPT, Universidade Federal do Rio de Janeiro — We show that Chern insulators with and without inversion symmetry respond differently to strong disorder. We consider a Haldane model with Anderson disorder and use a real-space numerical approach to calculate the conductivity tensor of a Haldane model in the presence of Anderson disorder. The inversion symmetry is explicitly broken by adding a sub-lattice potential $\Delta_{AB}$. While disorder closes the gap and destroys the Chern insulator in the system with inversion symmetry, the quantum anomalous Hall effect is insensitive to increasing Anderson disorder in the case of broken symmetry. In this case, the symmetry breaking works as a valley filter that protects the topological state from inter-valley scattering and strong disorder gives rise to a novel topological state that is similar to the topological Anderson insulator.

9:00AM Y10.00006 Topological phase transition in the Hofstadter- Hubbard model. HSIANG-HSUAN HUNG, Department of Physics, University of Texas at Austin, LEI WANG, MATTHIAS TROYER, Theoretische Physik, ETH — We study the interplay between topological and conventional long-range order of attractive fermions in a time-reversal-symmetric Hofstadter lattice using quantum Monte Carlo simulations, focusing on the case of one-third flux quantum per plaquette. At one-third filling, the noninteracting system is a topological insulator, and a nonzero critical interaction strength is needed to drive a transition from the quantum spin Hall insulator to a superfluid. We probe the topological signature of the phase transition by threading a magnetic flux through a cylinder and observe quantized topological charge pumping.

9:12AM Y10.00007 Non-trivial edge physics in a featureless Mott insulator. BRAYDEN WARE, Univ of California - Santa Barbara, ITAMAR KIMCHI, Univ of California - Berkeley, SIDDHARTH PARMESWARAN, Univ of California - Irvine, BELA BAUER, Station Q, Microsoft Research, Santa Barbara, CA — While the Lieb-Schultz-Mattis theorem forbids the existence of fully symmetric quantum paramagnetic phases on lattices with fractional filling of particles per unit cell, such a phase is in principle allowed with certain fractional numbers of particles per site on non-Bravais lattices, including half-filling on the honeycomb lattice. It has been shown that a non-interacting Hamiltonian of spinless fermions or bosons cannot have such a symmetric insulating ground state, and an explicit construction using interactions is challenging. Recently, Kimchi et al. constructed a wavefunction for bosons at half-filling that does not break any symmetries and is not topologically ordered—and in this sense is a featureless insulator in the bulk. Here, however, we reveal that this wavefunction exhibits non-trivial structure at the edge. We apply recently developed techniques based on a tensor network representation of the wavefunction to demonstrate the presence of a gapless entanglement spectrum and a non-trivial action of combined charge-conservation and spatial symmetries on the edge. We will also discuss the possibility of finding a parent Hamiltonian and analyzing the existence of a symmetry-protected topological phase around this state.

9:24AM Y10.00008 ABSTRACT WITHDRAWN
9:36AM Y10.00009 Bound states of three fermions forming symmetry-protected topological phases. CHONG WANG, Massachusetts Inst of Tech-MIT — We propose a simple theoretical construction of certain short-range entangled phases of interacting fermions, by putting the bound states of three fermions (which we refer to as clustons) into topological bands. We give examples in two and three dimensions, and show that they are distinct from any free fermion state. We further argue that these states can be viewed as combinations of certain free fermion topological states and bosonic symmetry-protected topological (SPT) states. This provides a conceptually simple understanding of various SPT phases.

9:48AM Y10.00010 Generalized Dirac points and topological surface states in a three-dimensional nonsymmorphic photonic crystal. LING LU, CHEN FANG, TIMOTHY HSIEH, LIANG FU, JOHN JOANNOPOULOS, MARIN SOLJACIC. Massachusetts Institute of Technology — In condensed matter physics, the three-dimensional (3D) Dirac equation describes low-energy excitations of spin-$\frac{1}{2}$ electrons in quantum materials ranging from topological insulators to Dirac semimetals. Here we discover, in photonic crystals, the existence of robust 3D linear point degeneracies between two pairs of band crossings with different velocities. Based on symmetry considerations, we demonstrate that such dispersion is governed by a generalization of 3D Dirac equation for spin-$\frac{1}{2}$ photons propagating in a periodic medium. This 3D Dirac phase in photonic crystals represents a new topological phase of matter protected by nonsymmorphic crystal symmetry and exhibits novel two-dimensional surface states, which we characterize. Time-reversal symmetry is preserved but not required in our photonic system.

10:00AM Y10.00011 Accurate band gaps of semiconductors and insulators from Quantum Monte Carlo calculations. ROMAN NAZAROV, RANDOLPH HOOD, MIGUEL MORALES, LLNL — Ab initio calculations are useful tools in developing materials with targeted band gaps for semiconductor industry. Unfortunately, the main workhorse of ab initio calculations – density functional theory (DFT) in local density approximation (LDA) or generalized gradient approximation (GGA) underestimates band gaps. Several approaches have been proposed starting from empirical corrections to more elaborate exchange-correlation functionals to deal with this problem. But none of these work well for the entire range of semiconductors and insulators. Deficiencies of DFT as a mean field method can be overcome using many-body techniques. Quantum Monte Carlo (QMC) methods can obtain a nearly exact numerical solutions of both total energies and spectral properties. Diffusion Monte Carlo (DMC), the most widely used QMC method, has been shown to provide gold standard results for different material properties, including spectroscopic constants of dimers and clusters, equation of state for solids, accurate descriptions of defects in metals and insulators. To test the accuracy in a wider range of semiconductors and insulators we have computed band gaps of several semiconductors and insulators. We show that DMC can provide superior agreement with experiment compared with more traditional DFT approaches including high level exchange-correlation functionals (e.g. HSE).

10:12AM Y10.00012 ABSTRACT WITHDRAWN —

10:24AM Y10.00013 ABSTRACT WITHDRAWN —

Friday, March 6, 2015 8:00AM - 10:48AM — Session Y11 GSNP: Statistical Mechanics of Social Systems 007B - Manolis Antonoyiannakis, Columbia University

8:00AM Y11.00001 Transition between different search patterns in human online search behavior1. XIANGWEN WANG, MICHEL PLEIMLING, Virginia Tech — We investigate the human online search behavior by analyzing data sets from different search engines. Based on the comparison of the results from several click-through data-sets collected in different years, we observe a transition of the search pattern from a Lévy-flight-like behavior to a Brownian-motion-type behavior as the search engine algorithms improve. This result is consistent with findings in animal foraging processes. A more detailed analysis shows that the human search patterns are more complex than simple Lévy flights or Brownian motions. Notable differences between the behaviors of different individuals can be observed in many quantities.

1This work is in part supported by the US National Science Foundation through grant DMR-1205309.

8:12AM Y11.00002 Social consensus and tipping points with opinion inertia2, CASEY DOYLE, SAMEET SREENIVASAN, BOLESLAW SZYMANSKI, GYORGY KORNISS, Rensselaer Polytech Institute — When opinions, behaviors or ideas diffuse within a population, some are invariably more sticky than others. The stickier the opinion, the greater an individual’s inertia to replace it with an alternative. Here we study the effect of stickiness of opinions in a two-opinion model, where individuals change their opinion only after a certain number of consecutive encounters with the alternative opinion. We focus on the scenario where initially a minority of the population adopts an opinion that is as sticky or stickier than that of the majority, and investigate how the critical size of the initial minority required to tip the entire population over to its opinion, depends on the stickiness of the minority opinion. We analyze this scenario for a complete-graph topology through simulations, and through a semi-analytical approach which yields an upper bound for the critical size of the minority. We present analogous simulation results for the case of the Erdos-Rényi random network. Finally, we investigate the coarsening properties of sticky opinion spreading on two-dimensional lattices, and show that the presence of stickiness gives rise to an effective surface tension that causes the coarsening behavior to become curvature-driven.

2Supported in part by ARL NS-CTA, ARO, ONR, and NSF.

8:24AM Y11.00003 A Universal Power Law Governing Pedestrian Interactions3. IOANNIS KARAMOUIZAS, Univ of Minn - Minneapolis, BRIAN SKINNER, Argonne National Laboratory, STEPHEN J. GUY, Univ of Minn - Minneapolis — Human crowds often bear a striking resemblance to interacting particle systems, and this has prompted many researchers to describe pedestrian dynamics in terms of interaction forces and potential energies. The correct quantitative form of this interaction, however, has remained an open question. Here, we introduce a novel statistical-mechanical approach to directly measure the interaction energy between pedestrians. This analysis, when applied to a large collection of human motion data, reveals a simple power law interaction that is based not on the physical separation between pedestrians but on their projected time to a potential future collision, and is therefore fundamentally anticipatory in nature. Remarkably, this simple law is able to describe human interactions across a wide variety of situations, speeds and densities. We further show, through simulations, that the interaction law we identify is sufficient to reproduce many known crowd phenomena.

3Work at Argonne National Laboratory is supported by the U.S. Department of Energy, under contract no. DE-AC02-06CH11357. Work at the University of Minnesota is supported by MnDRIVE Initiative on Robotics, Sensors, and Advanced Manufacturing.
8:36AM Y11.00004 Finite size scaling analysis on Nagel-Schreckenberg model for traffic flow
, ASHKAN BALOUCHI, DANITA BROWNE, Department of Physics & Astronomy, Louisiana State University — The traffic flow problem as a many-particle non-equilibrium system has caught the interest of physicists for decades. Understanding the traffic flow properties and their resulting effects on the human behavior has been a critical field of study in the 21st century. Here we study the critical value for the density of vehicles to achieve the jammed phase in the Nagel-Schreckenberg model. We present our results for different system sizes and compare our findings with the exact solution for infinite systems. We find that the critical value changes with the system size and that the finite size effects become more pronounced as the size of the network is increased.

, VRINKANT YADAV, ARSHAD KUDROLLI, Clark University — We model the behavior of traffic using Self Propelled Particles (SPPs). Granular rods with asymmetric mass distribution confined to move in a circular channel on a vibrated substrate and interact through elastic collisions act as our model vehicle. Motion of a single vehicle is observed to be composed of 2 parts, a linear velocity in the direction of lighter end and a non-Gaussian asymmetric mass distribution confined to move in a circular channel on a vibrated substrate and interact through inelastic collisions serve as our model vehicle. Our model captures the behavior of traffic congestion in a low-dimensional network, and we conclude by analyzing the scaling behavior of the non-equilibrium system has caught the interest of physicists for decades. Understanding the traffic flow properties and their resulting effects on the human behavior have been a critical field of study in the 21st century. Here we study the critical value for the density of vehicles to achieve the jammed phase in the Nagel-Schreckenberg model. We present our results for different system sizes and compare our findings with the exact solution for infinite systems. We find that the critical value changes with the system size and that the finite size effects become more pronounced as the size of the network is increased.

9:00AM Y11.00006 Dynamics of influence and social balance in spatially-embedded regular and random networks
, P. SINGH, S. SREENIVASAN, B. SZYMANSKI, G. KORNIS, RPI — Structural balance affects deradicalization in an otherwise polarized population of leftists and rightists constituting the nodes of a low-dimensional social network. Specifically, assuming an externally moderating influence that converts leftists or rightists to centrists with probability $p$, we study the critical value $p_c$, below which the presence of metastable mixed population states exponentially delay the achievement of centrist consensus. Above the critical value, centrist consensus is the only fixed point. Complementing our previous results on complete graphs, we present results for the process on low-dimensional social networks, and show that the low-dimensional embedding of the underlying network significantly affects the critical value of probability $p$. Intriguingly, on low-dimensional networks, the critical value $p_c$ can show non-monotonicity as the dimensionality of the network is varied. We conclude by analyzing the scaling behavior of the temporal variation of unbalanced triad density in the network for different low-dimensional network topologies.

9:12AM Y11.00007 Self-organization of divided hierarchy
, TAKASHI ODAKAGI, KEIGO KITADA, KENTA OMIZO, Tokyo Denki University, RYO FUJIE, The University of Tokyo — There are two types of extreme form of hierarchy, one is the plutonomy where small fraction of winners and losers and many people in the middle class appear and the other a divided hierarchy where half of population become winners and the remaining half become losers. We study the emergence of the divided hierarchy in a model society which consists of bellicose individuals who always try to fight and fight with the strongest or the weakest individual. In our model society $(1)$ individuals make random walk on a square lattice, $(2)$ when two individuals encounter they fight each other and $(3)$ the winner deprives wealth from the loser. By a Monte Carlo simulation, we show that there are two transitions when the population density is increased; one is a transition from the egalitarian society to a hierarchical society I where winners, losers and middle classes coexist and the other is a transition from the hierarchical society I to a hierarchical society II where winners and losers exist but no middle classes exist, that is the divided hierarchy. We also show that clusters consisting mostly of bellicose individuals appear in the hierarchical society I.

9:24AM Y11.00008 Canonical Sectors and Evolution of Firms in the US Stock Markets
, LORIEN HAYDEN, RICKY CHACHRA, ALEXANDER ALEMI, PAUL GINSZPARG, JAMES SETHNA, Cornell University — In this work, we show how an unsupervised machine learning can provide a more objective and comprehensive broad-level sector decomposition of stocks. Classification of companies into sectors of the economy is important for macroeconomic analysis, and for investments into the sector-specific financial indices and exchange traded funds (ETFs). Historically, these major industrial classification systems and financial indices have been based on expert opinion and developed manually. Our method, in contrast, produces an emergent low-dimensional structure in the space of historical stock price returns. This emergent structure automatically identifies “canonical sectors” in the market, and assigns every stock a participation weight into these sectors. Furthermore, by analyzing data from different periods, we show how these weights for listed firms have evolved over time.

9:36AM Y11.00009 Lead-lag relationships between stock and market risk within linear response theory
, STANISLAV BORYSOV V, ALEXANDER BALATSKY Y, Nordita, KTH Royal Institute of Technology and Stockholm University, Roslagstullsbacken 23, SE-106 91 Stockholm, Sweden — We study historical correlations and lead-lag relationships between individual stock risks and the market risk (standard deviation of daily returns) and market risk (standard deviation of daily returns of a market-representative portfolio) in the US stock market. We consider the cross-correlation functions averaged over stocks, using historical stock prices from the Standard & Poor’s 500 index for 1994-2013. The observed historical dynamics suggests that the dependence between the risks was almost linear during the US stock market downturn of 2002 and after the US housing bubble in 2007, remaining at that level until 2013. Moreover, the averaged cross-correlation function often had an asymmetric shape with respect to zero lag in the periods of high correlation. We develop the analysis by the application of the linear response formalism to study underlying causal relations. The calculated response functions suggest the presence of characteristic regimes near financial crashes, when individual stock risks affect market risk and vice versa.

, XIAOXIANG YANG, CONAN ZHAO, IRINA MAZILIU, Washington and Lee University — Due to incomplete information available in the market and uncertainties associated with the price determination process, the stock prices fluctuate randomly during a short period of time. In the long run, however, certain economic factors, such as the interest rate, the inflation rate, and the company’s revenue growth rate, will cause a gradual shift in the stock price. Thus, in this paper, a differential equation model has been constructed in order to study the effects of these factors on the stock prices. The model obtained accurately describes the general trends in the AAPL and XOM stock price changes over the last ten years.
used for the identification of large transitions for various threshold distributions. The transition point is independent of the system size, while the contribution of the rest of the initiators converges to zero at infinite system size. This property is largely independent of the system size in the network. There is a critical fraction of initiators for which a transition from small to large cascades occurs, which for Erdős-Rényi (ER) graphs is a uniform threshold in the network. Opinion dynamics is the Threshold Model (TM) aiming to model the spread of a new opinion based on the social drive of peer pressure. Under the TM a node adopts a new opinion only when the fraction of its first neighbors possessing that opinion exceeds a pre-assigned threshold. Cascades in the TM depend on multiple parameters, such as the number and selection strategy of the initially active nodes (initiators), and the threshold distribution of the nodes. For a uniform threshold in the network there is a critical fraction of initiators for which a transition from small to large cascades occurs, which for ER graphs is largely independent of the system size [2]. Here, we study the spread contribution of each newly assigned initiator under the TM for different initiator selection strategies for synthetic graphs of various sizes. We observe that for ER graphs when large cascades occur, the spread contribution of the added initiator on the transition point is independent of the system size, while the contribution of the rest of the initiators converges to zero at infinite system size. This property is used for the identification of large transitions for various threshold distributions.

2 Supported in part by ARL NS-CTA, ARO, ONR, and DARPA.

The work was financially supported by Grant-in-Aid for Scientific Research (C) of Japan Society for the Promotion of Science (JSPS) No. 253302703 and Grant-in-Aid for Scientific Research on Innovative Area No. 2512001313.

10:12AM Y11.00012 Cascades in the Threshold Model for varying system sizes, PANAGIOTIS KARAMPOURNITOS, SAMEET SREENIVASAN, BOLESLAW SZYMANSKI, GYORGY KORNISS, Rensselaer Polytechnic Institute — A classical model in opinion dynamics is the Threshold Model (TM) aiming to model the spread of an idea, opinion, or disease based on the social drive of peer pressure. Under the TM a node adopts a new opinion only when the fraction of its neighbors possessing that opinion exceeds a pre-assigned threshold. Cascades in the TM depend on multiple parameters, such as the number and selection strategy of the initially active nodes (initiators), and the threshold distribution of the nodes. For a uniform threshold in the network there is a critical fraction of initiators for which a transition from small to large cascades occurs, which for ER graphs is largely independent of the system size [2]. Here, we study the spread contribution of each newly assigned initiator under the TM for different initiator selection strategies for synthetic graphs of various sizes. We observe that for ER graphs when large cascades occur, the spread contribution of the added initiator on the transition point is independent of the system size, while the contribution of the rest of the initiators converges to zero at infinite system size. This property is used for the identification of large transitions for various threshold distributions.

1 Supported in part by ARL NS-CTA, ARO, ONR, and DARPA.

10:24AM Y11.00013 Collective behavior in the evolution of scientific research interests, TAO JIA, Department of Physics and Computer Science, Rensselaer Polytechnic Institute, Troy, NY, 12180 USA, DASHUN WANG, IBM Thomas J. Watson Research Center, Yorktown Heights, NY, 10598 USA, GYORGY KORNISS, Department of Physics, Rensselaer Polytechnic Institute, Troy, NY, 12180 USA, BOLESLAW SZYMANSKI, Department of Computer Science, Rensselaer Polytechnic Institute, Troy, NY, 12180 USA — Scientific research is strongly associated with the researchers’ interests in particular areas or disciplines. On one hand, the stable research interest enables one to gain the expertise by repetitive practices specialized in a certain field. On the other hand, occasional change on the area of interest may reinvigorate one’s research. To date, we lack a quantitative understanding on the likelihood of the research interest change, the consequent impact and the internal mechanism of this dynamical process. Here we analyze the publication records of over 14,000 scientists and quantitatively measure their research interest transitions. Our result shows that the fraction of scientists drops exponentially with the extent of transition, indicating that most scientists keep their interests quite stable. While it is rare, those who change demonstrate a higher-than-average chance to increase the productivity and impact. We propose a theoretical model that reproduces not only the observations in interest evolution but also the patterns of publication activities, allowing us to probe the short-term benefits of exploitation on the established field and the long-term returns of exploration on the new lines of inquiry.

Supported in part by ARL NS-CTA, ONR and ARO.

10:36AM Y11.00014 Median Citation Index vs Journal Impact Factor, MANOLIS ANTONOYIANNAKIS, JUN-ICHI INOUE, HE CHEN, Kokaido University — We discuss social inequalities in labor markets for university graduates in Japan by using the Gini and k-indices [1]. Feature vectors which specify the abilities of candidates (students) are built into the probabilistic labor market model [2]. Here we systematically examine what kind of selection processes (strategies) by companies according to the weighted feature vector of each candidate could induce what type of inequalities in the number of informal acceptances leading to a large mismatch between students and companies.


The work was financially supported by Grant-in-Aid for Scientific Research (C) of Japan Society for the Promotion of Science (JSPS) No. 2533027803 and Grant-in-Aid for Scientific Research on Innovative Area No. 2512001313.

10:48AM Y11.00015 Cascades in the Threshold Model for varying system sizes, PANAGIOTIS KARAMPOURNITOS, SAMEET SREENIVASAN, BOLESLAW SZYMANSKI, GYORGY KORNISS, Rensselaer Polytechnic Institute — A classical model in opinion dynamics is the Threshold Model (TM) aiming to model the spread of an idea, opinion, or disease based on the social drive of peer pressure. Under the TM a node adopts a new opinion only when the fraction of its neighbors possessing that opinion exceeds a pre-assigned threshold. Cascades in the TM depend on multiple parameters, such as the number and selection strategy of the initially active nodes (initiators), and the threshold distribution of the nodes. For a uniform threshold in the network there is a critical fraction of initiators for which a transition from small to large cascades occurs, which for ER graphs is largely independent of the system size [2]. Here, we study the spread contribution of each newly assigned initiator under the TM for different initiator selection strategies for synthetic graphs of various sizes. We observe that for ER graphs when large cascades occur, the spread contribution of the added initiator on the transition point is independent of the system size, while the contribution of the rest of the initiators converges to zero at infinite system size. This property is used for the identification of large transitions for various threshold distributions.

1 Supported in part by ARL NS-CTA, ARO, ONR, and DARPA.

Median Citation Index vs Journal Impact Factor, MANOLIS ANTONOYIANNAKIS, (1) Columbia University (2) American Physical Society — The Journal Impact Factor is an arithmetic mean: It is the average number of citations, in a year, to a journal’s articles that were published the previous two years. But for the vast majority of scholarly journals, the distribution of these citations is skewed (non-symmetric). We argue that a more representative member of the skewed distribution of citations is its median, not the mean. We thus introduce the Median Citation Index (MCI) and compare it to the Journal Impact Factor (JIF) as a potentially more suitable choice of the “center” of the distribution, or its typical value. Unlike the JIF, the MCI is far less sensitive to outlier (very highly cited) papers or to gaming, and does not lend itself to the hype of calculating it to three decimal digits.

Supported in part by ARL NS-CTA, ONR and ARO.

Friday, March 6, 2015 8:00AM - 10:48AM – Session Y12 DCMP: Spectroscopy on Topological Insulators 007C - Andrew Wray, New York University

8:00AM Y12.00001 Surface Plasmons in 3D Topological Insulators, ANSHUL KOGAR, SEAN VIG, GIL CHO, ALEXANDER THALER, YIRAN XIAO, TAYLOR HUGHES, MAN-HONG WONG, TAI-CHANG CHANG, GREG MACDOUGALL, PETER ABBAMONTE, Univ of Illinois - Urbana — Most studies of three-dimensional (3D) topological insulators have concentrated on their one-electron properties as exhibited by angle-resolved photoemission spectroscopy (ARPES) or by scanning tunneling microscopy (STM). Many-body interactions are often neglected in the treatment of models of topological insulators, such as in the Kane-Mele and Bernevig-Hughes-Zhang models. Using angle-resolved inelastic electron scattering from the surface, I will present data on the collective mode that owes its existence to the presence of many-body interactions, the surface plasmon (SP), in two known 3D topological insulators, Bi2Se3 and Bi0.5Sb1.5Se1.5-xTe1.5-x. Surprisingly, the SP was prominent even after depressing the Fermi energy into the bulk band gap. Having studied the SP as a function of doping, momentum transfer and its aging properties, I will present evidence to suggest that bulk-surface coupling is crucial in explaining many of its properties. A simple model with dynamic bulk screening will be presented showing qualitative agreement with the observations. Lastly, the relation of the observed surface plasmon to the predicted spin-plasmon mode and to the kinks seen in the electronic dispersion as measured by ARPES will be discussed.

The work was supported as part of the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science.

8:00AM Y12.00001 Surface Plasmons in 3D Topological Insulators, ANSHUL KOGAR, SEAN VIG, GIL CHO, ALEXANDER THALER, YIRAN XIAO, TAYLOR HUGHES, MAN-HONG WONG, TAI-CHANG CHANG, GREG MACDOUGALL, PETER ABBAMONTE, Univ of Illinois - Urbana — Most studies of three-dimensional (3D) topological insulators have concentrated on their one-electron properties as exhibited by angle-resolved photoemission spectroscopy (ARPES) or by scanning tunneling microscopy (STM). Many-body interactions are often neglected in the treatment of models of topological insulators, such as in the Kane-Mele and Bernevig-Hughes-Zhang models. Using angle-resolved inelastic electron scattering from the surface, I will present data on the collective mode that owes its existence to the presence of many-body interactions, the surface plasmon (SP), in two known 3D topological insulators, Bi2Se3 and Bi0.5Sb1.5Se1.5-xTe1.5-x. Surprisingly, the SP was prominent even after depressing the Fermi energy into the bulk band gap. Having studied the SP as a function of doping, momentum transfer and its aging properties, I will present evidence to suggest that bulk-surface coupling is crucial in explaining many of its properties. A simple model with dynamic bulk screening will be presented showing qualitative agreement with the observations. Lastly, the relation of the observed surface plasmon to the predicted spin-plasmon mode and to the kinks seen in the electronic dispersion as measured by ARPES will be discussed.

The work was supported as part of the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science.
8:12AM Y12.00002 Scanning tunneling spectroscopy investigation of the topological phase transition in (Bi$_{1-x}$In$_x$)$_2$Se$_3$. - DANIEL WALKUP, WENWEN ZHOU, ILIJA ZELIKOVIC, Boston College, YOSHINORI OKADA, Tohoku University, ZHENSONG REN, KANE SCIPIONI, Boston College, STEPHEN WILSON, Boston College and University of California Santa Barbara, VIDYA MADHAVAN, Boston College and University of Illinois Urbana-Champaign — The three-dimensional topological insulator (Bi$_{1-x}$In$_x$)$_2$Se$_3$ undergoes a phase transition to a trivial insulator as Bi atoms are replaced with In. This chemical substitution is expected to reduce the spin-orbit coupling, lift the bulk band inversion and thus destroy the Dirac surface states present in the end-member Bi$_2$Se$_3$. Although photoemission and transport measurements have provided evidence for this phase transition in thin films, the nature of the surface state transformation across the critical point remains unclear, especially near the transition point where the surface state penetration depth becomes comparable to film thicknesses. Here, we present scanning tunneling spectroscopy experiments on single crystals of (Bi$_{1-x}$In$_x$)$_2$Se$_3$ for $x \approx 0\text{--}10\%$. Using Landau Level spectroscopy, we map the surface state dispersion across the phase transition. Additionally, we use local density of states mapping to reveal the local influence of the In dopants near the critical point.

8:24AM Y12.00003 Andreev Reflection Spectroscopy of Nb-doped Bi$_2$Se$_3$ Topological Insulator$^*$ - C. KURTER, Missouri University of Science and Technology, A.D.K. FINCK, University of Illinois at Urbana Champaign, Y. QIU, Missouri University of Science and Technology, E. HUEMILLER, A. WEIS, J. ATKINSON, University of Illinois at Urbana Champaign, J. MEDVEDEVA, Y.S. HOR, Missouri University of Science and Technology, D.J. VAN HARLINGEN, University of Illinois at Urbana Champaign — Doped topological insulators are speculated to realize p-wave superconductivity with unusual low energy quasiparticles, such as surface Andreev bound states. We present point contact spectroscopy of thin exfoliated flakes of Nb-doped Bi$_2$Se$_3$ where superconductivity persists up to $\sim 1$ K, compared to 3.2 K in bulk crystals. The critical magnetic field is strongly anisotropic, consistent with quasi-2D behavior. Andreev reflection measurements of devices with low resistance contacts result in prominent BTK-like behavior with an enhanced conductance plateau at low bias. For high resistance contacts, we observe a split zero bias conductance anomaly and additional features at the superconducting gap. Our results suggest that this material is a promising platform for studying topological superconductivity.

$^*$We acknowledge support from Microsoft Project Q.

8:36AM Y12.00004 Andreev Reflection Spectroscopy on Bismuth-Chalcogenide Topological Insulators$^*$ - C.R. GRANSTROM, I. FRIDMAN, University of Toronto, J.Y.T. WEI, University of Toronto, Canadian Institute for Advanced Research, H. LEI$^*$, C. PETROVIC, Brookhaven National Laboratory, R.X. LIANG, University of British Columbia — Andreev reflection (AR) is the basic mechanism underlying the superconducting proximity effect which, at the interface between a topological insulator (TI) and a spin-singlet superconductor, can give rise to Majorana-like states. Despite this basic importance, little is known about how AR is affected by the unique attributes of a three-dimensional TI, namely the near degeneracy at the Dirac point, its warped bands, and additional features at the superconducting gap. Our results suggest that this material is a promising platform for studying topological superconductivity.

$^*$Work supported by NSERC, CFI-OIT, CIFAR, and the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. DOE, Office for Basic Energy Science.

8:48AM Y12.00005 STM/S studies of BiSbTeSe$_2$ alloys: Intrinsic topological insulators with robust Fermi level in the bulk band gap. - HYOUNGDO NAM, Department of Physics, University of Texas at Austin, Austin, Texas 78712, USA, YANG XU, IRENEUSZ MIOTKOWSKI, JIFIA TIAN, YONG CHEN, Department of Physics and Astronomy, Purdue University, West Lafayette, IN 47907, USA, CHIH-KANG SHIH, Department of Physics, Department of Physics of Texas at Austin, Austin, Texas 78712, USA. — Topological insulators (TI) have been attracting a lot of interest in spin chirality topological surface state (TSS). One of the major material challenges has been the difficulty to create a topological insulator with true insulating bulk so that the topological surface states dominate the transport properties. There has been effort in creating the quaternary compounds, Bi$_{2-x}$Sb$_{x}$Te$_3$Se$_3$ (BSTS) with intrinsic bulk states. Namely the Fermi level is inside the bulk band gap with Dirac point also in the bulk band gap. Angle resolved photoemission has been used to show that 1112 compound, Bi$_2$Sb$_x$Te$_3$Se$_2$, possess this desirable property. Recent observation of topological surface state quantum Hall effect in this compound marks another important milestone. This work focuses on investigations of the electronic structure of BiSbTeSe$_2$ using scanning tunneling microscopy and spectroscopy (STM/S). With the second derivative of tunneling current, we accurately observed the locations of Dirac point (DP), valence band maximum point, and conduction band minimum point, which consist with previous ARPES studies. The investigation confirms the intrinsic bulk states with Fermi level is very close to the DP. We will further discuss the potential correlation of the DP fluctuation with respect to the local compositional fluctuations.

9:00AM Y12.00006 Visualizing the native atomic defects in Bi$_2$Se$_3$ with scanning tunneling microscopy$^*$ - JIXIA DAI, Department of physics and astronomy, Rutgers University, DAMIEN WEST, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, XUEYUN WANG, YAZHONG HANG, DANIEL KWOK, SANG WOOK CHEONG, Department of physics and astronomy, Rutgers University, SHENGBAI ZHANG, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, WEIDA WU, Department of physics and astronomy, Rutgers University — In topological insulators such as Bi$_2$Se$_3$ the existence of native atomic defects is one of the major bottlenecks for potential applications utilizing the topologically protected surface states. Native defects such as vacancies or antisites are believed to be responsible for the metallic transport observed in Bi$_2$Se$_3$. In this study, we examined a series of Bi$_2$Se$_3$ samples that were grown with different conditions using atomically resolving scanning tunneling microscopy. We have successfully identified several types of intrinsic defects, including Se vacancies and Bi-Se antisites. The individual defect images are corroborated by first principle calculations. The densities of these defects across different samples are correlated with their growth conditions. Preliminary results suggest the defect densities can account for the charge carrier density estimated from tunneling spectroscopy.

$^*$This work is supported by NSF grant # DMR-0844807.

9:12AM Y12.00007 Observation of Fermi Arcs in a Doped Pseudospin-1/2 Heisenberg Antiferromagnet Strontium Iridate$^*$ - Y. K. KIM, O. KRUPIN, J. D. DENLINGER, A. BOSTWICK, E. ROTENBERG, Lawrence Berkeley Natl Lab, Q. ZHAO, J. F. MITCHELL, MSD, Argonne Natl Lab, J. W. ALLEN, Ranall Lab of physics, Univ. of Michigan, B. J. KIM, MSD, Argonne Natl Lab, Ranall Lab of physics, Univ. of Michigan, Max Plank institute for Solid state research, Stuttgart — Emergent properties of two microscopically different systems can be similar. Despite manifestly different underlying microscopic electronic structures, the effective low-energy physics of SrZrO$_4$ has been shown to be remarkably similar to that of the parent insulators of superconducting cuprates. However, whether the parallel with the cuprates continues to hold for a metallic phase induced by carrier doping remains unclear, which holds the key to the realization of a new high temperature superconductor. In this presentation, we will report that the evolution of the fermiology of SrZrO$_4$ with doping and temperature reproduces that observed for the cuprates. Upon surface electron doping through in situ deposition of alkali-metal atoms, angle-resolved photoemission spectra of SrZrO$_4$ display disconnected segments of zero-energy states, known as ‘Fermi arcs’, and a gap as large as 80 meV. The Fermi arc smoothly evolves to a closed Fermi surface at higher surface coverage and at higher temperature.
9:24AM Y12.00008 A Scanning Tunnelling Microscopy Study on an Alloyed Topological Insulator, Bi$_{1.5}$Sb$_5$Te$_7$Se$_{1.3}$, WONHEE KO, INSU JEON, HYO WON KIM, HYEOKSHIN KWON, YOUNGTEK OH, Samsung Advanced Institute of Technology, SE-JONG KAHNG, Korea University, JOONBUM PARK, JUN SUNG KIM, Pohang University of Science and Technology, SUNG WOO HWANG, HWANSOO SUH, Samsung Advanced Institute of Technology — Efficient doping of topological insulators while protecting its topological nature is key ingredient to realize topological devices. Engineering the chemical potential in the alloyed compound Bi$_{2-x}$Sb$_5$Te$_7$Se$_{1.3}$ has been achieved by tuning its chemical composition. However, the effect of alloying in microscopic scale has not yet been fully investigated with local probes. Here we report on the atomic and electronic structures of Bi$_{1.5}$Sb$_5$Te$_7$Se$_{1.3}$ studied using scanning tunnelling microscopy/spectroscopy (STM/STS). Although there is significant surface disorder due to the alloying of constituent atoms, cleaved surfaces of the crystals present a well-ordered hexagonal lattice in STM topographs with 1 nm high quintuple layer steps. STS results reflect the band structure and indicate that the surface state and Fermi energy are both located inside the energy gap. The surface states do not show any electron back-scattering; due to their topological nature they are extremely robust. Landau levels generated by perpendicular magnetic field follow the massless Dirac fermions. This finding demonstrates that alloying is a promising route for efficient doping of topological insulators whilst keeping the topological surface state intact.

9:36AM Y12.00009 Circular photocurrent response of a topological insulator thin film probed by scanning photocurrent microscopy, DONG-XIA QU, Lawrence Livermore National Lab, XUFENG KOU, MURONG LANG, University of California, Los Angeles, JONATHAN CROWHURST, MICHAEL ARMSTRONG, JOSEPH ZAUG, Lawrence Livermore National Lab, KANG L. WANG, University of California, Los Angeles, GEORGE CHAPLINE, Lawrence Livermore National Lab — The remarkable nature of surface states in topological insulators is expected to have a unique photocurrent response to electromagnetic radiation. However, the surface and bulk photo-excited charge transport mechanisms, in relation to the band bending at the electrode-topological insulator interface, have not been well understood. Here, we present scanning photocurrent microscopy measurements on a gated topological insulator microdevice and show that the spin-polarized photocurrent displays direction reversal near the electrical contact interfaces. We discuss two possible mechanisms, which alternatively play dominant roles in the helicity-dependent photocurrent map. Our analysis determines the magnitude of each contribution, and reveals the governing process under different gate conditions.

9:48AM Y12.00010 Rapid high-resolution spin- and time-resolved ARPES, CHU-YUN LIN, Department of Physics, University of California, Berkeley, KENNETH GOTTLIKE, Graduate Group in Applied Science and Technology, University of California, Berkeley, CHRIS JOZWIAK, ZAHID HUSSAIN, AARON BOSTWICK, Advanced Light Source, Lawrence Berkeley National Laboratory, ALESSANDRA LANZARA, Department of Physics, University of California, Berkeley and Material Science Division, Lawrence Berkeley National Laboratory, ADVANCED LIGHT SOURCE, LAWRENCE BERKELEY NATIONAL LABORATORY COLLABORATION, GRADUATE GROUP IN APPLIED SCIENCE AND TECHNOLOGY, UNIVERSITY OF CALIFORNIA, BERKELEY COLLABORATION, GRADUATE GROUP IN APPLIED SCIENCE AND TECHNOLOGY, UNIVERSITY OF CALIFORNIA, BERKELEY, CHRISTOPHER JOZWIAK, ZAHID HUSSAIN, Lawrence Berkeley National Laboratory, ALESSANDRA LANZARA, University of California Berkeley, Lawrence Berkeley National Laboratory — Significant experimental and theoretical interest has followed the observation that the spin polarization of photoelectrons from a topological surface state can be measured with photoemission spectroscopy. Here, we report on the first observation of spin resolved photoemission spectroscopy with a fast time-resolving spectrometer, coupled with a lab-based 6 eV laser, which is capable of demonstrating its potential for simultaneous spin- and time-resolved ARPES with pump-probe based measurements.

10:00AM Y12.00011 Photoelectron Spin Control in Spin-Orbit Systems, KENNETH GOTTLIKE, University of California Berkeley, CHRISTOPHER JOZWIAK, Lawrence Berkeley National Laboratory, KENNETH GOTTLIKE, University of California Berkeley, ZAHID HUSSAIN, Lawrence Berkeley National Laboratory, ALEXANDRA LANZARA, University of California Berkeley, Lawrence Berkeley National Laboratory — The remarkable nature of surface states in topological insulators is expected to have a unique photocurrent response to electromagnetic radiation. However, the surface and bulk photo-excited charge transport mechanisms, in relation to the band bending at the electrode-topological insulator interface, have not been well understood. Here, we present scanning photocurrent microscopy measurements on a gated topological insulator microdevice and show that the spin-polarized photocurrent displays direction reversal near the electrical contact interfaces. We discuss two possible mechanisms, which alternatively play dominant roles in the helicity-dependent photocurrent map. Our analysis determines the magnitude of each contribution, and reveals the governing process under different gate conditions.

10:12AM Y12.00012 Direct Observation of the Fermi Arc Surface State in the Three-Dimensional Dirac Semimetal Na$_3$Bi, AIJI LIANG, ZHIJUN WANG, CHAOYU CHEN, YOUGUO SHI, HEMIAN YI, YA FENG, ZHUOJIN XIE, SHAOLONG HE, JUNFENG HE, YINGYING PENG, CU LIU, YAN LIU, LIN ZHAO, GUODONG LIU, JUN ZHANG, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, M. NAKATAKE, M. ARITA, K. SHIMADA, H. NAMATAME, M. TANIGUCHI, Hiroshima Synchrotron Radiation Center, Hiroshima University, Hiroshima 739-8526, Japan, ZUAN YUAN CHU, CHUANGTIAN CHEN, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, China, XI DAI, ZHONG FANG, XINGJIANG ZHOU, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — The three dimensional (3D) Dirac semimetals have linearly dispersive 3D Dirac nodes where the conduction and valence bands connect to each other. Here we report the direct observation of the linearly dispersive 3D bulk Dirac points at the natural (001) cleaving surface of Na$_3$Bi single crystal by high resolution ARPES. In addition, we have directly observed two separated 3D bulk Dirac nodes by elaborately cleaving Na$_3$Bi samples at a non-natural-cleavage (100) crystalline surface. We further unveil the unusual Fermi-arc surface states connecting the two 3D Dirac nodes. At this unique (100) crystalline surface, the identification of the 3D Dirac semimetal state in Na$_3$Bi paves the way for systematically exploring rich exotic topological physics such as topological insulator and Weyl semimetal state.

10:24AM Y12.00013 Magnetism-induced massive Dirac fermions and topological defects in the surface state (SS) of binary and ternary topological insulators (TIs)1, CHIEN-CHANG CHEN, M. L. TEAGUE, N. WOODWARD, W. FAN, N.-C. YEH, Dept. of Physics, Caltech, Pasadena, CA 91125, L. HE, X. KOU, M. LANG, K. L. WANG, Dept. of Electrical Engineering, UCLA, Los Angeles, CA 90095 — Magnetic doping effects on the SS of Bi$_2$Se$_3$ and (Bi$_{1-y}$Sb$_y$)$_2$Te$_3$ are studied by scanning tunneling microscopy/ spectroscopy (STS) on MBE-grown bilayers of Bi$_2$Se$_3$/(Bi$_{1-x}$Sb$_x$)$_2$Se$_3$ and (Bi$_{1-y}$Sb$_y$)$_2$Te$_3$/(Bi$_{1-x}$Sb$_x$)$_2$Te$_3$ on InP (111) as a function of the undoped layer thickness (d) and the Cr-doping level (x). For x = 5% and 10%, magnetic proximity effect is induced in the SS of Bi$_2$Se$_3$ for d < 4-QL, leading to gapped Dirac spectra for temperatures (T) below a 3D Curie temperature $T_C = (210 \pm 10) K$ and (240 \pm 10) K for x = 5% and 10%, respectively, which are much higher than the bulk T$_C \approx 25 K$ where anomalous Hall effect occurs. The gap (Δ) is spatially inhomogeneous in zero magnetic field (H = 0), and reaching a maximum Δ $= (0.4 \pm 0.1) eV$ at T $< T_C$. The gap inhomogeneity decreases with increasing $x$, H and decreasing T. Moreover, localized sharp impurity resonances are found occasionally near the boundaries of gapped and gapless regions, which are attributed to isolated Cr impurities that couple with the spins of Dirac fermions and form long-lived topological defects. With increasing interlayer H, the resonance peaks diminish as the spatial gap homogenizes. These findings in the bilayer binary TIs are compared with those in the bilayer ternary TIs of more uniform bulk ferromagnetism.

1Supported by DARPA and NSF.
Park (TEM) showed presence of corrugations and wisps in the carbon nanotubes framework attributed to the curvature induced by nitrogen atoms. XPS results. High pressure adsorption of CO\textsubscript{2} properties (thermoelectric power and resistivity) and the phonon modes of the CNTs and the trapped gaseous nitrogen are used to further substantiate the carbon nanotubes skeletal structure and 1 atomic% present as gaseous nitrogen trapped inside the nanotubes. Investigation of the temperature dependent transport in Carbon Nanotubes.

This Work is Supported by Penn State Altoona Undergraduate Research Sponsored Program and Penn State Materials Research Institute, University Park.

Friday, March 6, 2015 8:00AM - 11:00AM
Session Y16 DMP: Focus Session: Carbon Nanotubes, Graphene, & Related Materials: Chemical Properties and Sensing

8:00AM Y16.00001 Measurement of electronic perturbations in the surface of a carbon nanotube by adsorbed atoms and molecules\textsuperscript{1}, DAVID COBDE, BORIS DZYUBENKO, HAO-CHUN LEE, OSCAR VILCHES, University of Washington, Seattle — The physisorption of atoms and molecules onto a surface such as carbon involves small hybridization with the substrate electron states which have not previously been accessible to experiments. Suspended single-walled carbon nanotube devices are a good system for studying the electronic perturbations, as they combine a perfect carbon surface with single-atom mass sensing capability and single-electron-transistor sensitivity. By monitoring both the conductance and the adsorbed mass, derived from the mechanical frequency shift, in equilibrium with the vapor, we are able to detect for the first time the very small charge transfer from adsorbates to the surface. It is found to be of a similar magnitude for all gases tested (4He, Ar, Kr, Xe, N\textsubscript{2}, CO and O\textsubscript{2}), and depends on coverage and temperature. Although it is only $10^{-5} - 10^{-3}$ e per atom, at gate voltages near threshold it can produce a large change in conductance. It can thus be used to sense tiny amounts of adsorbates and to explore the phase transitions of atoms on a cylinder.

\textsuperscript{1}This work supported by NSF DMR 1206208

8:12AM Y16.00002 Argon Adsorption on Open Carbon Nanohorns\textsuperscript{1}, ANGEL CALVILLO, BRICE RUSSELL, ALDO MIGONE, Department of Physics, Southern Illinois University, Carbondale, IL 62901, USA, SUMIO IIJIMA, MASAKO YUDASAKA, National Institute of Advanced Industrial Science and Technology, Tsukuba 305-8565, Japan — We have measured adsorption isotherms for argon adsorbed on a 0.1692 g sample of chemically-opened carbon nanohorns. Two clear substeps are visible in the adsorption data, corresponding to groups of stronger binding sites (lower pressure substep) and weaker binding sites (higher pressure substep). We have measured adsorption at five different temperatures in the range between 70 and 90 K. The chemically-opened nanohorns have the space at the interior of the individual nanohorns accessible to adsorbates. Consequently, higher loadings are obtained on these samples compared to those for unopened (as-produced) nanohorns. Results for the kinetics of adsorption, the effective specific surface area, and the isosteric heat of adsorption as a function of sorbent loading will be presented and compared to results from other studies on nanohorns.

\textsuperscript{1}This work was supported by the NSF through grant DMR-1006428.

8:24AM Y16.00003 Computer simulations of Ne and CO\textsubscript{2} adsorbed in carbon nanohorns\textsuperscript{1}. SILVINA GATICA, Howard University, ADAM SCRIVENER, University of Rochester — We computed the equilibrium properties of Ne and CO\textsubscript{2} adsorbed on carbon nanohorns. We modeled the nanohorns as an arrangement of nanometer-size cones composed of carbon atoms. Our method of calculation is the Grand Canonical Monte Carlo technique, where the substrate is considered rigid. We calculate the adsorption isotherms for various temperatures (18K-50K for Ne and 147K - 200K for CO\textsubscript{2}). We also calculate the isosteric heat of adsorption and compare with available experimental results.

\textsuperscript{1}Partially supported by the Research Experience for Undergraduates (REU) summer program (NSF Grant PHY-1358727) and Partnership for Reduced Dimensional Materials (PRDM), (NSF DMR-1205608)

8:36AM Y16.00004 Ethane Adsorption on Carbon Nanohorns\textsuperscript{1}, BRICE RUSSELL, ALDO MIGONE, Department of Physics, Southern Illinois University, Carbondale, IL 62901, USA, SUMIO IIJIMA, MASAKO YUDASAKA, National Institute of Advanced Industrial Science and Technology, Tsukuba 305-8565, Japan — We have measured adsorption isotherms for ethane adsorbed on as-produced single-walled carbon nanohorns. Measurements have been completed for nine temperatures between 123.66 K and 221.32 K. The kinetics of adsorption will be compared to results previously obtained for ethane adsorption on purified HiPco single-walled carbon nanotubes. On nanotubes it was found that equilibration times for ethane decreased with increasing sorbent loading (coverage). By contrast, for adsorption on the as-produced nanohorns, equilibration times increased with increasing sorbent loading. The kinetic results for sorbent mass loading will be compared to an expression with only one rate-controlling mechanism. The point-B method was used to determine monolayer completion values at each temperature. Results will also be presented for the isosteric heat values, which were determined for the full range of loadings covered by the isotherms.

\textsuperscript{1}This work was supported by the NSF through grant DMR-1006428

8:48AM Y16.00005 Transport and Optical Investigations of Substitutional and Trapped Nitrogen in Carbon Nanotubes\textsuperscript{1}, ALI QAJAR, University of Texas, Austin, DANHANG MA, The Pennsylvania State University, RAMAKRISHAN RAJAGOPALAN, The Pennsylvania State University-DuBois, KOFI ADU, The Pennsylvania State University-Altoona College, GAMINI SUMANASEKERA, University of Nevada — Multiwall carbon nanotubes that contain nitrogen were synthesized using acetonitrile as the precursor and ferrocene as the catalyst. X-ray photoelectron spectroscopy detected ~ 2 atomic% nitrogen in the carbon nanotubes with ~ 1 atomic% of the nitrogen as substitutionally doped in the carbon nanotubes skeleton structure and 1 atomic% present as gaseous nitrogen trapped inside the nanotubes. Investigation of the temperature dependent transport properties (thermoelectric power and resistivity) and the phonon modes of the CNTs and the trapped gaseous nitrogen are used to further substantiate the XPS results. High pressure adsorption of CO\textsubscript{2} at room temperature also confirmed no porosity accessible for CO\textsubscript{2} molecules. Transmission electron microscopy (TEM) showed presence of corrugations and wisps in the carbon nanotubes framework attributed to the curvature induced by nitrogen atoms.

\textsuperscript{1}This Work is Supported by Penn State Altoona Undergraduate Research Sponsored Program and Penn State Materials Research Institute, University Park
9:00AM Y16.00006 Spectroscopic Investigations into the Redox Sorting of Carbon Nanotubes, JASON STREIT, National Institute of Standards and Technology, HUI GUI, University of Southern California, JEFFERY FAGAN, ANGELA HIGHT WALKER, National Institute of Standards and Technology, CHONGWU ZHOU, University of Southern California, MING ZHENG, National Institute of Standards and Technology — Charge-transfer reactions have been shown to alter the electronic structure of single-wall carbon nanotubes (SWCNTs) in a bandgap-dependent fashion. Such electronic modification shows great promise for chiral selective separations. This study investigates the role of redox chemistry in the aqueous two-phase extraction of SWCNTs. We demonstrate a multi-step oxidative extraction procedure to successfully separate SWCNTs both by semiconducting bandgap and metallicity. We propose that electron transfer between redox molecules and the nanotubes induces reorganization of the surfactant coating layer, which in turn affects the partitioning of the SWCNTs between the two different aqueous polymer phases. Spectroscopic measurements are applied to probe surfactant structure reorganization in different redox environments. We suggest that redox-induced modulation of the surfactant coating is a generally observed phenomenon in many different nanotube sorting processes which can be further controlled to improve separation reproducibility and purity.

9:12AM Y16.00007 Rotations and vibrations of water molecule inside the fullerene cage: infrared study of H2O@C60, TOOMAS ROOM, A. SHUGAI, U. NAGEL, NIPCPB, Tallinn, Estonia, S. MAMONE, A. KRACHMALNICOFF, R.J. WHITBY, M.H. LEVITT, Chemistry, Univ. of Southampton, UK, T. NISHIDA, Y. MURATA, Inst. of Chem. Research, Kyoto Univ., Uji, Japan, XUEGONG LEI, YONGJUN LI, N.J. TURRO, Dep. of Chemistry, Columbia Univ., New York — Water is the second molecule after hydrogen what has been trapped inside the cage of a C60 molecule by the molecular surgery method [Kurotobi and Murata, Science 333, 613 (2011)]. We studied isolated water molecule isotopeologs H2O, D2O, and HD2O in the solid phase at cryogenic temperatures using IR spectroscopy. The water molecule rotation transitions were observed in the THz [Beduz et al., PNAS 109, 12894 (2012)] and vibration-rotation transitions in the mid-IR range. The slow conversion between ortho and para water allowed us to record the time evolution of spectra and to separate ortho and para absorption lines of water. The similarity of the rotation spectrum of caged water to water in the gas phase indicates that water is free to rotate in the C60 cage even at temperature as low as 3 K. However, spectral lines show a splitting of about 0.5 meV what is not compatible with the icosahedral symmetry of C60. Different models (e.g. crystal field effects in solid C60, C60 cage distortions) will be discussed.

1This work was supported by institutional research funding IUT23-3 of the Estonian Ministry of Education and Research.

9:24AM Y16.00008 Adsorption of Ar on individual carbon nanotubes, graphene, and graphite, BORIS DZYUBENKO, JOSHUA KAHN, OSCAR VILCHES, DAVID COBDEN, Department of Physics, University of Washington — We compare and contrast results of adsorption measurements of Ar on single-walled carbon nanotubes, graphene, and graphite. Adsorption isotherms on individual suspended nanotubes were obtained using both the mechanical resonance frequency shift (sensitive to mass adsorption) and the electrical conductance. Isotherms on graphene mounted on hexagonal boron nitride were obtained using only the conductance. New volumetric adsorption isotherms on bulk exfoliated graphite were also obtained, paying special attention to the very low coverage region (less than 2% of a monolayer). This allowed us to compare the degree of heterogeneity on the three substrate types, the binding energies, and the van der Waals 2D parameters. Research supported by NSF DMR 1206208.

9:36AM Y16.00009 Ortho-para conversion of endohedral water in the fullerene C60 at cryogenic temperatures, ANNA SHUGAI, U. NAGEL, T. RÖÖM, NIPCPB, Tallinn, Estonia, S. MAMONE, M. CONCISTRÈ, B. MEIER, A. KRACHMALNICOFF, R.J. WHITBY, M.H. LEVITT, Chemistry, Univ. of Southampton, UK, XUEGONG LEI, YONGJUN LI, N.J. TURRO, Dep. of Chemistry, Columbia Univ., New York — Water displays the phenomenon of spin isomerism in which the two proton spins either couple to form a triplet (ortho water, I = 1) or a singlet nuclear spin state (para water, I = 0). Here we study the interconversion of para and ortho water. The exact mechanism of this process is still not fully understood. In order to minimize interactions between molecules we use a sample where a single H2O is trapped in the C60 molecular cage (H2O@C60) and H2O@C65 is crystallized. H2O@C65 has long-lived ortho state [Beduz et al., PNAS 109, 12894 (2012)] and ortho-para conversion kinetics is non-exponential. At some temperatures the kinetics is exponential. Models are discussed in order to explain the T and concentration dependence of ortho-para interconversion kinetics.

1This work was supported by institutional research funding IUT23-3 of the Estonian Ministry of Education and Research.

9:48AM Y16.00010 Effect of intercalated molecules on graphene sensing behavior, TAO SUN, KIYOUNGMIN MIN, NARAYANA ALURU, Univ of Illinois - Urbana, COMPUTATIONAL MULTISCALE NANO SYSTEM TEAM — The physical mechanism of graphene humidity sensor based upon capacitance measurement is explored by atomic/ab-initio simulations. Our simulations show that molecules intercalated between graphene and substrate (H2O) can have large influence on graphene sensing behavior. We find that oxygen vacancies on the surface of the substrate can induce an N-type doping in graphene, while oxygen molecules entering between the substrate and graphene will fill the vacancies and eliminate the N-type doping effect. We also observe that water molecules trapped at the interfacial layer can change the interlayer distance, thus changing the measured capacitance. Our simulations uncover the effect of intercalated molecules, which is helpful to better understand the operation process of graphene sensing devices.

1Lead by Professor N R Ahlu, we do multiscale simulations to explore mechanical and electronic properties of materials.

10:00AM Y16.00011 Determining the thermal noise floor of graphene biosensors, MICHAEL CROSSER, Linfield College, MORGAN BROWN, ETHAN MINOT, Oregon State University — The use of graphene field-effect transistors (GFETs) as biosensors in aqueous environments is fundamentally limited by voltage noise. In many GFET devices, noise is dominated by the fluctuating occupancy of charge traps in the substrate. Fabrication techniques have been found to reduce this substrate effect, but thermally-driven charge transfer across the graphene liquid interface has yet to be characterized and addressed. In this report we present the first characterization of this noise source. We show that the power spectral density of this noise scales inversely with frequency and inversely with interface area. Our results are in quantitative agreement with recent measurements of voltage noise in clean, suspended graphene.

1This work is supported by NSF award number 1459067.

10:12AM Y16.00012 Spatial Self-Phase Modulation in Graphene and Graphene Oxide Water Suspensions, YANAN WANG, Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, ZHUAN ZHU, Department of Electrical and Computer Engineering, University of Houston, XUFENG ZHOU, Ningbo Institute of Materials Technology & Engineering, Chinese Academy of Sciences, ZHIMING WANG, Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, JIMING BAO, Department of Electrical and Computer Engineering, University of Houston, UESTC & UH COLLABORATION — With promising potential in photonic and optoelectronic applications, nonlinear optical properties of graphene based materials have attracted enormous interest. In this work, we observed spatial self-phase modulation (SSPM) of propagating laser beams in both graphene and graphene oxide (GO) water suspensions. The formation and temporal evolution of far-field diffraction rings have been investigated systematically. It is found that alignment of graphene or GO flakes is controlled by water convection rather than the polarization of laser. We further discovered that SSPM can be mainly attributed to the thermo-optic effect of water instead of graphene or GO.
10:24AM Y16.00013 Asymmetric behavior in electrowetting of electrolyte solutions on graphene at the nanoscale: A molecular dynamics simulation. FERESHTE TAHERIAN TABASI, Postdoctoral Research Fellow, NICO VAN DER VECT, Professor of Physical chemistry at Technical University of Darmstadt — Using molecular dynamics simulations, electrowetting of aqueous solutions on graphene are studied. By doping the surface with the positive or negative charges, the counter-ions are adsorbed at the solid-liquid interface, and the co-ions are repelled from the interface, leading to the decrease of the solid-liquid surface tension and therefore the contact angle (known as electrowetting). Our simulation results show that at zero surface charge density, water molecules at the interface (located between the surface and first ionic layer) are mainly oriented parallel to the surface. However due to the smaller size of the hydrogen, there is a slight tendency of the water dipole moment to orient into the surface. On the charged surfaces, the orientation polarization of the interfacial water molecules are shown to be stronger on the negative surfaces than the positive ones. Such asymmetric orientation polarization of water leads to different screening of the graphene surface charge and therefore different contact angles of the solution with opposite charges. Simulations results show more spreading of the liquid on the positively charged surfaces than the negative ones.

10:36AM Y16.00014 Ionic transport across atomically-thin graphene membranes. LAUREN CANTLEY, Dept. of Mechanical Engineering, Boston University, SCOTT BUNCH, Dept. of Mechanical Engineering, Division of Materials Science and Engineering, Boston University — Graphene is an attractive material for applications in single molecule sensing and molecular sieving, in part due to its atomic thinness, strength and barrier properties. In this study, we examine ionic transport across a suspended single-layer graphene membrane separating two reservoirs of aqueous ionic solution. Molecularly sized, sub-nm pore(s) are introduced by chemical etching, which allow for only proton transport across the graphene membrane. The pore is further opened and ionic conductance measurements are carried out to further investigate and characterize ionic transport across sub-nm and nm-scale pores.

10:48AM Y16.00015 Synthesis, characterization and application of highly crystalline sp2–bonded boron nitride aerogels. THANG PHAM, Materials Science and Engineering, Physics Department, UC Berkeley, ANNA GOLSTEIN, Chemistry, Physics Department, UC Berkeley, MARCUS WORSLEY, LETA WOO, Physical Science Directorate, Lawrence Livermore National Laboratory, WILLIAM MICKESELON, Center of Integrated Nanomechanical System (COINS), UC Berkeley, ALEX ZETTL, Physics Department, COINS, UC Berkeley, Kavli Energy Nanosciences Institute, UC Berkeley, Materials Science Division, Lawrence Berkeley National Lab — Aerogels have much potential in both research and industrial applications due to high surface area, low density and fine pore size distribution. Here we report a versatile synthesis and thorough structure characterization of three-dimensional aerogels composed of highly crystalline sp2–bonded BN layers formed by carbothermal reaction. The structure, crystallinity and bonding of the as-prepared BN aerogels were elucidated by x-ray diffraction, nuclear magnetic resonance of 11B, transmission electron microscopy (TEAM) and resonant soft x-ray scattering. The macroscopic roughness of the aerogel’s surface causes it to be superhydrophobic with a contact angle of 155 ± 3° and high oil uptake (up to 1500 wt%). The used BN aerogel can be regenerated by different heat treatments and still maintain the crystalline porous structure and adsorption capacity. The highly crystalline, chemically pure, thermally stable and porous sp2–boron nitride aerogel is an ideal host for liquids, gases and other nanomaterials.

Friday, March 6, 2015 8:00AM - 10:48AM – Session Y17 DMP: Focus Session: Graphene Devices: Optical and Opto-electronics 102AB - Xiao Li, University of Maryland

8:00AM Y17.00001 Graphene- and quantum well-based dipolariton nanodevices for integrated optical circuits. GERMAN V. KOLMAKOV, New York City College of Technology CUNY, TIM BYRINES, New York University, ROMAN YA. KEZERASHVILI, New York City College of Technology CUNY — Application of dipolaritons, which are a quantum superposition of photons, direct excitons and indirect excitons, in an optical microcavity for the design of nanoscale devices for optical computing is considered. In the proposed setup, a dipolariton condensate is formed in a patterned microcavity with an embedded two-layer gapped graphene. The condensate propagates in quasi-one dimensional channels formed by the pattern, and its propagation is controlled by the gate voltage applied to a positively-charged hole-carrying graphene layer. The advantage of the dipolaritons, compared to the conventional polaritons formed by the direct excitons and photons, is in the possibility to drive the condensate by the electric force since the latter is directly applied the dipolaritons. A dipolariton switch based on a Y-shaped channel is considered and its performance is determined via numerical simulations of the dipolarition condensate dynamics. The tunability of the device functions by the application of an external electric field is discussed. The simulations for a Y-shaped switch is also performed for a patterned microcavity with embedded coupled quantum wells and the results are compared with those for a microcavity with graphene.

8:12AM Y17.00002 Terahertz hot electron bolometric detectors based on graphene quantum dots1. A EL FATIMY, Department of Physics, Georgetown University, Washington, DC 20057, USA, R.L. MYERS-WARD, A. K. BOYD, K. M. DANIELS, D.K. GASKILL, U.S. Naval Research Laboratory Washington, DC 20375, USA, P. BARBARA, Department of Physics, Georgetown University, Washington, DC 20057, USA — We study graphene quantum dots patterned from epitaxial graphene on SiC with a resistance strongly dependent on temperature. The combination of weak electron-phonon coupling and small electronic heat capacity in graphene makes these quantum dots ideal hot-electron bolometers. We measure and characterize the THz optical response of devices with different dot sizes, at operating temperatures from 2.5K to 80K. The high responsivity, the potential for operation above 80 K and the process scalability show great promise towards practical applications of graphene quantum dot THz detectors.

1 This work was sponsored by the U.S. Office of Naval Research (award number N000141310865)

8:24AM Y17.00003 Position dependent photodetection of graphene field effect transistors. BIDDUT SARKER, Purdue University. EDWARD CAZALAS, Pennsylvania State University, ISAAC CHILDRES, Purdue University, IGOR JOVANOVIC, Pennsylvania State University, YONG CHEN, Purdue University — The extraordinary optical and electronic properties of graphene make it a promising component of high-performance photodetectors. Most graphene photodetectors studied so far require light illumination either on the graphene or at the graphene/metal interface. In this talk, we report a study of the spatial dependence of photoresponse in back-gated graphene field effect transistors (GFET) on undoped semiconductor substrates by scanning a focused laser spot across and away from the GFETs. We find that the photocurrent and photoresponsivity can be varied by a few orders of magnitude depending on the laser illumination position. Our observation can be explained using a numerical model based on the charge transport of photoexcited carriers in the substrate. This work may enable position sensitive photodetectors and further developments of graphene-based optoelectronic devices.
8:36AM Y17.00004 Optical rectification at visible frequency in biased bilayer graphene, F. HIPOLITO, NUS Graduate School for Integrative Sciences and Engineering, VITOR M. PEREIRĂ, Department of Physics, National University of Singapore — The second order response of the electrical current to an electromagnetic field is analyzed within the framework of non-equilibrium many-body perturbation theory for the case of a two-dimensional electronic system such as graphene and its bilayer. The absence of inversion symmetry in a biased graphene bilayer allows finite DC response in second order to an AC electromagnetic wave. The induced DC current is evaluated for biased bilayer at finite temperature, and its tunability is analyzed as a function of electron density, which can be experimentally varied by means of a global gate voltage applied to the sample. Both intrinsic and photon drag microscopic processes are considered, as they contribute on similar footing to the photocurrent in general. However, the dependencies of these two contributions on the polarization state of the incident light are different, which allows the manipulation of the relative contribution of intrinsic versus photon drag contributions by tuning the experimental parameters. For example, the photocurrent emerging from circularly polarized light stems entirely from photon drag, as the circular photogalvanic effect is forbidden by the $C_{3v}$ rotation symmetry of the honeycomb lattice.

8:48AM Y17.00005 Graphene-Boron Nitride Heterostructure Based Electro-Optical Modulator, YUANDA GAO, Columbia University, REN-JYE SHIUE, Massachusetts Institute of Technology, XUETAO GAN, JAMES HONE, Columbia University, DIRK ENGLUND, Massachusetts Institute of Technology — Graphene, a two-dimensional atomic-scale carbon based material, exhibits uniform absorption of the incident light over a broad spectrum range from visible to mid-infrared. This absorption can be tuned by electrostatic doping, resulting in electro-absorptive modulation of the incident light. We propose and demonstrate a high-speed electro-optical modulator structure by using a high-mobility dual-layer graphene capacitor integrated with a planar silicon photonic crystal nanocavity. Strongly enhanced light-matter interaction of graphene in a sub-micron meter cavity enables efficient electrical tuning of the cavity reflection. We achieved a modulation depth of 3.2 dB within a voltage swing of only 2.5 V; we measured a 3dB cut-off frequency up to 1.2 GHz.

9:00AM Y17.00006 Asymmetric transmission of terahertz waves in graphene-loaded photonic systems, YU ZHOU, REN-HAO FAN, Nanjing University, QING HU, Massachusetts Institute of Technology, RU-WEN PENG, MU WANG, Nanjing University — In this work, we have proposed two types of graphene-loaded photonic systems, through which terahertz(THz) waves present asymmetric transmission tuned by external magnetic field. One is a graphene-loaded metal grating. It is found that resonant modes in the system can be converted between transverse-electric and transverse-magnetic polarizations due to Hall conductivity of graphene. As a consequence, asymmetric transmission of THz waves through these graphene-loaded metal gratings is achieved. The other is a photonic crystal cavity integrated with graphene. Non-reciprocal propagation of THz waves has been verified in this system. By adjusting the external magnetic field or the Fermi level of graphene, asymmetric wave propagation can be significantly tuned. Our investigations offer unique approaches to achieve potentially applications in the design of the graphene-loaded tunable devices such as THz isolators and diodes.


9:12AM Y17.00007 Photoresponse and light trapping in nanowire array-graphene interfaces, TITO HUBER, SCOTT JOHNSON, QUINTON BARCLIFT, TINA BROWER, Howard University, JEFFREY H. HUNT, JOHN H. BELK, The Boeing Company — Graphene is emerging as an optical material that features tunability by electrostatic doping and a photothermoelectric response, however it features low optical absorption. We studied interfaces between nanowire arrays and graphene and also other transparent electrodes such as indium tin oxide films. The nanowire arrays were fabricated using a template method. Graphene was transferred from copper substrates. The interfaces were characterized with a number of tools including Scanning Electron microscopy, Raman spectroscopy and optical reflectance. We also studied the photocurrent through the interface in particular the temporal and wavelength dependence that are revealing of the characteristic thermoelectric origin of the signal. In the photocurrent tests we employed devices composed of nanowire arrays which are capped with the transparent electrode. Interestingly, we observed that the interface has low optical reflectivity and high optical absorption, which we will discuss in terms of enhanced optical trapping.

9:24AM Y17.00008 Terahertz modulators based on multiple non-Bernal graphene layers, IOANNIS CHATZAKIS, ZHEN LI, University of Southern California Electrical Engineering, ALEXANDER BENDERSKII, University of Southern California Department of Chemistry, STEPHEN CRONIN, University of Southern California Electrical Engineering — We investigate a THz modulator based on a stack of disoriented the non-Bernal stacks graphene layers (GLs) grown by chemical vapor deposition method (CVD) on SiO2 substrate [1]. The non-Bernal stacking GLs results in the electron decoupling of the GLs, higher interband absorption and exhibit the same energy spectrum of the charge carriers to that in individual GLs. The detection efficiency in room temperature is high due low probability of the high energy of the optical phonons (~ 0.2 eV) absorption. Using terahertz time-domain spectroscopy, we show that the multi graphene layers exhibit fairly high responsivity due to high quantum efficiency.


9:36AM Y17.00009 Optical Plasmonic Switch based on Graphene, KYUNGSONG MOON, SUK-YOUNG PARK, Dept. of Physics, Yonsei University — We have studied an electro-optical plasmonic waveguide, which controls the transmission of incident light by switching the coupling of the surface plasmon polariton (SPP) localized on graphene. It has been previously shown that the propagation length of the SPP localized on the copper surface can be effectively reduced by a factor of two or three by applying external bias potential. In our study, we have demonstrated that the propagation length of the SPP localized on graphene can be dramatically reduced by a factor of ten or so and the wavelength of SPP can be reduced by several hundreds of that of the incident light as well. We have also investigated the effect of scattering times of graphene and active Si layer on switching line shape. Switching occurs upon varying the carrier density of Si layer by $\Delta n/n \sim 15\%$ in the vicinity of switching region. For a fixed bias voltage applied just below the critical value, signal laser beam shone into the metal nano-particles may increase the carrier density as such, which will induce switching. This may help develop an all-optical nano-scale plasmonic switch.

This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(NRF-2012R1A1A006927).
Many-Body Problem

9:48AM Y17.00010 Time-of-flight photoconductivity in polymer/graphene blends, GVIDO BRATINA, EGGON PAVLICA, SRINIVASA RAO PATHIPATI, ROBERT NAWROCKI, RAVEENDRA PENUMALA, Laboratory for Organic Matter Physics, University of Nova Gorica, Slovenia — We have used time-of-flight (TOF) photoconductivity measurements to assess the electric charge transport parameters in thin layers of poly(3-hexyl thiophene-2,5-diyl) (P3HT) mixed with single and multiple-layer graphene nanoflakes. Thin layers were cast from a solution and two co-planar metal electrodes were deposited by vacuum evaporation on top. An electric field was set up between the electrodes A laser pulse was used to photogenerate charge carriers near the biased electrode, and time dependence of the photocurrent (I(t)) was measured at the opposite electrode. I(t) curves were confronted to I(t) obtained by a Gaussian-disorder Monte Carlo simulations, adapted to thin-film geometry. The simulations included a position-dependent electric field between two coplanar electrodes, which importantly affects the charge carrier transport through the blend between the electrodes. Comparison between the simulated and measured I(t) results in values for charge carrier mobility, average charge velocity and variation of charge velocity. Our results show that the hole mobility in blends is increased by more than an order of magnitude in comparison to the hole mobility of a neat layers of P3HT.

10:00AM Y17.00011 Optical and electronic properties study of bottom-up graphene nanoribbons for photovoltaic applications1, CESAR E.P. VILLEGAS, ALEXANDRE ROCHA, Instituto de Física Teórica, Universidade Estadual Paulista, São Paulo, SP, Brazil — Graphene nanoribbons (GNRs), turn out to be serious contender for several optoelectronic applications due to their physical properties. Recently, bottom-up methods, using the assembly of appropriate precursor molecules were shown to be an exciting pathway towards making precise nanoribbons. In particular, it has been demonstrated that so-called cove-shaped GNRs absorb light in the visible part of the spectrum, suggesting they could be used for photovoltaic applications. In solar cells, the key ingredient is the presence excitions and their subsequent diffusion along a donor material. This is influenced by the character of the different excitations taking place, as well as, the exciton binding energy. Thus, in this work we use many-body corrected density functional theory to simulate the optical properties of these nanoribbons. We elucidate the most important transitions occurring in these systems, and identify types of excitations that have not been previously observed in conventional nanoribbons. We also find that the exciton binding energies for all the structures we considered are in the eV range, which enhances the diffusion lengths for the particle-hole pairs. Finally, we estimate the potential of these systems as solar cells by calculating the short-circuit current. The Authors thank FAPESF for financial support.

10:12AM Y17.00012 Graphene Oxide Liquid Crystals for Reflective Display without Polarizing Optics, ZHUAN ZHU, University of Houston, LIQUIN HE, University of Science and Technology of China, JIAN YE, Guangdong University of Technology, MIN SHUI, Texas A&M University, XUFEI ZHOU, Chinese Academy of Sciences, YANAN WANG, YANG LI, ZHIHUA SU, University of Houston, HAIYAN ZHANG, YING CHEN, Guangdong University of Technology, ZHAOPIING LIU, Chinese Academy of Sciences, ZHENDONG CHENG, Texas A&M University, JIMING BAO, University of Houston — The recent emergence of liquid crystals of atomically thin two-dimensional (2D) materials not only has allowed us to explore novel phenomena of macroscopically aligned 2D nanomaterials but also has provided a route toward their controlled assembly into three-dimensional functional macrostructures. Using flow-induced mechanical alignment, we prepared flakes of graphene oxide (GO) in different orientational orders and demonstrated that GO liquid crystal (LC) can be used as a rewritable medium for reflective display without polarizing optics. With a wire or stick as a pen, we can make the surface of GO LC reflective and bright, and we can then manually draw lines, curves, and any other patterns with dark appearance. The contrast between bright and dark features is due to anisotropic optical responses of ordered GO flakes. Since optical anisotropy is an intrinsic property of 2D structures, our observations and demonstration represent one of many potential applications of macroscopically aligned 2D nanomaterials.

10:24AM Y17.00013 Development of graphene oxide materials with controllably modified optical properties, ANTON NAUMOV, Central Connecticut State University, CHARUDATTA GALANDE, Rice University, ADITYA MOHITE, Los Alamos National Laboratory, PULICKE A. AJAYAN, R. BRUCE WEISMAN, Rice University — One of the major current goals in graphene research is modifying its optical and electronic properties through controllable generation of band gaps. To achieve this, we have studied the changes in optical properties of reduced graphene oxide (RGO) in water suspension upon the exposure to ozone. Ozonation for the periods of 5 to 35 minutes has caused a dramatic bleaching of its absorption and the concurrent appearance of strong visible fluorescence in previously nonemissive samples. These observed spectral changes suggest a functionalization-induced band gap opening. The sample fluorescence induced by ozonation was found to be highly pH-dependent: sharp and structured emission features resembling the spectra of molecular fluorophores were present at basic pH values, but this emission reversibly broadened and red-shifted in acidic conditions. These findings are consistent with excited state protonation of the emitting species in acidic media. Oxygen-containing addends resulting from the ozonation were detected by XPS and FTIR spectroscopy and related to optical transitions in localized graphene oxide fluorophores by computational modeling. Further research will be directed toward producing graphene-based optoelectronic devices with tailored and controllable optical properties.

10:36AM Y17.00014 Determination of graphene layer thickness using optical image processing, MONICA COOK, R.G. MANI, Georgia State University — Graphene, a single atomic layer of carbon arranged in a hexagonal lattice structure, is a valuable material in a wide range of research. A significant impediment to graphene research is the need to manually characterize the thickness of high-quality graphene produced via mechanical exfoliation. Traditional methods of characterizing the layer thickness of graphene, including Raman spectroscopy and atomic force microscopy, require expensive equipment and can be damaging to the graphene sample. We examine here a known alternative method for quantitatively determining the layer thickness of graphene on SiO2/Si based on optical image processing, which is quick, inexpensive, and non-invasive [1]. Using RGB images of a candidate graphene sample and a background image, taken with a simple optical microscope and charge-coupled device (CCD) camera, we process the images with an algorithm based on Fresnel’s law to obtain the contrast spectrum. Each layer of graphene exhibits a unique contrast spectrum for its particular substrate, which is measured and used for accurate layer identification. We also discuss how this algorithm can be generalized to characterize the thickness of other promising two-dimensional materials as well as more complex structures on a variety of substrates.


Friday, March 6, 2015 8:00AM - 11:00AM –
Session Y18 DCOMP: Invited Session: New Approaches to the Non-Equilibrium Quantum Many-Body Problem Mission Room 103A - Andrew Millis, Columbia University
8:00AM Y18.00001 Bold-line Monte Carlo and the nonequilibrium physics of strongly correlated many-body systems¹, GUY COHEN, Columbia Univ — This talk summarizes real time bold-line diagrammatic Monte-Carlo approaches to quantum impurity models, which make significant headway against the sign problem by summing over corrections to self-consistent diagrammatic expansions rather than a bare diagrammatic series. When the bold-line method is combined with reduced dynamics techniques² both local single-time properties³ and two time correlators such as Green function⁴ can be computed at very long timescales, enabling studies of nonequilibrium steady state behavior of quantum impurity models⁵ and creating new solvers for nonequilibrium dynamical mean field theory.

¹This work is supported by NSF DMR 1006282, NSF CHE-1213247, DOE ER 46932, TG-DMR120085 and TG-DMR130036, and the Yad Hanadiv-Rothschild Foundation.


8:36AM Y18.00002 The time-dependent Gutzwiller approximation¹, MICHELE FABRIZIO, SISSA — The time-dependent Gutzwiller Approximation (t-GA) [1,2] is shown to be capable of tracking the off-equilibrium evolution both of coherent quasiparticles and of incoherent Hubbard bands. The method is used to demonstrate that the sharp dynamical crossover observed by time-dependent DMFT in the quench-dynamics of a half-filled Hubbard model can be identified within the t-GA as a genuine dynamical transition separating two distinct physical phases [3]. This result, strictly variational for lattices of infinite coordination number, is intriguing as it actually questions the occurrence of thermalization. Next, we shall present how t-GA works in a multi-band model for V₂O₃ that displays a first-order Mott transition. We shall show that a physically accessible excitation pathway is able to collapse the Mott gap down and drive off-equilibrium the insulator into a metastable metal phase [4].


Work supported by the European Union, Seventh Framework Programme, under the project GO FAST, Grant Agreement no. 280555.

9:12AM Y18.00003 Thermalization and long-time behavior of nonequilibrium correlated quantum systems¹, HERBERT F. FOTSO, Ames Laboratory — Nonequilibrium dynamical mean field theory and nonequilibrium self-consistent strong coupling expansion[1] are used to study the relaxation of correlated quantum systems driven out of equilibrium by DC electric fields[2]. Both the Falicov-Kimball and the Hubbard model are found to exhibit regimes of monotonic or oscillatory thermalization as well as regimes where they evolve in a monotonic or oscillatory manner towards a non-thermal state. This suggests that driven quantum systems have a richer behavior than their quenched counterparts and that integrability does not play as critical a role. In the monotonic thermalization scenario, the system evolves through successive quasi-thermal states and it is possible to extrapolate its long time properties from its transient; bridging the gap between the transient and the steady state with very little computational cost. Furthermore, regardless of the relaxation scenario, it is interesting to ask how the particles are distributed as the system evolves in time. We will show that non-trivial parameter-dependent patterns are formed when the system is visualized in momentum space [3]. These features should be observable in current cold atom experiments.


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9:48AM Y18.00004 New Perspectives for Time-Evolution with DMRG, ULRICH SCHOLLWOECK, Dept of Physics University of Munich — In the last 10 years, time-evolution with DMRG has revealed itself to be a very powerful technique for low-dimensional strongly interacting quantum systems both near and far from equilibrium. We show how new techniques, mainly based on the use of Chebyshev polynomials allowing to use DMRG for obtaining real-frequency spectral information in multi-band DMFT calculations, also allow to use it as an impurity solver for far-from-equilibrium DMFT in a Hamiltonian formulation, strongly increasing the time range of non-equilibrium DMFT, and to attack time-evolutions efficiently in far from equilibrium settings.
10:24AM Y18.00005 Nonequilibrium Dynamical Mean Field Theory for Inhomogeneous and Photo-Excited Systems1. PHILIPP WERNER, University of Fribourg — Photodoping of a Mott insulator triggers a nonequilibrium phase transition from a correlation induced insulating state to a nonthermaling conducting state with electron- and hole-like carriers. Using the nonequilibrium extension of (inhomogeneous) dynamical mean field theory2,3 in combination with a strong-coupling impurity solver4 we study the relaxation and diffusion of photo-doped carriers in Mott insulating bulk systems and hetero-structures. In large-gap insulators, the life-time of the carriers depends exponentially on the gap size5 while in small-gap insulators, strongly pulse-energy dependent impact ionization processes lead to a double-exponential relaxation6. In the paramagnetic phase, the photo-doped carriers spread through the insulator in a diffusive manner, while the scattering with an antiferromagnetic background leads to a rapid loss of kinetic energy7. In the presence of strong fields, as realized e. g. in polar heterostructures, the ability to dissipate energy locally in an antiferromagnetic system enables fast carrier transport8. These insights should be relevant for designing Mott insulating solar cells and light-controlled devices which operate on an ultra-fast timescale.

1This work is supported by ERC/FP7 Starting Grant No. 278023
8:36AM Y20.00002 Spin transport across ferromagnetic tunnel contacts to semiconductors — questions and answers, RON JANSEN, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan — Ferromagnetic tunnel contacts to semiconductors are key building blocks of spintronic semiconductor devices. Such contacts allow the transport of spins from the ferromagnetic source into the semiconductor, driven either electrically or thermally, but also provide a means to detect spins in the semiconductor and convert the spin information into an electrical signal. Reproducible results have been obtained using either a local (3-terminal) or non-local (4-terminal) measurement geometry, and the electrical spin signals in both cases exhibit all the characteristic features of a current-induced non-equilibrium spin population. Nevertheless, the quantitative analysis has revealed surprising discrepancies with the existing theory. I will address several relevant questions about the nature of the spin transport in ferromagnetic tunnel contacts on semiconductors, and discuss the answers using the experimental observations that have been obtained over the last years and their comparison with available theories, including those involving localized states in the contact. The aim is to clarify what is established and understood and what is not, the latter pointing to interesting new physics yet to be uncovered.


9:12AM Y20.00003 3-terminal Hanle measurements in metals: spin accumulation or novel magnetoresistance effect?, FELIX CASANOVA, CIC nanoGUNE, 20018 San Sebastian (Basque Country, Spain) — A simple device to study spin injection and transport in semiconductors uses a 3-terminal (3T) geometry, in which spin accumulation is induced and probed by a single magnetic tunnel contact, through the Hanle effect [1]. Since this geometry does not require submicron-sized fabrication, 3T-measurements have become very popular [1-3]. However, many of the reported results disagree with the standard theory of spin injection and have put these measurements into question [4-6]. Our recent work shines some light to this controversy. First, we fabricated ferromagnetic-insulator-nonmagnetic (FIN) 3T devices with metallic electrodes to avoid the complications brought by the Fermi-level pinning when using a semiconductor, and demonstrate that measured Hanle and inverted Hanle-like features are not compatible with spin injection in these metals [5]. Subsequently, we detect this effect in nonmagnetic-insulator-nonmagnetic (NIN) tunnel junctions for the first time and we demonstrate experimentally beyond any doubt that the measured Hanle-like signals are due to impurities in the oxide layer [7]. We support these results with a theory for impurity-assisted tunneling which takes into account spin interactions and Coulomb correlations. We show that this is actually a novel magnetoresistance effect, which is general to any impurity-assisted tunneling process regardless of the oxide thickness or materials used. The presented work will thus be used as a benchmark to spin injection experiments to any nonmagnetic material, and specially will redirect research of semiconductor spintronics, with all the implications in such a technologically relevant area. [1] S. P. Dash et al., Nature 462, 491 (2009); [2] C. H. Li et al., Nature Commun. 2, 245 (2011); [3] A. Jain et al., Phys. Rev. Lett. 109, 106603 (2012); [4] Y. Aoki et al., Phys. Rev. B 86, 081201(R) (2012); [5] O. Txoperena et al., Appl. Phys. Lett. 102, 192406 (2013); [6] H. N. Tinkey et al., Appl. Phys. Lett. 104, 232410 (2014); [7] O. Txoperena et al., Phys. Rev. Lett. 113, 146601 (2014).

9:48AM Y20.00004 New interpretation for recent spin injection experiments1, HANAN DERY, University of Rochester — We elucidate the large discrepancy between known spin relaxation theory and the findings of recent spin injection experiments that make use of a single ferromagnetic-insulator-nonmagnetic junction for both injection and detection of spin-polarized currents. This local setup scheme gained popularity since 2009 when Dash et al. claimed to achieve room temperature spin injection in silicon [1], followed by avalanche of similar experiments in silicon and other materials that resort to this measurement technique. We show that those enhanced signals and their dependence on temperature are set by impurities embedded in the tunnel barrier with large on-site Coulomb repulsion compared with the voltage bias [2]. Depending on the electron occupation of the resonance level, the magnetoresistance effect is established by the interplay between the Zeeman energy and the impurity coupling to the ferromagnetic material. Considering molecular fields due to hyperfine and exchange interactions, we capture the shape and sign dependence of the signal on magnetic field orientation. The findings are used to explain both conventional spin injection [1], and cases where the bias voltage is distributed across the junction while the net charge current is zero (the so-called local Seebeck spin tunneling [3]). Finally, we extend the theory to impurity-rich tunnel junctions, showing that a similar magnetoresistance effect can persist in completely nondopant junctions [4]. The extension beyond electrical spin injection from ferromagnetic electrodes paves the way for a new class of 1D nanometer-size memory cells which represents the ultimate scaling of memories (leaving no room in the bottom).


1This work is supported by NSF and DTRA Contracts No. ECCS-1231570 and No. HDTRA1-13-1-0013, respectively.

10:24AM Y20.00005 Crossover from Spin Accumulation into Interface States to Spin Injection in the Germanium Conduction Band1, MATHIEU JAMET, CEA and University Grenoble Alpes — Electrical spin injection from ferromagnetic metals to silicon (Si) and germanium (Ge) is the first and basic requirement for the development of spintronic devices and their integration with mainstream semiconductor (SC) technology. The main obstacle to efficient spin injection is the conductivity mismatch between the ferromagnetic metal and Si or Ge and requires tunneling spin injection through an oxide barrier (Ox). However, tunneling spin injection raises other important issues in the interpretation of spin signals obtained in three-terminal geometry. In particular, the possible presence of localized states within the Ox or at the Ox/SC interface may lead to wrong conclusions. To study the exact origin of the spin signals measured in three-terminal geometry, we have grown Ta/CoFeB/MgO/SoI and GeO1 substrates with n and p type doping using variable MgO thicknesses. The use of SOI and GeOI substrates allows us to apply back gate voltages to the SC channel to vary its resistivity. Moreover we have used three different techniques to grow the MgO tunnel barrier: by sputtering of MgO or Mg followed by a plasma oxidation and e-beam evaporation of MgO. Using the Mg and plasma oxidation growth of the tunnel barrier, though less flexible than the other techniques, allowed us to show the temperature transition from the spin accumulation into interface states to the spin accumulation into the conduction band of n-Ge. Above 150 K, the magnitude of the spin RA product agrees well with the spin diffusion theory predictions and is proportional to the injected current and to the channel resistivity as expected. Temperature dependent spin pumping measurements showed the same transition. Using the same spin injector, we also found radically different spin signals using p-Ge supporting the fact that spin accumulation occurs into the SC channel. In this presentation, we will extend our spin signal analysis using MgO tunnel barriers of different thicknesses and grown by different methods.

1Support by the French ANR project SiGeSPIN (ANR-13-BS10-0002) is acknowledged.

Friday, March 6, 2015 8:00AM - 11:00AM – Session Y21 DCMP: Vanadium Oxides I 201 - Jiang Wei, Tulane University
8:00AM Y21.00001 Oxygen Effect and Mechanism of Insulator-to-Metal Transition using Indirect Band in Vanadium Dioxide, TETIANA SLUSAR, ETRI-Elec Telecomm Rsch Inst in Korea, JIN CHEOL CHO, Korea University of Science and Technology, AHRUM SOHN, Ewha Womans University in Korea, JEONGYONG CHOI, ETRI-Elec Telecomm Rsch Inst in Korea, DONG-WOOK KIM, Ewha Womans University in Korea, HYUN-TAK KIM, ETRI-Elec Telecomm Rsch Inst in Korea — The vanadium dioxide VO$_2$ Science and Technology, AHRUM SOHN, Ewha Womans University in Korea, JEONGYONG CHOI, ETRI-Elec Telecomm Rsch Inst in Korea, DONG-WOOK KIM, Ewha Womans University in Korea, HYUN-TAK KIM, ETRI-Elec Telecomm Rsch Inst in Korea — The vanadium dioxide VO$_2$ is known as the Mott insulator and it undergoes the insulator-to-metal transition (IMT) near $T_c = 340$ K. Under the external influence (doping, strain etc.) the $T_c$ is reduced. To explain this behavior, we have used the Mott criterion proposing the critical carrier density $n_c$ at MIT (metal to insulator). In this case, Mott derived $n_c$ for the transition from metal to insulator. Therefore, $n_c$ is regarded as the minimum carrier density in metal phase. However, in the reverse transition (insulator to metal), $n_c$ cannot clarify the above behavior. Thus, a new model has been required. Here, we have grown VO$_2$ thin films under the different oxygen partial pressure conditions and studied the influence of oxygen deficiency on $T_c$ of the IMT. For the analysis, we have measured the Hall voltage near $T_c$ and a change of work function. Based on the experimental data we have proposed the model explaining $T_c$ changes in VO$_2$. This model describes the excitation process of bounded charges in direct and indirect energy bands as a criterion of the IMT. Moreover, it is shown that it can serve as universal mechanism that describes the physics of the IMT in many MIT materials from the new point of view, different from that, suggested by Mott. It is the fundament for operation of new devices.

8:12AM Y21.00002 First principles calculations of insulator-to-metal transition in photoexcited monoclinic VO$_2$, LEDE XIAN, University of the Basque Country, MATTEO GATTI, Ecole Polytechnique, PIERLUIGI CUDAZZO, University of the Basque Country, DANIEL WECKKAMP, MARC HERZOG, Fritz Haber Institute of the Max Planck Society, CHRISTINA MCGAHAN, ROBERT MARVEL, RICHARD HAGLUND, Vanderbilt University, MARTIN WOLF, JULIA STAHLER, Fritz Haber Institute of the Max Planck Society, ANGEL RUBIO, University of the Basque Country — The insulator-to-metal phase transition of VO$_2$ has been discovered for a long time, but its origin remains elusive. In recent experiments, ultrafast band gap collapse of monoclinic VO$_2$ upon photo excitation was observed through time resolved photoelectron spectroscopy (TRPES). In order to study this issue, we have performed first principles calculations based on many-body perturbation theory. We show that the band gap in monoclinic phase is extremely sensitive to small changes in the occupation of the localized d bands of V atoms. In particular, the photo-induced hole doping in VO$_2$ can strongly alter the dynamical screening, which then leads to a collapse of the band gap. Our results support the experimental findings and point to the electronic origin of the insulator-to-metal phase transition of monoclinic VO$_2$ in the TRPES experiments.

8:24AM Y21.00003 Extraordinary Inhibition of the Field-effect by Bound Quasiparticles at the Interface of a Dielectric and a Metal-Insulator Transition Material VO$_2$$_1$, KOEN MARTENS, KULeuven / imec / IBM Almaden, JAEWOO JEONG, NAGAPHANI AETUKURI, CHARLES RETTNER, IBM Almaden, NIHIL SHUKLA, EUGENE FREEMAN, Penn State University, DAVID ESHAHWI, FRANCOIS PEETERS, Universiteit Antwerpen, TEYA TOPURIA, PHIL RICE, IBM Almaden, ALEXANDER VOLODIN, KULeuven, WILDTED VANDERVORST, imec / KULeuven, MAHESH SAMANT, IBM Almaden, SUMAN DATTA, Penn State University, STUART PARKIN, IBM Almaden — An electric field applied normal to the interface of a dielectric and the prototypical, strongly-correlated semiconductor VO$_2$ is anticipated to lead to non-trivial phenomena. This field-effect allows for key insight into VO$_2$ physics. Field-effect modulation of channel current and carrier depletion in a field-effect device are found to be extraordinarily highly inhibited and no Metal-Insulator Transition is induced by the gate field for excess carriers up to $5 \times 10^{11}$cm$^{-2}$. The field-induced excess charge consists of bound quasi particles, as demonstrated by their activated and low excess carrier field-effect mobility. Small polarons as excess carriers in VO$_2$ consistently explain the observed field-effect, mobility and absence of depletion. The physics required to describe semiconducting VO$_2$’s field-effect is fundamentally different from classical semiconductor physics.

8:36AM Y21.00004 Phase inhomogeneity near the electrically driven insulator-metal transition in VO$_2$ nanobeams$^{1}$ , SUJAY SINGH, Department of Physics, University at Buffalo, State University of New York, Buffalo, NY 14260, USA, GREGORY HORROCKS, Department of Chemistry, Texas A&M University, College Station, TX 77843, USA, PETER MARLEY, Department of Chemistry, University at Buffalo, State University of New York, Buffalo, NY 14260, USA, ZHENZHONG SHI, Department of Physics, University at Buffalo, State University of New York, Buffalo, NY 14260, USA, SARBJIT BANERJEE, Department of Chemistry, Texas A&M University, College Station, TX 77843, USA, G. SAMBANDAMURTHY, Department of Physics, University at Buffalo, State University of New York, Buffalo, NY 14260, USA — Vanadium oxide (VO$_2$) exhibits an insulator to metal transition (IMT) at $T_c \approx 342$ K and this transition is amenable to triggering by voltage, light and strain. We present results from transport measurements (both AC and DC) on individual nanobeams of single crystalline VO$_2$ across the electrically driven transition from the insulating phase. Recent works in correlated electron systems have debated the individual roles of mechanisms such as Joule heating, percolation and avalanche in driving the transition. In our samples, the calculated average temperature of the nanobeams due to Joule heating is less than $C_T$ near the IMT, suggesting that an inhomogeneous phase develops and filamentary conduction paths likely drive the transition. At low bias values, the conduction is dictated by Joule heating and avalanche processes. At high bias values, the conduction is dictated by the re-emission of quasiparticles. The occurrence of avalanche-type events at higher bias values induce the formation of filamentary pathways, thereby precluding further need for percolation.

8:48AM Y21.00005 An ultrafast nano-infrared study of the photo-induced insulator-to-metal transition in Vanadium Dioxide, AARON STERNBACH, University of California San Diego Department of Physics, MENGKUN LIU, University of California San Diego Department of Physics, Stony Brook University Department of Physics, MARTIN WAGNER, RUBEN IRAHETA, University of California San Diego Department of Physics, TETIANA SLUSAR, University of Science and Technology School of Advanced Device Technology, Metal-Insulator Transition Creative Research Center ETRI, ALFRED LEITENSTORFER, University of Konstanz, Center for Applied Photonics, HYUN-TAK KIM, University of Science and Technology School of Advanced Device Technology, Metal-Insulator Transition Creative Research Center ETRI, RICHARD AVERITT, DIMITRI BASOV, University of California San Diego Department of Physics — We have devised and implemented the technique of time resolved scanning near-field optical microscopy to study the inhomogeneous development of a phase transition in the time domain with 20 nanometer spatial resolution and 100 femtosecond temporal resolution. The subject of our study is Vanadium Dioxide (VO$_2$), which is a canonical correlated electron system that exhibits an insulator to metal transition (IMT). We observe an abrupt rise in the photoconductivity at several hundred femtoseconds followed by a slow rise, which takes place on the order of several hundred picoseconds. Our measurement resolves the rise time of the IMT in individual sites, and we further observe inhomogeneous dynamics that are dependent on local strain. Our results pave the way for studying a plethora of systems where phase transitions involve inhomogeneities and phase separation.

$^1$This work is supported by NSF DMR 0847324.

$^2$The FWO is acknowledged.
9:00AM Y21.00006 Anomaly in the Metal-to-Insulator Transition of $V_2O_3$ Thin Films Under Pressure1, ILYA VALMIANSKI, GABRIEL RAMIREZ, SIMING WANG, CHRISTIAN URBAN, Univ of California - San Diego, XAVIER BATTLE, University of Barcelona, IVAN K. SCHULLER, Univ of California - San Diego, CENTER FOR ADVANCED NANOSCIENCE TEAM, GROUP OF MAGNETIC NANOMATERIALS TEAM — We present results of electrical transport measurements in highly textured $V_2O_3$ thin films of varying thickness under hydrostatic pressure from 100 kPa to 1.6 GPa. All films presented ~ 4 orders of magnitude resistance change at the Metal-to-Insulator Transition (MIT). Morphological and structural characterization was performed using in- and out-of-plane X-ray diffractometry and Atomic Force Microscopy before and after pressurization. We found an anomalous pressure dependence of the MIT for pressures above 500 MPa that deviates from the bulk behavior. Furthermore, we found an irreversible change in the MIT temperature, which coincides with a morphological but not crystal structure change in the film. The obtained anomalous pressure dependence suggests a difference between bulk and thin film MIT mechanisms.

1Work supported by AFOSR Project #: FA 9550-10-1-0409, Spanish MINECO MAT2012-33037 and European Feder Funds (Una manera de hacer Europa)

9:12AM Y21.00007 Neutron and x-ray scattering studies of the lattice dynamics in VO2, OLIVER DELAIRE, JOHN D. BUDAI, JIAWANG HONG, MICHAEL MANLEY, CHEN LI, ELIOT SPECHT, Oak Ridge National Laboratory, AYMAN SAID, BOGDAN LEU, JON TISCHEL, Argonne National Laboratory, DOUGLAS ABERNATHY, LYNN BOATNER, ROBERT MCMINNEKEY, Oak Ridge National Laboratory, ORNL-ANL COLLABORATION — Vanadium dioxide exhibits a metal-insulator transition at 340K, concomitant with a structural distortion from rutile to monoclinic on cooling. While much attention has been given to purely electronic aspects of the transition and the band-gap opening, less information has been available about the lattice dynamics (phonons), and their role in the thermodynamics of this important phase transition. We report detailed x-ray and neutron scattering measurements of the phonon dispersions and density of states in VO2, and their influence on the thermodynamics [1]. We show that the entropy of the transition is controlled by the large phonon entropy of the rutile phase, which stabilizes it at high temperature. This phonon entropy arises from soft, strongly-anharmonic phonons across much of the Brillouin zone. The origin of this softness and strong anharmonicity are discussed. [1] J. D. Budai*, J. Hong*, M. E. Manley, E. D. Specht, C. W. Li, J. Z. Tischler, D. L. Abernathy, A. H. Said, B. M. Leu, L. A. Boatner, R. J. McQueeney, and O. Dellaire, Nature 2014, DOI:10.1038/nature13865 Support by DOE Office of Basic Energy Sciences, Materials Sciences and Engineering Division; APS and SNS facilities supported by DOE-BES.

9:24AM Y21.00008 Toward Nano-Electronics Applications of Metal-Insulator Transition Materials - Atomic Layer Deposition of VO2 and a Selector Device Concept, ANTONY PETER, imec, KOEN MARTENS, imec / KULeuven, IVILIANA RADU, imec, NUO XU, UC Berkeley, GEERT RAMPHELBERG, Universiteit Gent, CHRISTOPH ADELMANN, imec, CHISTOPHE DETAVERNIER, Universiteit Gent, MARC HEYNS, imec / KULeuven, MALGORZATA JURCZAK, imec — We discuss advances toward applications of Metal-Insulator Transition (MIT) materials in nano-electronics based on the prototypical MIT material VO2. A fabrication friendly method to deposit VO2 is required for VO2 applications. VO2 films deposited by techniques suitable for manufacturing, including Atomic Layer Deposition (ALD), have typically been non-continuous and have shown a strongly degraded MIT when film thickness was below 40-50 nm. We show how the nanoscale morphology of VO2 films can be controlled to realize smooth ultrathin (thinner than 10 nm) crystalline films with ALD. We demonstrate that the films possess both a structural and an electronic transition. The film resistivity of ultrathin films changes by more than two orders of magnitude across the MIT. Incipient nanoelectronics based on Metal-Insulator-Transition (MIT) materials currently features promising device concepts that require further development and understanding. A candidate first nanoelectronic application for MIT materials is a selector element, which is used to prevent sneak currents in dense cross bar memory arrays. Making use of simulations we elaborate a device concept for a selector element based on MIT materials such as VO2 and SmNiO3.

9:36AM Y21.00009 Tungsten-doped vanadium dioxide thin films for THz analog optical applications1, GULTEN KARAOGLAN-BEBEK, NADIM HOQUE, Texas Tech University, MARK HOLTZ, Texas State University, ZHAOYANG FAN, AYRTON BERNUSSI, Texas Tech University — The Mott transition of vanadium dioxide (VO2) has been widely studied, with abrupt changes in electrical and optical properties at temperature approximately 70 C. The phase transition properties of thin vanadium dioxide films can be changed by doping with tungsten making it a prospective candidate to realize tunable optical devices at terahertz (THz) frequencies. Tungsten incorporation into the vanadium dioxide film yields a wider transition window and a lower transition temperature allowing practical use in analog-like continuous applications. Our results reveal characteristic metal-insulator phase temperature and width of 40 C and 35 C, respectively, for the film with the highest W content. We show that the refractive index of W-doped vanadium dioxide can be continuously tuned and this provides precise control of the transmission properties of the vanadium dioxide films and discuss future active THz optical devices for analog applications. We demonstrate that W-doped vanadium dioxide films can be also used as anti-reflective coating at THz frequencies but at temperatures much lower than that observed for undoped films.

1National Science Foundation (ECCS 1128644)

9:48AM Y21.00010 Distinct substrate effects on the gate-induced metallic states in VO2 thin films, MASAKI NAKANO, University of Tokyo, DAISUKE OKUYAMA, Tohoku University, MASAICHIRO MIZUMAKI, SPRing-8, HIROYUKI OSUMI, RIKEN SPRing-8 Center, MASARO YOSHIDA, TAKAHISA ARIMA, University of Tokyo, MASAKI TAKATA, RIKEN SPRing-8 Center, MASASHI KAWASAKI, University of Tokyo, YOSHINORI TUKURA, RIKEN Center for Emergent Matter Science (CEMS), YOSHIHIRO IWASA, University of Tokyo — The idea of utilizing electric-double layers for controlling electronic phases of condensed matters by external voltages, namely EDLT, has attracted growing attention. Of particular interest is EDLT based on VO2, enabling electrical control of “bulk” electronic phases over the electrostatic screening length, as proven by transport, optical, and structural measurements [1-3]. We attributed this unique feature to electrostatic effects, but there are other models proposed from electrochemical viewpoints. Here we show that the reversibility of the device operation strongly depends on the substrates, suggesting a governing mechanism can differ depending on the substrates. We found that EDLT with VO2 films grown on lattice-matched TiO2 substrates show reversible gating effects, whereas those on hexagonal Al2O3 substrates become irreversible, although in both cases metallic states can be induced electrically. X-ray absorption spectra taken before and after the gating experiments also indicated distinct substrate effects on the valence states of vanadium at the gate-induced metallic states.

10:00AM Y21.00011 Platform for applying uniform strain to VO2 nanobeams and other small crystals1, BOSONG SUN, Department of Physics, University of Washington, ANA SANCHEZ, RICHARD BEANLAND, Department of Physics, University of Warwick, TAIUNO PALOMAKI, DAVID COBDEN, Department of Physics, University of Washington — Many properties of crystals, including symmetry, equilibrium phase, band structure, and Bloch state properties such as Berry curvature and even topology, can be modified by strain. Conversely, controlling strain properly is essential for determining the intrinsic properties of many complex materials. We are therefore exploring ways to apply uniaxial stress to small crystals, ranging from two-dimensional materials to nanowires. For example, we have developed a platform for making samples with controlled built-in stress. In the case of VO2 nanobeams, this allows us to perform systematic studies on each of the several phases (R, M1, M2 and T) involved in the metal-insulator transition in a single sample using multiple microscopies, including transmission electron microscopy. Amongst other things we can image the T phase, study the propagation of interphase boundaries, explore the origin of putative noncentrosymmetry, and seek diffuse contrast to locate the spinodal lines of the transition.

1Supported By DoE BES (DE-SC0002197).

10:12AM Y21.00012 ABSTRACT WITHDRAWN

10:24AM Y21.00013 Phase Transitions in Electron Beam Deposited Cr-doped VO2 Thin Films2, DOMINIC ROTA, Belmont University, KENT HALLMAN, Vanderbilt University, DAVON FERRARA, Belmont University, RICHARD HAGLUND, Vanderbilt University — Three phases of the semiconducting state of VO2 are known, denoted M1, M2 and T; the M2 phase in particular has alternating vanadium chains arranged in antiferromagnetic pairs. This suggests potentially interesting magnetic and optical properties, motivating our interest in developing a robust protocol for preparing thin films of the M2 and T phases for studies of the optically induced semiconductor-to-metal transition (SMT). A protocol for electron beam deposition of Cr-doped VO2 (Cr$_x$V$_{1-x}$O$_2$) thin films was developed, allowing for low-cost and efficient fabrication of homogeneous films, beginning with powder precursors for vanadia and chromia in appropriate proportions. The films were characterized by resistivity and reflectivity measurements of the SMT with concentrations of Cr dopant ranging from x=0 to x=0.04. Raman spectroscopy was used to identify the structural phase transitions and revealed that the structural phases M1, T, and M2 can be determined by comparing differences in the spectrum. Comparing the resistivity hysteresis curves to the Raman spectroscopic measurements, we find that single-phase structures occur for x=0 (M1) and x=0.04 (M2) while concentrations between the x=0 and x=0.04 exhibit a mixture of at least two structural phases, including the T phase.

2We gratefully acknowledge research support from the National Science Foundation (KAH, DMR-1207507) and through the NSF Research Experiences for Undergraduates program (DR, PHY-1263045)

10:36AM Y21.00014 Ab Initio phonon calculations in metallic and insulating phases of VO$_2$1, CHRISTOPHER HENDRIKS, ERIC WALTER, HENRY KRAKAUER, William and Mary College — Vanadium dioxide (VO$_2$) undergoes a first-order metal-insulator transition (MIT) from the high-temperature rutile phase (R) to an insulating, low-temperature monoclinic phase (M1). Several competing insulating phases exist, with phase boundaries in a narrow temperature and strain range close to the MIT. Recently, novel IR and Raman measurements of micro- and nano-structured VO$_2$ samples have become increasingly available; this allows the phases to be studied while avoiding many difficulties with bulk samples, such as twinning and cracking on cycling through the MIT. Theoretical calculations of vibrational properties can assist in the interpretation of such experiments1. We will present ab initio DFT+U calculations of phonon frequencies for the various phases and compare these to reported measurements for the R, M1, M2 and T phases.

1Supported by ONR
4T. J. Huffman et al., PRB 87, 115121 (2013).
6C. Marini et al., PRB 77, 235111 (2008).

10:48AM Y21.00015 Heterogeneous Nucleation and Growth Dynamics in the Light-induced Phase Transition in Vanadium Dioxide. NATHANIEL BRADY, Univ of Alabama - Birmingham, KANNATASSEN APPAVOO, JOYEE NAG, Vanderbilt University, MIN-AH SEO, ROHIT PRASANKUMAR, Los Alamos National Lab, RICHARD HAGLUND, Vanderbilt University, DAVID HILTON, Univ of Alabama - Birmingham — Vanadium dioxide is a well-known transition metal oxide that undergoes an insulator-to-metal phase transition at $T_C = 340$ K that is accompanied by a structural distortion from monoclinic [P2_1/c for $T < T_c$] to rutile [P42/mnm for $T > T_c$]. The heterogeneous nature of this phase transition is evident from the significantly smaller the thermal energy at $T_c$ when compared to the energy barrier for homogenous nucleation [see: Phys. Rev. B 65, 224113 (2002)]. The identity of the relevant defect that locally lowers this barrier enabling this phase transition, however, is currently unclear. In our talk, we will report on ultrafast optical investigations of the light-induced insulator-to-metal phase transition in samples with controlled disorder generated by substrate mismatch. Our results reveal several common features of this optical phase transition that are independent of this disorder and a small variation in threshold fluence needed to drive this phase transition that depends on the sample morphology.

Friday, March 6, 2015 8:00AM - 11:00AM —
Session Y22 DMP: Focus Session: Carbon Nanotubes: Optical, Mechanical, Magnetic & Other Properties — 202A — Michael S. Arnold, University of Wisconsin-Madison

...decay pathways arising from exciton mobility. [1] S. Ghosh, et al., Science, 330, 1656 (2010). [2] Y. Piao, et al., Nature Chem., 5, 840 (2013). [3] Y. Miyauchi, a function of dopant species. We also report photoluminescence decay dynamics obtained at the ensemble and single tube levels. We find that localization of dopant sites. Relevant to their potential uses in imaging and as novel photon sources, we demonstrate blinking behaviors and discuss a range of response as...studies have furthermore elucidated the associated chemical and electronic structure. [4] We report here photoluminescence studies of dynamic behaviors of the being introduced by chemically stable oxygen [1,2] and aryl diazonium dopants [3] that increase photoluminescence quantum yields. Recent low-temperature optical study, we demonstrated conclusively a robust Luttinger liquid in metallic SWNTs at room temperature. [3] Shun-Wen Chang, Kevin Bergemann, Rohan Dhall, Jeramy Zimmerman, Stephen Forrest, Stephen Cronin, “Non-ideal Diode Behavior and Band Gap Quadratically with Field, while Measurements with Different Excitation Powers and Energies Show that Effects from Heating and Relaxation Pathways are Small. We attribute the shifts to the Stark effect, and characterize nanotubes with different chiralities. By taking into account exciton binding energies for air-suspended tubes, we find that theoretical predictions are in quantitative agreement.

8:00AM Y22.00001 Stark effect of excitons in individual air-suspended carbon nanotubes1. MASASHIRO YOSHIDA, YUSUKE KUMAMOTO, AKIHIRO ISHI, AKIO YOKOYAMA, YUICHIRO K. KATO, The University of Tokyo — We investigate electric-field induced redshifts of photoluminescence from individual single-walled carbon nanotubes (SWNTs) under an application of symmetric bias voltages on source and drain contacts. We find that redshifts scale quadratically with field, while measurements with different excitation powers and energies show that effects from heating and relaxation pathways are small. We attribute the shifts to the Stark effect, and characterize nanotubes with different chiralities. By taking into account exciton binding energies for air-suspended tubes, we find that theoretical predictions are in quantitative agreement.

1Work supported by KAKENHI, the NSF, Asahi Glass Foundation, and KDDI Foundation, as well as the Photon Frontier Network Program of MEXT, Japan. M.Y. is supported by ALPS, and A.I. is supported by MERIT and JSPS Research Fellowship.

8:12AM Y22.00002 ABSTRACT WITHDRAWN

8:24AM Y22.00003 In-situ TEM study of collapsing, reinflating and twisting of multi-walled carbon nanotubes. AIMING YAN, Dept. of Physics, Univ of California - Berkeley; Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, HAMID BARZEGAR, Dept of Physics, Univ of California, 90187 Umea, Sweden, CLAUDIA OJEDA-ARISTIZABAL, GABRIEL DUNN, Dept. of Physics, Univ of California - Berkeley; THOMAS WAGBERG, Dept of Physics, 90187 Umea, Sweden. — Since the first observation of collapsed carbon nanotubes (CCNTs) by Chopra et al., CCNTs have attracted a lot of attention due to their potentially modified electrical properties caused by structural changes compared to their tubular counterparts. We study the transition of multi-walled carbon nanotubes (MWCNTs) from tubular to collapsed form and the reverse process in-situ by Transmission Electron Microscope (TEM) and monitor the whole process by imaging and electron diffraction. We show that we are able to collapse the tubular CNT by extracting the inner core of the tube and reinflate the collapsed carbon nanotube by applying a voltage at the tip of the CNT. We also observe the twisting of the collapsed multi-walled CNT in-situ. The nano-scale manipulation of carbon nanotubes inside TEM enables us to tailor the transition between tubular and collapsed forms of a CNT.

8:36AM Y22.00004 Optoelectronic Properties and Electromechanical Resonance Behavior in Individual Suspended Carbon Nanotube pn-Junctions and Devices, STEPHEN CRONIN, University of Southern California — In carbon nanotubes pn-junctions, we observe Zener tunneling behavior and photocurrent generation in quasi-metallic nanotubes [1], which have smaller band gaps than most known bulk semiconductors. These carbon nanotube-based devices deviate from conventional bulk semiconductor device behavior due to their low-dimensional nature. We observe rectifying behavior based on Zener tunneling of ballistic carriers instead of ideal diode behavior, as limited by the diffusive transport of carriers. We observe substantial photocurrents at room temperature, suggesting that these quasi-metallic pn-devices may have a broader impact in optoelectronic devices. We also explore the role of weak clamping forces, typically assumed to be infinite, in the electromechanical resonance behavior of these suspended carbon nanotubes [2]. Due to these forces, we observe a hysteretic clamping and unclamping of the nanotube device that results in a discrete drop in the mechanical resonance frequency on the order of 5–20 MHz, when the temperature is cycled between 340 and 375 K. This instability in the resonant frequency results from the nanotube unpinning from the electrode/trench sidewall where it is bound weakly by van der Waals forces. Interestingly, this unpinning does not affect the Q-factor of the resonance, since the clamping is still governed by van der Waals forces above and below the unpinning. For a 1 µm device, the drop observed in resonance frequency corresponds to a change in nanotube length of approximately 50–65 nm. On the basis of these findings, we introduce a new model, which includes a finite tension around zero gate voltage due to van der Waals forces and shows better agreement with the experimental data than the perfect clamping model. From the gate dependence of the mechanical resonance frequency, we extract the van der Waals clamping force to be 1.8 pN. The mechanical resonance frequency exhibits a striking temperature dependence below 200 K attributed to a temperature-dependent slack arising from the competition between the van der Waals force and the thermal fluctuations in the suspended nanotube.


9:12AM Y22.00005 Near-field optical study of individual single-walled carbon nanotubes. ZHIWEN SHI, XIAOPING HONG, UC Berkeley, HANS BECHTEL, MICHAEL MARTIN, Lawrence Berkeley National Laboratory, YUEN-RON SHEN, FENG WANG, UC Berkeley — Quantum-confined electrons in one dimension (1D) behave as Luttinger liquid, a strongly correlated electronic matter distinctly different from Fermi liquid. Metallic single-walled carbon nanotubes (SWNTs), with their strong quantum confinement and structural simplicity, provide the ideal model system for Luttinger liquid. Direct experimental observation of Luttinger liquid in SWNTs, however, proves to be surprisingly challenging. Through near-field optical study, we demonstrated conclusively a robust Luttinger liquid in metallic SWNTs at room temperature.

9:36AM Y22.00007 Plasmon enhanced Raman scattering effect for an atom near a carbon nanotube. ALEX GULYUK, IGOR BONDAREV, North Carolina Central University — A quantum theory of the resonance Raman scattering is developed for a two-level dipole emitter, two-level system (TLS), coupled to a low-energy inter-band plasmon resonance of a carbon nanotube (CN). This resonance Raman scattering is a manifestation of the general Surface Enhanced Raman Scattering (SERS) effect received much of attention due to a very broad range of its applications in nanophotonics, biochemistry, and medicine. Here[1], the SERS effect comes about as a near-field effect in which strong local-field enhancement occurs due to the inter-band plasmon excitation when the TLS is located near the CN surface and its transition energy matches the plasmon resonance energy of the CN. Raman cross-section derived covers both weak and strong TLS-plasmon coupling, and shows a dramatic increase by a factor ~ 10^3 in the strong coupling regime. The effect may be used to detect individual atomic type objects trapped near CNs. More advanced applications, which require further theoretical development, may include highly efficient CN based SERS substrates for single molecule/atom/ion detection, precision spontaneous emission control, and manipulation. – [1] V.Bondarev, arXiv:1407.5142

9:48AM Y22.00008 Optical Field Enhancement by Semiconducting Graphene Nanoribbons. YOSHIYUKI MIYAMOTO, AIST, Japan, HONG ZHANG, Sichuan University, China — Graphene nano-ribbons are known to have energy gap depending on direction of ribbon edge and ribbon width having optical property different from that derived from Dirac cone of the graphene. When the edges are in armchair orientation, the ribbons are semiconducting with energy gaps at their Γ points. In this presentation, we report an enhancement of an optical electric field (E-field) by an armchair graphene nanoribbon by means of the first-principles simulation. The polarization of the E-field was set as parallel to the graphene sheet and perpendicular to ribbon axis. By performing the time-dependent density functional theory (TDDFT) simulation under dynamical E-field, an enhancement of E-field was seen with optical frequencies near the resonance of absorption peaks of the nano-ribbon. The enhancement was not persistent but showed an amplitude modulation with frequencies of few (tens) terahertz depending on E-field frequencies. In this presentation, we discuss mechanisms of field-enhancement and possible applications.

1This work was supported by a fund from the Science of Atomic Layers (SATL), MEXT

10:00AM Y22.00009 Novel quasi-1D Y-junction carbon with anisotropic conductance and changeable magnetization. BHALCHANDRA PUJARI, Centre for Modeling and Simulation, Savitribai Phule Pune University, Pune 411007 India, ANDREY TOKAREV, DST Hydrogen Infrastructure Center of Competence (HySA Infrastructure), Faculty of Engineering, North-West University, Potchefstroom, South Africa — We propose two conformations of a novel quasi-1D carbon allotrope designed by tailoring three graphene nanoribbons to form a Y-shaped junction. The armchair and zigzag conformations arise due to chirality of underlying ribbons. While armchair Y-junction carbon (YJC) is formed by three identical “arms” of the graphene nanoribbons the zigzag conformation has one distinguishable arm. The result in the later configuration is the broken symmetry of the structure, in which the arms are no longer separated by 120° each. Interestingly the broken structural symmetry of zigzag YJC is also associated with magnetic moment. It is shown that the magnetism is due to underlying nanoribbons and not symmetry breaking. Moreover the magnetism is also affected by the nature of edge passivation. Based on the analysis of density of states, we conjecture that the mixture of sp^2- and sp^3-bonded atoms results three conducting ribbons joined together by the insulating carbon chain. Thus making the structure an anisotropic conductor, with conductivity of armchair conformation being higher than that of zigzag. Armchair and zigzag conformations are energetically extremely stable with binding energy of 11.44 eV/atom and 8.39 eV/atom respectively.

10:12AM Y22.00010 Non-saturating Linear Magnetoresistance in 3-dimensional Carbon Nanostructure. LEI WANG, University of South Carolina, Columbia, MING YIN, FOUZI ARAMMASH, Benedict College, TIMIR DATTA, University of South Carolina, Columbia — Magneto-transport of carbon nanostructure with periodic spherical voids was investigated in magnetic field up to 9.4T in the temperatures range from 2K to 50K. With increase of magnetic field, transverse magnetoresistance crosses over from quadratic to a non-saturating linear dependence. Furthermore, longitudinal magnetoresistance which is negligible in most materials exhibits the same value as transverse magnetoresistance in our system. We demonstrate linear magnetoresistance (LMR) is proportional to the carrier mobility. Over the entire B-T phase region studied, MR data is observed to be a universal function of B/T. Orientation independent linear response is an attractive feature for applications.

10:24AM Y22.00011 Anomalous magnetization of a carbon nanotube as an excitonic insulator. MASSIMO RONTANI, CNR-NANO Research Center S3, Modena, Italy — We show theoretically that an undoped carbon nanotube might be an excitonic insulator—the long-sought phase of matter proposed by Keldysh, Kohn, and others fifty years ago. We predict that the condensation of triplet excitons, driven by intervalley exchange interaction, spontaneously occurs at equilibrium if the tube radius is sufficiently small. The signatures of exciton condensation are its sizable contributions to both the energy gap and the magnetic moment per electron. The increase of the gap might have already been measured, albeit with a different explanation [2]. The enhancement of the quasiparticle magnetic moment is a pair-breaking effect that counteracts the weak paramagnetism of the ground-state condensate of excitons. This property could rationalize the anomalous magnitude of magnetic moments recently observed in different devices close to charge neutrality. [1] M. Rontani, Phys. Rev. B 90, 195415 (2014). [2] V. V. Deshpande et al., Science 323, 106 (2009).

1I acknowledge support from EU-FP7 Marie Curie ITN INDEX and MIUR AbNano

10:36AM Y22.00012 Carbon nanotubes coupled to superconducting impedance matching circuits. SCHONENBERGER CHRISTIAN, MINKYUNG JUNG, VISHAL RANJAN, Department of Physics, Univ. of Basel, GABRIEL PUEBLA-HELMANN, Department of Physics, ETH-Zurich, THOMAS HASLER, ANDREAS NUNNENKAMP, Department of Physics, Univ. of Basel, MATTHIAS MUOTH, CHRISTOPHER HIEROLD, Micro- and Nanosystems, ETH-Zurich, ANDREAS WALLRAFF, Department of Physics, ETH-Zurich, RF-HYBRID-COLLABORATION COLLABORATION — Coupling carbon nanotube devices to microwave circuits offers a significant increase in bandwidth and signal-to-noise ratio. These facilitate fast non-invasive readouts important for quantum optics, shot noise and correlation measurements. Here, we successfully couple a carbon nanotube (CNT) double quantum dot to a GHz superconducting matching circuit using a mechanical transfer technique. The device shows a tunable bipolar double dot behavior, reaching the few-electron/hole regime. The resonance response reflected by the matching circuit is a sensitive probe of the charge state of the device, allowing a determination of the absolute charge number. The resonance response at the interdot charge transitions enables quantitative parameter extraction. Presented results open the path for novel studies of microwave photons interacting with electrons in carbon nanotubes.

1Research at Basel is supported by the NCCR-Nano, NCCR-QIST, ERC project QUEST, and FP7 project SE2ND.
10:48AM Y22.00013 Interplay of Magnetism of Superconductivity in Graphitic Nanostructures, YAO AN, ROBERT MEULENBERG, Department of Physics and Astronomy and Laboratory for Surface Science and Technology, University of Maine — The main foci in modern high temperature superconductivity (HTS) research are two-fold: (a) in conventional HTS finding new machinable materials necessary for any real world applications and (b) discovering new materials for that elusive room temperature superconductivity (RTS). It is quite evident that the potential applications for HTS or RTS are immense, and could show tremendous cost savings in various industries. To date, most reports of RTS have been eventually disproved; however, recent work has suggested that graphite flakes can exhibit RTS when treated with water. This extraordinary claim, if true, offers a wide range of stimulating physics to be studied in RTS; A main obstacle toward RTS in carbon based materials is ruling out whether one is truly observing superconductivity, or simply magnetism. In this talk, we will discuss effects of solution exfoliation of graphite powders. Not surprisingly, drastic changes to the graphite powder are observed. These changes, mainly in the form of graphene sheet exfoliation and defect formation, suggest a form of magnetism and not superconductivity in the treated powders via SQUID magnetometry measurements. A method for preparing graphitic monoliths that allow for transport measurements will be presented.

Friday, March 6, 2015 8:00AM - 10:24AM –

Session Y23 DCOMP: Focus Session: Petascale Science and Beyond: Applications and Opportunities in Materials Science and Chemistry III 202B - Thomas Schulthess, Swiss Federal Institute of Technology (ETH)

8:00AM Y23.00001 Aneesur Rahman Prize Talk: Working at the Speed of Light, JOHN JOANNOPOLOS, Massachusetts Institute of Technology — Photonic crystals are periodic dielectric structures possessing a photonic band gap that forbids propagation of a certain frequency range of light. This gap, and other curious properties of these systems, enable control of light with amazing facility and produce effects that are impossible to achieve with conventional optics. By combining analytical theory with state-of-the-art numerical calculations, examples of novel, and even anomalous, light behavior will be presented.

8:36AM Y23.00002 Scale-Bridging Modeling of Material Dynamics: Petascale Assessments of the Road to Exascale, TIMOTHY GERMANN, Los Alamos National Laboratory, EXMATEX TEAM — Within the multi-institutional, multi-disciplinary Exascale Co-design Center for Materials in Extreme Environments (ExMatEx), we are engaging domain (computational materials) scientists, applied mathematicians, computer scientists, and hardware architects, in order to establish the relationships between algorithms, software stacks, and architectures needed to enable exascale-ready materials science application codes within the next decade. We anticipate that we will be able to exploit hierarchical, heterogeneous architectures to achieve more realistic large-scale simulations with adaptive physics refinement, and are using tractable application scale-bridging proxy application testbeds to assess new approaches and requirements. Our focus has been on scale-bridging strategies that accumulate (or recompute) a distributed response database from fine-scale calculations, in a top-down rather than bottom-up multiscale approach. To evaluate and exercise the task-based programming models, databases, and runtime systems required to perform such many-task computation workflows, we are carrying out petascale demonstrations in 2015 which I will describe in this talk.

8:48AM Y23.00003 Large Scale Molecular Dynamics Simulation of Polymeric Materials, MONOJOY GOSWAMI, JAN-MICHAEL CARRILLO, RAJEEV KUMAR, BOBBY SUMPTER, Oak Ridge National Lab — In this talk, I will present a series of large-scale molecular simulations of polymer nanocomposites and block copolymers (BCP). We will discuss three different problems in this talk that requires large-scale computation: 1) hydrated RNA dynamics on a nanodiamond (ND) surface for drug-delivery applications, 2) poly(3-hexylthiophene) (P3HT) and PCBM nanocomposites for the application in organic photovoltaics (OPV) and (3) amphiphilic BCP self assembly in surfactant solution for membrane separation technology applications. We simulate problem (1) using fully atomistic NAMD simulation and discuss the puzzling discovery of faster RNA dynamics on ND surface. LAMMPS MD code is used to simulate problems (2) and (3). Here we explain the importance of nano-domains in P3HT:PCBM nanocomposites in designing OPV and the criterion for surfactant mediated self-assembly of amphiphilic BCP in solution.

9:00AM Y23.00004 Fast Analysis of Time-Resolved Scattering Data, ALEXANDER HEXEMER, DINESH KUMAR, SINGANALLUR VENKATAKRISHNAN, ABHINAV SARJE, SIMON PATTON, SHERRY LI, JACK DESLIPPE, CRAIG TULL, Lawrence Berkeley Natl Lab, ELI DART, ESNET, FENG LIU, THOMAS RUSSELL, Amherst UMass, ENRIQUE GOMEZ, The Pennsylvania State University, CHENHUI ZHU, ERIC SCHAIBLE, POLITE STEWART, Lawrence Berkeley Natl Lab, CAMERA TEAM, ESNET TEAM, SPOT SUITE TEAM, UMASS COLLABORATION, PENNSTATE COLLABORATION — Organic Photovoltaics hold promise to reduce costs and increase efficiency. Most efforts have focused on spin-coating to fabricate high performance devices, a process that is not amenable to large scale fabrication. This mismatch in device fabrication processes makes it difficult to translate quantitative results obtained from laboratory scale devices to commercially prepared large area devices. Using a mini-slot die coater, designed and build in house, we address this issue, where the commercial process is translated to the laboratory setting. Grazing Incidence Small Angle X-ray Scattering was used to probe the change in morphology during the printing process. HIPGISAXS was used to fit the data in real-time by utilizing different ASCR facilities. SPOT orchestrated the workflow for the data: the transfer from the beamline to NERSC and subsequently to the TITAN supercomputer for fitting and back to NERSC.

9:12AM Y23.00005 Real-time calculations of dynamical effects in x-ray spectra, J.J. REHR, J.J. KAS, A.J. LEE, Univ of Washington — An understanding of dynamical effects and inelastic losses in x-ray spectra due to the sudden creation of a core-hole and photonelectron has long been of interest. Here we present a real-time approach for calculations of core level x-ray absorption and x-ray photoemission spectra that account for the dynamic response in terms of a spectral function that includes intrinsic, extrinsic and interference terms. Our approach is based on a factorization in terms of the core-hole Green’s function and a time-correlation function that avoids the need for ultra-short time-steps. The approach extends a time-correlation function approach for XAS, factorization in terms of the core-hole Green’s function and a time-correlation function that avoids the need for ultra-short time-steps. The approach extends an adaptation of the Crank-Nicholson time-evolution algorithm with PAW transition matrix elements. Illustrative examples are presented for a number of systems.

1Supported by DOE BES DE-FG03-97ER45623.
9:24AM Y23.00006 Atomistic Materials Modeling on Petascale Platforms Using SNAP\(^1\). AIDAN THOMPSON, LAURA SWILER, CHRISTIAN TROTT, STEPHEN FOILES. Sandia National Laboratories, GARRITT TUCKER, Drexel University — The growing availability of capacity computing for atomistic materials modeling has encouraged the use of high-accuracy computationally intensive interatomic potentials, such as SNAP. These potentials also happen to scale well on petascale computing platforms. SNAP has a very general form and uses machine-learning techniques to reproduce the energies, forces, and stress tensors of a large set of small configurations of atoms, which are obtained using high-accuracy quantum electronic structure (QM) calculations. The local environment of each atom is characterized by a set of bispectrum components of the local neighbor density projected onto a basis of hyperspherical harmonics in four dimensions. The computational cost per atom is much greater than that of similar potentials such as Lennard-Jones or EAM, while the communication cost remains modest. We discuss a variety of strategies for implementing SNAP in the LAMMPS molecular dynamics package. We present several results obtained running SNAP on three different classes of machine: a conventional Intel Xeon CPU cluster; the Titan GPU-based system; and the combined Sequoia and Vulcan BlueGene/Q.

\(^1\)Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corp., for the U.S. Dept. of Energy’s National Nuclear Security Admin. under contract DE-AC04-94AL85000

9:36AM Y23.00007 Molecular dynamics simulation: at a crossroad between molecular biophysics and petascale computing\(^1\). XIAOLIN CHENG, Oak Ridge National Laboratory — High-performance computing (HPC) has become crucial for most advances made in chemistry and biology today. In particular, biophysical simulation is capable of helping generate critical new insights and drive the direction of experimentation. In this talk, I will discuss our work towards addressing some fundamental membrane biophysical questions using HPC capabilities at Oak Ridge National Laboratory. I will first provide a synopsis of our current progress in developing molecular dynamics (MD) techniques that make efficient use of massively parallel supercomputers. I will then discuss a few examples of large-scale MD simulations of biomembrane vesicles, an effort aimed at shedding light on the lateral organization and cross-layer coupling in biologically-relevant membranes. In conclusion, I will discuss a few scientific and technical challenges faced by MD simulation at the exascale.

\(^1\)This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No.DE-AC05-00OR22725.

9:48AM Y23.00008 Large-scale atomistic simulations of surface nanostructuring by short pulse laser irradiation\(^1\). CHENGPING WU, MAXIM SHUGAEV, LEONID ZHIGILEI, University of Virginia — The availability of petascale supercomputing resources has expanded the range of research questions that can be addressed in the simulations and, in particular, enabled large-scale atomistic simulations of short pulse laser nanostructuring of metal surfaces. A series of simulations performed for systems consisting of 10\(^9\) ~ 10\(^9\) atoms is used in this study to investigate the mechanisms responsible for the generation of complex multiscale surface morphology and microstructure. At low laser fluence, just below the spallation threshold, a concurrent occurrence of fast laser melting, dynamic relaxation of laser-induced stresses, and rapid cooling and resolidification of the transiently melted surface region is found to produce a sub-surface porous region covered by a nanocrystalline layer. At higher laser fluences, in the spallation and phase explosion regimes, the material disintegration and ejection driven by the relaxation of laser-induced stresses and/or explosive release of vapor leads to the formation of complex surface morphology that can only be studied in billion-atom simulations. The first result from a billion atom simulation of surface nanostructuring performed on Titan will be discussed in the presentation.

\(^1\)Financial support is provided by NSF (DMR-0907247 and CMMI-1301298) and AFOSR (FA9550-10-1-0541). Computational support is provided by the OLCF (MAT048) and NSF XSEDE (TG-DMR110090).

10:00AM Y23.00009 Retention of hydrogen and helium in monocrystal of tungsten\(^1\). JACK WELLS, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, PREDRAG KRSTIC, State University of New York, Stony Brook, NY 11794 — Beginning with either perfect or damaged mono-crystal of tungsten, we bombard the surface with a mix of isotopes of H and He at the impact energy range from 1-100 eV in order to predict the retention rate of the impinging atoms as well as their distribution inside the material, in particular inside the vacancies. Our calculation is based on molecular dynamics simulation using high-performance computing and bond-order potentials. The goal is to distinguish between the following alternative outcomes: (1) the retention rate is proportional to the number of vacancies — consistent with recent experiments on the retention of H in damaged W, (2) vacancies will be filled by aggregates of H or He, leading to unstable surfaces, e.g., bubbling and blistering of the surface, and (3) some fraction of hydrogen and helium will fill the interatomic space in the W crystal lattice, creating a “protective layer” or bubbles and blisters close to the surface, even in absence of significant tungsten lattice defects, and (4) the impact direction and the crystal surface cut influence significantly ratio of effects 1-3.

\(^1\)Used resources of the Oak Ridge Leadership Computing Facility, which is supported by DOE Office of Science.

10:12AM Y23.00010 Teraflops and beyond: GPU-based MD exploration of emergent phenomena\(^1\). DENNIS RAPAPORT, Bar-Ilan University — Molecular dynamics (MD) simulation of emergent phenomena can be computationally demanding because of the broad range of length and time scales that must be covered, ranging from the individual particles out to where the collective behavior is expressed; the fact that simulations of this type are often subject to unpredictable outcomes is a further complication. Examples of MD studies of emergent behavior include discrete-particle modeling of hydrodynamic instabilities (e.g., thermal convection cells), complex segregation processes in granular systems modeled with inelastic particles (e.g., in a rotating drum), and supramolecular self-assembly (e.g., the growth of icoshedral shells corresponding to viral capsids). The comparatively large and long simulations required for these problems benefit substantially from massively parallel GPU-based implementation, with even a single GPU typically providing an order of magnitude speedup over a conventional CPU. A sampling of newly obtained exploratory results for these and similar problems [arXiv:1409.5958] will be described, along with the methodology; the results offer a tantalizing hint of the kinds of phenomena that can be explored, and what might be achieved given the appropriate resources.

Friday, March 6, 2015 8:00AM - 11:00AM – Session Y25 DCMP: Superconductivity in Cuprates (mostly): Theory II 203B - Wei Ku, Brookhaven National Laboratory
order due to hole doping, through exact finite temperature phase diagram of the model. [1] M. H. Fischer, S. Wu, M. Lawler, A. Paramekanti, and E.-A. Kim, temperature properties as well as unbiased determination of ground state spin and charge configuration. As a function of system parameters, we obtain a rich understand the phase diagram of broken symmetry states using a simple model that captures the essence of hole doped cuprates [1]. The model consists of phase coherence around 25%, giving rise to a dome shape of superconducting transition temperature in excellent agreement with experimental observations.

1 This research was carried out with resources of the Oak Ridge Leadership Computing Facility (OLCF), the Swiss National Supercomputing Center (CSCS), and the Center for Nanophase Materials Sciences (CNM).
9:24AM Y25.00008 Enchancement of superconductivity in a three-dimensional hotspot model of competing orders in the cuprates. — ZACHARY RAINES, VALENTIN STANEV, VICTOR GALITSKI, Univ of Maryland-College Park — Recent experiments in the cuprates have shown evidence of a transient superconducting state upon optical excitation polarized along the c-axis. Motivated by these experiments we considered a hotspot model of competing superconductivity and bond density order in a system of stacked planes. We generally find an enhancement of superconductivity in the coexistent phase as a function of c-axis coupling strength. Furthermore, we propose a simple Floquet system which takes advantage of this enhancement.

9:36AM Y25.00009 Collective modes in the hot spot model of cuprates1. — VALENTIN STANEV, ZACH RAINES, VICTOR GALITSKI, Univ of Maryland-College Park — We study the collective modes of the possible order parameters of cuprate high-temperature superconductors. Observing and analyzing these modes provide insights into the nature of the ordered state. Using the hot spot model of cuprates, we explore the amplitude oscillations of both charge density wave (CDW) and superconducting states. Especially interesting is the region, in which CDW and superconductivity coexist, in which the two amplitude oscillations become mixed in a single mode with energy inside the single-particle gap. We compare these results with the recent data extracted from reflectivity measurements.

1Work supported by DOE-BES (DESC0001911) and Simons Foundation.

9:48AM Y25.00010 Can short-ranged orders enhance superconductivity of cuprates?1. — KYUNGMIN LEE, EUN-AH KIM, Cornell University — Recent advances in experiments established short-ranged orders associated with tendencies for spatial symmetry breaking as universal phenomena of undoped cuprates. This brings the question of the relationship between these short-ranged orders and superconductivity to the forefront of the study of high Tc superconductivity. Here we study this issue paying special attention to the role form-factors play. Using both non-self-consistent and self-consistent Bogoliubov-de Gennes equation with real-space realization of short-range order we investigate how the short-ranged order affects the electronic structure as well as superconducting tendencies. Typically an inhomogeneous potential due to short-ranged ordering patterns will act as a scatterer that is detrimental to unconventional superconductor which is not protected through Anderson's theorem. However we find that that form factor of the short-ranged ordering form can make consequential differences in the way short-range order interact with superconductivity, with the possibility of enhancing superconductivity.

1This work has been supported by DOE with grant number DE-SC0010313.

10:00AM Y25.00011 ABSTRACT WITHDRAWN —

10:12AM Y25.00012 Amplitude mode oscillations in pump-probe photoemission spectra of electron-phonon mediated superconductors1. — ALEXANDER KEMPER, Lawrence Berkeley National Laboratory, MICHAEL SENTEUF, Universitt Bonn, BRIAN MORITZ, Stanford Institute for Materials & Energy Sciences, JAMES FREERICKS, Georgetown University, THOMAS DEVEREAU, Stanford Institute for Materials & Energy Sciences — The amplitude, or Higgs mode is deeply intertwined with the historical development of the BCS theory of superconductivity. Although the presence of the Higgs mode is fundamental to superconductivity, it remained elusive for many decades, and its presence and observability is still under debate in many contexts. We present results for time-dependent photoemission spectra to directly probe the dynamics of the superconducting gap edge where the fingerprint of superconductivity is strongest. The pumping of a superconductor is simulated by solving the two-time Gor’kov equations of motion for the Migdal-Eliashberg model, which is a minimal gauge-invariant model for superconductivity with a pairing boson and dissipation. The Higgs mode can be directly detected without the requirement of any additional symmetry breaking and is clearly visible as oscillations of the gap edge spectra at twice the gap frequency, a hallmark of amplitude modes.

1A.F.K. was supported by the Laboratory Directed Research and Development Program of Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. DE-AC02-05CH11231

10:24AM Y25.00013 Angle-dependent magnetoresistance and the presence of fluctuating hot spots on the Fermi surface of Tl2201. — SYLVIA LEWIN, JAMES ANALYTIS, University of California, Berkeley — The normal-state transport properties of cuprate high-temperature superconductors are not well understood. While the Hall angle in such materials is typically proportional to T2, the in-plane resistivity has a more complicated temperature dependence. This has led to many theories of the scattering processes in such materials, including several that posit the existence of two or more independent scattering lifetimes. Here, we propose a model that may explain the cuprates’ complicated normal-state behavior without the need to invoke multiple scattering channels: fluctuating hot spots on the Fermi surface, a result of transient antiferromagnetic order. We will demonstrate that this model can accurately simulate angle-dependent magnetoresistance data from Tl2Ba2CuO6+δ, and discuss what additional calculations and experiments will be performed in order to further test this model.

1This research used resources of the National Energy Research Scientific Computing Center and was supported by a fellowship from the NSF Graduate Research Fellowship Program.

10:36AM Y25.00014 Polar Kerr effect from chiral-nematic charge order. — YUXUAN WANG, Univ of Wisconsin, Madison, ANDREY CHUBUKOV, University of Minnesota, RAHUL NANDKISHORE, Princeton University — We analyze the polar Kerr effect in an itinerant electron system on a square lattice in the presence of a composite charge order proposed for the pseudogap state in underdoped cuprates. This composite charge order preserves translational symmetries, and is “chiral-nematic” in the sense that it breaks time-reversal symmetry, mirror symmetries in x and y directions, and C4 lattice rotation symmetry. The Kerr angle \( \theta_K \) in C4-symmetric system is proportional to the antisymmetric component of the anomalous Hall conductivity \( \sigma_{xy} - \sigma_{yx} \). We show that this result holds when \( C_4 \) symmetry is broken. We show that chiral-nematic charge order satisfies all symmetry requirements by a polar Kerr effect. We further show that to get a non-zero \( \theta_K \) in a one-band spin-fluctuation scenario, in the absence of disorder, one has to extend the spin-mediated interaction to momenta away from (\( \pi, \pi \)) and has to include particle-hole asymmetry. Alternatively, in the presence of disorder one can get a non-zero \( \theta_K \) from impurity scattering; either due to skew scattering (with non-Gaussian disorder) or due to particle-hole asymmetry in case of Gaussian disorder. We finally discuss the effect of an external magnetic field on the Kerr signal.
10:48AM Y25.00015 Finite T spectral function of a single carrier injected into an Ising chain: a comparison of 3 different models\(^1\), MIRKO MOELLER, MONA BERCIU, Univ British Columbia — When studying the properties of complex, magnetic materials it is often necessary to work with effective Hamiltonians. In many cases the effective Hamiltonian is obtained by mapping the full, multiband Hamiltonian onto a simpler, single band model. A prominent example is the use of Zhang-Rice singlets to map the multiband Emery model for cuprates onto the single band t–J-model. Such mappings are usually done at zero temperature (T) and it is implicitly assumed that they are justified at finite T, as well. We present results on 3 different models of a single charge carrier (electron or hole) injected into a ferromagnetic Ising chain. Model I is a two band, two sublattice model, Model II is a two band, single sublattice model, and Model III is a single band model, the so called t–J.,-model. Due to the absence of spin-flip terms, a numerically exact solution of all 3 Models is possible, even at finite T. A zero T mapping between all 3 models results in the same low energy physics. However, this is no longer true at finite T. Here the low energy behavior of Model III is significantly different from that of Models I and II. The reasons for this discrepancy and its implications for more realistic models (higher dimension, inclusion of spin-flip terms) are discussed.

\(^1\)This work was supported by NSERC, QMI and the UBC 4YF (M.M.).

Friday, March 6, 2015 8:00AM - 11:00AM — Session Y26 DCP: Surfaces, Interfaces, Colloids and Catalysis I

8:00AM Y26.00001 CO Adsorption on Pd(111) at 0.5ML: a First Principles Study\(^1\), ZAHRA HOOSHAMOND GHAREHBAGH, DUY LE, TALAT S. RAHMAN, University of Central Florida, Department of Physics, Orlando FL 32816-2385, USA — While the adlayer structures formed by CO molecules on Pd(111) are well-understood both experimentally and theoretically, for low and high coverages, it is still a matter of discussion for medium coverage (0.5ML). At this medium coverage, it is well-known that the c(4 × 2) phase is formed but the adsorption sites of CO molecules have been reported differently by various studies: at the bridge sites, at the hollow sites, or at both bridge and hollow sites. Using density functional theory calculations we studied the overlayer structure of CO at 0.5ML on Pd(111) with all possible highly symmetric adsorption sites leading to c(4 × 2) structures. We will show that, on the same surface, CO molecules adsorb either only on bridge or hollow sites and that there is no overlayer structure in which CO binds at both bridge and hollow sites. By means of \textit{ab initio} thermodynamics simulation, we will also report the conditions (temperature, pressure) in which each overlayer structure exists.

\(^1\)Work support in part by NSF Grant CHE-1310327

8:12AM Y26.00002 Theoretical investigation of oxygen adsorption on Pu-Ga alloy (111) surface\(^1\), SARAH C. HERNANDEZ, University of Texas at Arlington, THOMAS J. VENHAUS, Los Alamos National Laboratory, MUHAMMAD N. HUDA, University of Texas at Arlington — All electron density functional theory was implemented to study the adsorption of atomic oxygen on a 3.125 at. % Ga stabilized δ-Pu (111) surface. A 4-layer periodic slab, with 8 atoms per layer, was used to model the surface, and the location of the Ga within the surface was considered. High symmetry on-surface and interstitials adsorption sites were explored, which also included the adatom placed in different local environments (i.e. oxygen coordinated with/without a Ga atom). Full relaxation of the atomic positions of the Pu-Ga slab and O atom were employed. The inclusion of spin-orbit-coupling was preferred for the lowest energetic structure. The goal of these calculations was to test the probe the effects that Ga may have within the surface when O is adsorb. We found that oxygen binds strongly at an on-surface site with chemisorption energy of -5.06 eV and prefers to be three-fold coordinated either on bridge or hollow sites. It is well-known that the c(4 × 2) phase is formed but the adsorption sites of CO molecules have been reported differently by various studies: at the bridge sites, at the hollow sites, or at both bridge and hollow sites. Using density functional theory calculations we studied the overlayer structure of CO at 0.5ML on Pd(111) with all possible highly symmetric adsorption sites leading to c(4 × 2) structures. We will show that, on the same surface, CO molecules adsorb either only on bridge or hollow sites and that there is no overlayer structure in which CO binds at both bridge and hollow sites. By means of \textit{ab initio} thermodynamics simulation, we will also report the conditions (temperature, pressure) in which each overlayer structure exists.

\(^1\)We gratefully acknowledge support by the US Department of Energy through the Los Alamos National Laboratory LDRD Program.

8:24AM Y26.00003 Stabilization of CH\(_2\) on Ru(0001) by hydrogen co-adsorption, SERGEY V. LEVCHENKO, XUNHUA ZHAO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, FRITZ-HABER-INSTITUT DER MPG, BERLIN TEAM — Based on indirect experimental evidence, CH\(_2\) was proposed as a building block for hydrocarbon chain growth on the Ru(0001) surface during the Fischer-Tropsch process. However, previous calculations agreed that CH\(_2\) is not stable on Ru(0001) at the reaction conditions, and should quickly convert into CH. Employing density-functional theory, we show that this disagreement can be reconciled if coadsorbed hydrogen is present on the surface. The atomic structure of various CH\(_2\)+H\(_2\) phases is obtained with genetic algorithm. CH\(_2\) dissociation barriers are calculated using the string method. We further demonstrate, by calculating the surface phase diagram for one-carbon species on Ru(0001) as a function of H\(_2\) chemical potential, that the stabilization of CH\(_2\) by co-adsorbed hydrogen requires non-equilibrium conditions. The calculated barrier for the CH\(_2\) dissociation in the presence of hydrogen is significantly increased, and is close to the one recently measured by vibrational sum-frequency generation spectroscopy [1]. Our results also explain why CH\(_2\) was not observed when C or CH are hydrogenated on Ru(0001), although it is observed after methane decomposition.


8:36AM Y26.00004 ABSTRACT WITHDRAWN

8:48AM Y26.00005 ABSTRACT WITHDRAWN

9:00AM Y26.00006 Structure and Electron Localization of Reduced Ceria Surfaces, RENAT SABIRIANOV, Univ of Nebraska - Omaha, KHALDOUN TARAWNEH, Princess Sumaya University for Technology, NABIL AL-AQTASH, NAN SHAO, WAI-NING MAI, Univ of Nebraska - Omaha, CHIN LI CHEUNG, Univ of Nebraska Lincoln — Ceria (CeO\(_2\)) is an extensively used industrial catalyst. However, the mechanism for its catalytic activity, especially in aqueous media, is not yet well-understood. While high density of oxygen vacancy defects (OVDs) are often cited as the major factor in enhancing the activity of nanostructured ceria, the synergistic influences between the surface defects, subsurface oxygen vacancies on the (100), (111) and (110) surfaces of ceria. The removal of a neutral surface oxygen atom leaves back excess electrons that are shown to localize on cerium ions neighboring the defect. The preferential defect formation and the different chemical reactivity of the (100), (111) and (110) surfaces are discussed in terms of defect formation energies. DFT-U calculations predict the preferential subsurface formation of OVDs for (111) surface by energy difference of 0.10 eV, in agreement with previous GGA+U results, while in case of (110) surface calculations predict the surface vacancy to be more stable by energy difference of 1.03 eV. The calculated atomic and electronic structures of ceria the reduced surfaces are shown to agree with spectroscopic and STM measurements.
Monolayer (Hydr)oxide-Metal Interfaces, ZHENHUA ZENG, JOSEPH KUBAL, JEFF GREELEY, Purdue University — Ultrathin specific example, we show how simultaneous NO$_x$ is general and can, in principle, be applied to many reactions, and for each case the choice of the transition oxide monolayer can be optimized. Here, as a ferroelectric substrate. The ferroelectric polarization switches the surface chemistry between strongly adsorptive and strongly desorptive regimes, circumventing sorbent loading dependence of the equilibration time is non-monotonic. This unusual characteristic appears to be related to the structural transition present in values. We have studied the adsorption kinetics for this system, i.e., how the equilibration times for adsorption change as a function of sorbent loading. The transition manifests itself as an additional (higher pressure) substep in the adsorption isotherm data. Xe isotherms measured above 145 K do not show the additional isotherm feature, while those measured below do. The extra adsorption step is a consequence of the “gate opening” transition that occurs due to the re-orientation of the organic linkers in the ZIF-8. This re-orientation increases the size of the apertures in the ZIF-8 structure, and consequently allows more Xe atoms to adsorb in the material, thus producing the additional adsorption step. The adsorption isotherm data were used to determine the effective surface area of ZIF-8 through application of the “point B” method. The isosteric heat of adsorption of Xe on ZIF-8 was determined from the isotherm data. We will also report on the kinetics of adsorption of Xe on ZIF-8.

Study of Xenon Adsorption on Zeolitic Imidazolate Framework – 8 (ZIF-8), DINUKA GALLABA, BRICE RUSSELL, ALDO MIGONE, Department of Physics, Southern Illinois University, Carbondale IL 62901 — We have investigated Xe adsorption on ZIF-8 for temperatures in the range between 138 and 150 K. ZIF-8 is known to undergo a transition (“gate-opening”) transition as a function of increasing pressure (or loading) for a number of adsorbates (N$_2$, Ar, CO, O$_2$). For isotherms measured at sufficiently low temperatures, the gate-opening transition manifests itself as an additional (higher pressure) substep in the adsorption isotherm data. Xe isotherms measured above 145 K do not show the additional isotherm feature, while those measured below do. The extra adsorption step is a consequence of the “gate opening” transition that occurs due to the re-orientation of the organic linkers in the ZIF-8. This re-orientation increases the size of the apertures in the ZIF-8 structure, and consequently allows more Xe atoms to adsorb in the material, thus producing the additional adsorption step. The adsorption isotherm data were used to determine the effective surface area of ZIF-8 through application of the “point B” method. The isosteric heat of adsorption of Xe on ZIF-8 was determined from the isotherm data. We will also report on the kinetics of adsorption of Xe on ZIF-8.

Ferroelectric based catalysis: Switchable surface chemistry$^1$, ARVIN KAKEHANI, SOHRAB ISMAIL-BEIJI, Yale University — We describe a new class of catalysts that uses an epitaxial monolayer of a transition metal oxide on a ferroelectric substrate. The ferroelectric polarization switches the surface chemistry between strongly adsorptive and strongly desorptive regimes, circumventing difficulties encountered on non-switchable catalytic surfaces where the Sabatier principle dictates a moderate surface-molecule interaction strength. This method is general and can, in principle, be applied to many reactions, and for each case the choice of the transition oxide monolayer can be optimized. Here, as a specific example, we show how simultaneous NO$_2$ direct decomposition (into N$_2$ and O$_2$) and CO oxidation can be achieved efficiently on Cr$_2$O$_3$ terminated PbTiO$_3$, while circumventing oxygen (and sulfur) poisoning issues. One should note that NO$_2$ direct decomposition has been an open challenge in automotive emission control technology. Our method could expand the range of catalytically active elements to those which are not conventionally considered for catalysis and which are more economical, e.g., Cr (for NO$_2$ direct decomposition and CO oxidation) instead of canonical precious metal catalysts.

Acceleration of non-PGM Electrocatalyst Design For Fuel Cells Through Site Specific XPS Predictions from First-principles Simulations, BORIS KIEFER, New Mexico State University, SADIA KABIR, KATERYNA ARTYUSHKOVA, PLAMEN ATANASSOV, University of New Mexico — One of the most pressing problems in the 21st century is the provision of environmentally consistent energy technologies especially for space limited non-stationary applications. Fuel Cells are promising candidates for addressing and mastering this challenge. Alternative materials to platinum catalysts which continue to attract significant attention are non-PGM FeN$_x$/C based materials. The understanding of the geometry and chemistry of catalytically active defect moieties is a prerequisite for the rational improvement and design of non-PGM electrocatalysts. XPS, a widely used surface analytical technique, generally shows broad N1s peaks with abundance weighted contributions from every defect motif. Due to the lack of appropriate reference materials it is currently impossible to de-convolute the N1s peak into defect specific contributions. In order to remove this limitation we have performed density-functional-theory (DFT) based calculations for a variety of in-plane FeN$_x$ ($x$=2-4) defects. Using DFT we predict, for the first time, defect chemistry and geometry induced N1s binding energy shifts in these materials. In combination with our XPS experiments and catalyst performance we find that higher FeN$_x$ defect abundance correlates with improved catalyst performance.

Electrolytes near structured dielectric interfaces, HUAXIN WU, YUEFEI JING, Northwestern University, FRANCISCO SOLIS, Arizona State University, MONICA OLVERA DE LA CRUZ, ERIK LUIJTEN, Northwestern University — The ion distribution in an electrolyte near a dielectric interface has important consequences for numerous applications. To date, most studies have focused on planar interfaces, where, e.g., simulations can take advantage of the image-charge method. However, for surfaces that display structure on the nanoscale, dielectric effects may be significantly different. Here, we investigate such interfaces via a combination of computer simulations and Poisson–Boltzmann theory. We demonstrate how, even for systems with piecewise uniform dielectric constant, surface structure affects the induced polarization charge as well as the ion distribution near the interface, in particular for asymmetric salts. We explore the role of ion concentration, dielectric mismatch and characteristic length scale of the surface structure.
10:36AM Y26.00014 Charge dependent condensation of macro-ions at air-water interfaces1. MRINAL BERA, MARK ANTONIO, Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL-60439, USA — Ordering of ions at and near air-water interfaces is a century old problem for researchers and has implications on a host of physical, chemical and biological processes. The dynamic nature of water surface and the surface fluctuations created by thermally excited capillary waves have always limited measurement of near surface ionic-distributions. We demonstrate that this limitation can be overcome by using macro-ions of sizes larger than the capillary wave roughness \( \sim 3\AA \). Our attempts to measure distributions of inorganic macro-ions in the form of Keggin heteropolyanions (HPAs) of sizes \(-10\AA\) have unraveled novel charge-dependent condensation of macro-ions beneath air-water interfaces. Our results demonstrate that HPAs with \(-3\) charges condense readily beneath air-water interfaces. This is in contrast to the absence of surface preference for HPAs with \(-4\) charges. The similarity of HPA-HPA separations near air-water interfaces and in bulk crystal structures suggests the presence of the planar Zundel ions (\( \text{H}_3\text{O}^+ \)), which interact with HPAs and the water surface to facilitate the charge dependent condensation beneath the air-water interfaces.

1This work and the use of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility at Argonne National Laboratory, is based upon work supported by the U.S. DOE, Office of Science, Office of Basic Energy Science, Divisio

10:48AM Y26.00015 Water-A New Player of the Solid Surface, YI GAO, YADONG LI, BEIEN ZHU, Shanghai Institute of Applied Physics (SINAP) — It is well-known that water configuration and behaviors are highly affected by the solid surface. On the other hand, water is generally considered to have negligible effects on the solid surface. But it might not be the case. Here, we theoretically present two examples to show water could significantly affect the surface. The first is the migration of the subsurface vacancies and the change of the surface elements population. These observations might give us a new perspective to understand the properties of liquid/solid interfaces.

Friday, March 6, 2015 8:00AM - 9:48AM — Session Y27 DCMP: Superconductivity and Spin Orbit Coupling 204B - Ke Chen, Temple University

8:00AM Y27.00001 Fraunhofer pattern arising from an edge-stepped topological surface Josephson current distribution, JAE HYEONG LEE, GIL-HO LEE1, JANGHEE LEE, JOONBUM PARK, SEUNG-GEOL NAM2, YUN-SOK SHIN3, JUN SUNG KIM, HU-JONG LEE, Pohang Univ of Sci & Tech — We report a surface-dominant Josephson effect in superconductor-topological insulator-superconductor (S–TI–S) devices, where a Bi$_2$Se$_3$ topologically trivial lead, like the fractional (4, PAVEL IOSELEVICH, Max Planck Institute for Solid State Research, MIKHAIL FEIGELMAN, Landau Institute for Theoretical Physics — Topological insulators’ edge-stepped nonuniform supercurrent distribution arising from the top and rough side surfaces of the BSTS flake. A Fraunhofer-like pattern was also observed for the local biasing. For the local biasing, the Fraunhofer signal was highly robust to the magnetic field up to the critical field of the Al electrodes, corresponding to the electrodes. We observed a Fraunhofer critical current modulation in a perpendicular magnetic field in an Al–TI–Al junction for both local and nonlocal current biasing. The Josephson effect in this case has an asymmetric dependence on the order parameters involved, and the critical current is suppressed very strongly in a typical situation, so that the product $I_c/R \ll \Delta$ even in a short contact.

8:12AM Y27.00002 Josephson junctions between topological and conventional superconductors, PAVEL IOSELEVICH, Max Planck Institute for Solid State Research, MIKHAIL FEIGELMAN, Landau Institute for Theoretical Physics — Topological superconductors host protected gapless modes at their boundaries. This leads to various robust phenomena when a topological superconductor is contacted to a topologically trivial lead, like the fractional (4π-periodic) Josephson effect or the zero-bias conductance peak in a tunneling NS-junction. Here we discuss phenomena arising in a Josephson contact between a topological and a trivial superconductor. The Josephson effect in this case has an asymmetric dependence on the order parameters involved, and the critical current is suppressed very strongly in a typical situation, so that the product $I_c/R \ll \Delta$ even in a short contact.

8:24AM Y27.00003 Microwave spectroscopy of Majorana bound states in S/TI/S junctions, JUKKA VAYRYNEN, Department of Physics, Yale University, GIANLUCA RASTELLI, WOLFGANG BELZIG, Fachbereich Physik, Universität Konstanz, LEONID GLAZMAN, Department of Physics, Yale University — We study the effects of microwave irradiation in a phase-biased topological Josephson junction, consisting of two s-wave superconductors linked by a quantum-spin-Hall insulator edge. A long topological junction supports multiple Andreev bound states, one of which (Majorana mode) has zero energy at phase difference $\phi = \pi$. We consider weak time-periodic modulation of the phase difference to study transitions between the discrete sub-gap levels of the junction. In a generic disordered junction all the degeneracies of single-particle levels are lifted but the zero-energy state remains and leads to a ground state degeneracy at $\phi = \pi$. Upon sweeping $\phi$ across the ground state degeneracy point, we show that the lowest excitation energy of the junction displays a prominent kink which can be observed in the absorption spectrum. To study this feature, we calculate the absorption power as a function of frequency, phase difference, and at finite temperature.

8:36AM Y27.00004 Zero-bias peak in InSb nanowires, PENG YU, JUN CHEN, School of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA, 15260, USA, MOIRA HOCEVAR, Institut Néel CNRS, Grenoble, France, SEBASTIEN PLISSARD, CNRS, LAAS, Toulouse, France, DIANA CAR, ERIK BAKKERS, Department of Applied Physics, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands, SERGEY FROLOV, Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA, 15260, USA — Zero-bias conductance peaks(ZBP) in InSb nanowires has been reported as a strong signature of Majorana bound states in semiconductors. We made similar superconductor-InSb nanowire-normal contact hybrid devices with NbTiN on bottom gates and found some features that may correspond to Majorana bound states. By setting a barrier and tuning gates under the nanowire that are in proximity of superconductors, ZBPs appear at finite magnetic field and usually persist for several hundred miliTesla. In different devices, ZBPs appear at different magnetic field, which may result from different chemical potentials. To achieve a so-called hard induced gap and cleaner devices, we are trying various contact materials and etching methods.

8:48AM Y27.00005 Anomalous Josephson Effect in Junctions with Rashba Spin-Orbit Coupling, KONSTANTIN NESTEROV, MANUEL HOUZET, JULIA MEYER, Univ. Grenoble Alpes, INAC-SPSMS, F-38000 Grenoble, France and CEA, INAC-SPSMS, F-38000 Grenoble, France — We study two-dimensional double-barrier SINIS Josephson junctions in which the inversion symmetry in the normal part is broken by Rashba spin-orbit coupling. In the presence of a suitably oriented Zeeman field in the normal part, the system displays the anomalous Josephson effect: the current is nonzero even at zero phase difference between two superconductors. We investigate this effect by means of the Ginzburg-Landau formalism and microscopic Green’s functions approach in the clean limit.

3This work was supported in part by the grants No. ANR-12-BS04-0016-03 and an EU-FP7 Marie Curie IRG.

9:00AM Y27.00006 Superconducting contacts to Ge/Si core/shell nanowires, ZHAOEN SU, AZARIN ZARASSI, DHARAMRAJ PATIL, SERGEY FROLOV, University of Pittsburgh, MOIRA HOCEVAR, Institute Neel CNRS, MINH NGUYEN, JINKYOUNG YOO, Los Alamos National Laboratory, SHADI DAYEH, University of California San Diego — Ge/Si core/shell nanowires are hosts to one dimensional hole gas. The spin-orbit interaction is expected to be much larger than that in electron systems such as InSb and InAs. Therefore, Ge/Si nanowires have great potential to demonstrate helical liquid. When strong superconductivity is induced in the nanowire, robust topological superconductivity may form in the system. We will show how to achieve semiconductor-superconductor contacts to the nanowire. The effects of a few surface cleaning methods and annealing process on the contact resistance will be shown. Superconducting contacts of NbTiN, Al, Ti and their combinations are studied. NbTiN may be suitable for hybrid device carrying Majorana fermions for its high critical temperature and magnetic field. Supercurrent through Josephson junctions with these contacts is measured.

9:12AM Y27.00007 Design and Implementation of a Josephson Junction Spectrometer, CAGLAR GIRIT, Collège de France & Quantronics Group, CEA-Saclay, MARCELO GOFFMAN, HUGUES POTHIER, CRISTIÁN URBINA, DANIEL ESTEVE, Quantronics Group, CEA-Saclay — A Josephson tunnel junction can be used as an on-chip absorption spectrometer at frequencies up to several hundred gigahertz. As a result of the AC Josephson effect, a voltage biased junction acts as a microwave source. When emitted photons are absorbed in the junction’s electromagnetic environment, a dc Cooper pair current flows (inelastic Cooper pair tunneling). By measuring this dc current as a function of applied voltage—the junction’s current-voltage characteristic—one obtains a spectrum of the electromagnetic environment. We describe the design of a Josephson junction spectrometer which seeks to optimize bandwidth, sensitivity, coupling and linewidth. We present measurements of the spectra of miniature on-chip $LC$ circuits with resonant frequencies in the 25-100 GHz range. Our Josephson junction spectrometer will be used to study level transitions in mesoscopic systems.

9:24AM Y27.00008 Domain walls in tetragonal superconductors: Andreev bound states and tunneling features, SOUMYA MUKHERJEE, KIRILL SAMOKHIN, Department of Physics, Brock University, KIRILL SAMOKHIN COLLABORATION — Domain walls can be formed in superconductors with a discrete degeneracy of the ground state, which breaks time reversal symmetry or a point group symmetry. We study all cases where the formation of domain walls is possible for the tetragonal point group symmetry D$_{4h}$. We discuss both triplet and mixed singlet order parameters. It is found that in all cases domain walls support subgap Andreev bound states, whose energies strongly depend on the direction of semiclassical propagation. We also study the density of states of these bound states and show that the formation of bound states near the domain wall strongly affects the tunneling conductance.

9:36AM Y27.00009 Anisotropic Andreev reflection in ferromagnet/s-wave superconductors (FS), PETRA HOEGL, University of Regensburg, ALEX MATOS ABIAGUE, IGOR ZUTIC, University at Buffalo, JAROSLAV FABIAN, University of Regensburg — Andreev reflection spectroscopy is a sensitive probe of the junction interface as well as of the spin polarization of the F region. By performing analytical and numerical calculations on widely accepted model systems, with interfacial Rashba and Dresselhaus spin-orbit fields, we show that Andreev reflection spectroscopy is also a sensitive tool of the interfacial spin-orbit coupling. In particular, we find a finite subgap conductance even in half-metallic systems due to the spin-flip Andreev reflection, imposing a triplet proximity effect. Furthermore, we predict a giant magnetic anisotropy of the Andreev reflection—anisotropic Andreev reflection (AAR)—with respect to the orientation of the F magnetization. We analyze the effects of the tunnel barrier strength, the F spin polarization, and the effective mass and Fermi wave vector mismatch. Our results should also have implications for designing Majorana states in semiconductor junctions with superconductors.

Friday, March 6, 2015 8:00AM - 11:00AM —
Session Y28 GMAG DMP FIAP: Focus Session: Spin-Hall Effect III

8:00AM Y28.00001 Spin pumping by magnetopolaritons, YUNSHAN CAO, PENG YAN, Delft Univ of Tech, HANS HUEBL, SEBASTIAN GOENNENWEIN, Walther-Meißner-Institut, GERRIT BAUER, Tohoku University and Delft Univ of Tech — Recent experiments report the strong coupling of microwaves to the magnetic insulator yttrium iron garnet with weakly damped magnetization dynamics [1]. We developed a scattering approach to study the coupled magnetization and microwave cavities beyond the paramagnetic/macrospin and rotating wave approximations that are implicit in the Tavis-Cummings model [2]. To this end we solve the coupled Landau-Lifshitz-Gilbert and Maxwell’s equations for a thin film magnet in a microwave cavity, leading to rich ferromagnetic spin wave resonance spectra of the transmitted or absorbed microwaves. Our method is valid for the full parameter range spanning the weak to strong coupling limits. We demonstrate strong coupling achievement not only for the FMR mode but also for standing spin waves, although the lowest excitation has a decisive leading role for coupling strength. Spin pumping in FI/N bilayers as detected by inverse spin Hall voltages provides additional access to study strong coupling electrically.

1Supported by grant ANR-10-IDEX-0001-02 PSL.

8:12AM Y28.00002 Spin Transport in Insulators Mediated by Magnetic Correlations Probed by $Y_3Fe_5O_{12}$-based Spin Pumping, CHUNHUI DU, HAILONG WANG, P. CHRIS HAMMEL, FENGYUAN YANG, The Ohio State University — Spin currents carried by mobile charges in ferromagnetic (FM) and nonmagnetic (NM) materials have been the central focus of spintronics, while spin transport in insulators is largely unexplored. FM spin pumping has awakened intense interest in magnon-mediated spin currents in both conducting and insulating FMs and in antiferromagnets (AF). Building on the large spin pumping signals enabled by our $Y_3Fe_5O_{12}$ (YIG) films, we report a systematic study of spin transport in six series of Pt/insulator/YIG trilayers where the insulators include one diamagnet, one paramagnet and four AFs. We observe remarkably robust spin transport in the AFs and a distinct linear relationship between the spin decay length in the insulator and the damping enhancement in the YIG, suggesting the critical role of magnonic coupling in AF insulators for spin transport. Strikingly, the insertion of a thin NIO layer between YIG and Pt significantly enhances the spin currents driven into Pt, suggesting exceptionally high spin transfer efficiency in YIG/NIO/Pt structures.
8:24AM Y28.00003 Spin pumping by time-dependent gate without magnetic field in a nanowire

LU-YAO WANG, Dept. of physics, Catholic Fu-Jen university, Taiwan, CHON-SAAR CHU, Dept. of Electrophysics, National Chiao-Tung university, Taiwan

We theoretically study that spin pumping by smooth profile time dependent gate in a Rashba type nanowire without magnetic field. The time dependent gate produces both spin dependent and spin-independent potentials. The spin dependent temporary potential inducing a dynamic Rashba coupling constant combining with the static Rashba coupling constant generate asymmetry spin dependent transmission. Such spin pumping can be enhanced by spin independent temporary potential.

8:36AM Y28.00004 Manipulation of Magnetic Insulators Using Spin Torque from the Spin Hall Effect , COLIN JERMINE, Cornell University, AARON ROSENBERG, Stanford University, HANJONG PAIK, SRIHARSHA ARADHYA, Cornell University, HAILONG WANG, Ohio State University, JOHN HERON, Cornell University, KATJA NOWACK, JOHN KIRTLIE, Stanford University, DARRELL SCHLOM, Cornell University, KATHRYN MOLER, Stanford University, PENGYUAN YANG, Ohio State University, DAN RALPH, Cornell University

We are exploring the possibility of current-induced switching driven by spin torque from the spin Hall effect for micron and nanoscale devices made from the magnetic insulators yttrium iron garnet (YIG) and lutetium iron garnet (LuIG). We will report on the fabrication of devices incorporating thin films of YIG or LuIG with thickness less than 20 nm and in-plane magnetization. We use electron beam lithography and ion milling to pattern the films into device structures with sizes ranging from 50 nm to 4 microns, integrated with a Ta or Pt layer, so that we can use the spin Hall effect to apply spin-transfer torque to the magnetic materials. With scanning SQUID magnetometry we measure the in-plane dipole orientation of the device magnetic moment at 4 K. By examining the magnetic orientation as a function of applied current we investigate whether the spin Hall torque can be used to drive reliable magnetic switching at low current levels.

8:48AM Y28.00005 Spin Torque Arising from the Spin Hall Effect within Ferromagnets , JONATHAN GIBBONS, Department of Physics, Cornell University, ROBERT BUHRMAN, School of Applied and Engineering Physics, Cornell University, DANIEL RALPH, Department of Physics, Cornell University

Recent spin-pumping measurements have indicated that ferromagnetic materials such as permalloy possess a significant inverse spin Hall effect, by which they convert an applied spin current to a charge current. We report experimental investigations of the inverse phenomenon, using the direct spin Hall effect within a ferromagnetic material to generate a spin current that can be used to apply a spin transfer torque to another nearby magnetic layer. Specifically, we measure spin-orbit-induced torques generated by an in-plane current in pinned ferromagnet/space/free ferromagnet multilayer structures. We quantify the strength of the torque using both non-resonant second harmonic magnetization tilting measurements and spin-torque ferromagnetic resonance. We focus on the dependence of the direction and strength of the spin torque on the relative orientation of the fixed-layer magnetization and the current.

9:00AM Y28.00006 Coupled spin-charge transport in two-dimensional electron gases from weak to strong spin-orbit couplings , YASUFUMI ARAKI, None, ALLAN H. MACDONALD, Department of Physics, University of Texas at Austin

We investigate the magnetoelectric response of two-dimensional electron gases with spin-orbit interactions of arbitrary strength. Rashba or Dresselhaus spin-orbit coupling in two-dimensional systems gives rise to the coupling of spin and charge transport, which may appear as spin Hall effect, spin-orbit induced torque, direct and inverse Edelstein effects, etc. We derive the diffusion equation for spin and charge densities microscopically with spin-independent disorder scattering and two types of spin-orbit interactions of arbitrary strength, and analyze the crossover in the coupled spin-charge transport from weak to strong spin-orbit coupling regimes. Our calculation connects the traditional perturbative treatment of the spin-orbit coupling in the weak spin-orbit coupling regime, where two spin states are nearly degenerate, to the relaxation time approximation estimate in the strong spin-orbit coupling regime, where the degeneracy is strongly lifted. The crossover becomes nontrivial when the Rashba and Dresselhaus spin-orbit interactions are comparable. Based on those calculations, we will give some comments on the spin-orbit induced torques induced in the heterostructure of ferromagnets and heavy metals.

9:12AM Y28.00007 ABSTRACT WITHDRAWN —

9:24AM Y28.00008 Testing Reciprocity of Spin Pumping and Spin Transfer Torque in Ferromagnet/Spin-Orbit Metal Heterostructures , CARL BOONE, SATORU EMORI, TIANXIANG NAN, NIAN SUN, North-eastern University

Spin pumping from a ferromagnet (FM) to a normal metal (NM) and spin transfer torque (STT) generated in a FM from an injected spin current should be reciprocal processes governed by the spin mixing conductance. The same should be true for the spin Hall effect (SHE) and inverse SHE, which are used to generate and measure spin currents. Past experiments on multilayer thin films involving FM and NM interfaces have measured only spin pumping or spin injection, and have utilized incomplete modeling that results in different effective values for the same parameter such as the spin mixing conductance or spin Hall angle. This gives rise to a large range of values reported in the literature. Here we develop a complete model for spin flow in the FM/NM system including SHE, spin diffusion and spin pumping that allows us to determine the true values of the spin transport parameters. To explore the physics we use STT-ferromagnetic resonance (FMR) experiments of NM/FM/NM trilayers, and FMR spectroscopy of FM/NM bilayers where we simultaneously measure damping changes due to spin pumping, voltage generated by inverse SHE, and STT generated by the SHE. These experiments, combined with the complete modeling, allow us to test the reciprocity of spin pumping and STT plus the SHE and its inverse.

9:36AM Y28.00009 Spin pumping with interface spin-orbit coupling , KAI CHEN, SHUFENG ZHANG, Univ of Arizona

The spin pumping has been formulated via a mixing conductance which characterizes the spin-dependent reflection coefficients [1]. The “mixing conductance” never mixes the spin at the interface, i.e., no spin-flip processes have been taken into account till now. We have recently reformulated the spin pumping via linear response approach in which the interface spin-orbit coupling as well as spin-diffusion driven backflow can be explicitly included. In some limiting cases, our formulation reduces to that of the previous theory. In the presence of the interface spin-orbit coupling, the electron spin traveling through an interface will receive a spin-orbit torque that rotates and absorbs the spin angular momentum. Among many distinctions with the previous theory [1], we predict a spatial dependent spin current in both magnetic and non-magnetic layers, an anisotropic enhanced damping parameter, and a plausible resolution on the controversial experimental results obtained by different methods such as the inverse spin Hall signal and the broadening of ferromagnetic resonance linewidth. This work is supported by NSF-ECS.

9:48AM Y28.00010 Quantifying Spin Hall and Rashba effect contributions to spin-orbit torque in magnetic bilayers. JOHN Q. XIAO1, Department of Physics and Astronomy, University of Delaware — Electrical control of magnetism has been energized by recent observation of spin-orbit torques in magnetic bilayers formed from a heavy metal (HM) and ferromagnet (FM). It has been demonstrated that the spin-orbit torques driven by an in-plane current can switch magnetization, manipulate magnetic domains and excite magnetization auto-oscillation. However, the microscopic mechanism for the spin-orbit torques is still under debate. The question being whether the dominating spin-orbit coupling (SOC) arises from the HM/FM interface due to the Rashba effect or arises in the bulk of HM due to the spin Hall effect, or a combination of the two. It has been theoretically demonstrated that both the Rashba effect and the spin Hall effect generate a field-like torque (T_{SOF}) and damping-like torque (T_{SOT}) on the magnetization, with only quantitative differences. Therefore, an accurate method to determine the T_{SOF} and T_{SOT} with various thicknesses of the FM and HM is needed. We present a newly developed, magneto-optic-Kerr-effect based spin-orbit torque magnetometer that measures both T_{SOF} and T_{SOT}, which can have both spatial and time resolution. We observed both T_{SOF} and T_{SOT} are nonlocal and does not require direct contact between FM and HM ...[1, 2]. By engineering the interface which modifies the Rashba interaction, we are able to show the co-existence of spin Hall and Rashba effect as well as quantifies both contributions to spin-orbit torques [1].


co-authors: Xin Fan, Halise Celik, Yumpeng Chen, Jun Wu1, Kyung-Jun Lee, and Virginia O. Lorenz

10:24AM Y28.00011 Magnonic Charge Pumping via Spin-Orbit Coupling. CHIARA CICCARELLI, University of Cambridge, KJETIL HALS, Norwegian University of Science and Technology, University of Copenhagen, ANDREW IRVINE, University of Cambridge, VIT NOVAK, Institute of Physics ASCR, YAROSLAV TSERKOVNYAK, University of California, Los Angeles, HIDEKAZU KUREBAYASHI, University College London, ARNE BRATAAS, Norwegian University of Science and Technology, ANDREW FERGUSON, University of Cambridge — The interplay between spin, charge and orbital degrees of freedom has led to the development of spintronic devices such as spin-torque oscillators and spin-transfer torque MRAM. In this development, spin pumping represents a convenient way to electrically detect magnetization dynamics. The effect originates from direct conversion of low-energy quantized spin waves in the magnet, known as magnons, into a flow of spins from the precessing magnet to adjacent leads. In this case, a secondary spin-charge conversion element, such as heavy metals with large spin Hall angle or multilayer layouts, is required to convert the spin current into a charge signal. Here, we report the observation of charge pumping in which a precessing ferromagnet pumps a charge current, demonstrating direct conversion of magnons into high-frequency currents via spin-orbit interaction. The generated electric current, unlike spin currents generated by spin-pumping, can be directly detected without the need of any additional spin-charge conversion mechanism. The charge-pumping phenomenon is generic and gives a deeper understanding of its reciprocal effect, the spin orbit torque, which is currently attracting interest for their potential in manipulating magnetic information.

10:36AM Y28.00012 Spin Circuit Representation for Spin Pumping Phenomena. KUNTAL ROY, SUPRIYO DATTA, School of Electrical and Computer Engineering, Purdue University — There has been enormous progress in the field of spintronics and nanomagnetics in recent years with the discovery of many new materials and phenomena and it remains a formidable challenge to integrate these phenomena into functional devices and evaluate their potential. To facilitate this process a modular approach has been proposed whereby different phenomena are represented by spin circuit components [1]. Unlike ordinary circuit components, these spin circuit components are characterized by 4-component voltages and currents (one for charge and three for spin). In this talk we will (1) present a spin circuit representation for spin pumping phenomena, (2) combine it with a spin circuit representation for the spin Hall effect [2] to show that it reproduces established results obtained earlier by other means, and finally (3) use it to propose a possible method for enhancing the spin-pumping efficiency by an order of magnitude through the addition of a spin sink layer. [1] Kerem Camsari, Samiran Ganguly and Supriyo Datta, Modular Approach to Spintronics, https://nanohub.org/groups/spintronics [2] Seokmin Hong, Shehrin Sayed and Supriyo Datta, Spin Circuit Representation for the Spin Hall Effect, in review.

1This work was supported by FAME, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA.

10:48AM Y28.00013 Dependence of the Spin Hall Torque Efficiency on the Transparency of Pt-Ferromagnetic Layer Interfaces. CHIARA CICCARELLI, University of Cambridge, KJETIL HALS, Norwegian University of Science and Technology, University of Copenhagen, ANDREW IRVINE, University of Cambridge — We report that spin current transport across Pt-ferromagnet (FM) interfaces is strongly dependent on the type and the thickness of the FM layer and on post-deposition processing protocols. By employing both harmonic voltage response measurements and spin-torque ferromagnetic resonance measurements on various Pt-Co and Pt-CoFe magnetic heterostructures, we find that the efficiency of the Pt spin Hall effect in exerting a damping-like spin torque on the FM ranges from < 0.05 to > 0.10 under different interfacial conditions. We also show that the temperature dependence of the spin torque efficiencies for both the damping-like torque and field-like torque is dependent upon the details of the Pt-FM interface. The “internal” spin Hall angle of the Pt thin films used in this study, after taking the interfacial spin transmission factor that is derived from the spin mixing conductance into account, is estimated to be ~0.20. This suggests that a careful engineering of Pt-FM interfaces can improve the spin-Hall-torque efficiency of Pt-based spintronic devices.

1Now at Massachusetts Institute of Technology

Friday, March 6, 2015 8:00AM - 11:00AM — Session Y29 GMAG DMP: Focus Session: Disordered and Glassy Magnets 206A - Daniel Silevitch, University of Chicago

8:00AM Y29.00001 Barkhausen noise in the Random Field Ising Magnet NdFeB. JIAN XU, DANIEL SILEVITCH, University of Chicago, THOMAS ROSENBAUM, California Institute of Technology — With the application of a magnetic field transverse to the magnetic easy axis, we performed magnetic measurements on an Nd-Fe-B thin film in which the magnetic moments are disordered, and a Random-Field Ising Model at room temperature. We study domain reversal and avalanche dynamics through an analysis of the Barkhausen noise. Power-law behavior with a cutoff is observed in the avalanche energy spectrum, consistent with theoretical predictions for disordered materials. Two regimes of behavior are found, one at low temperature and high transverse field where the system shows behavior consistent with randomness-dominated dynamics, and a high-temperature, low-transverse-field regime in which thermal fluctuations dominate the dynamics. In the randomness-dominated regime, the critical exponents are consistent with mean-field predictions for heavily disordered systems, whereas in the thermal-fluctuation regime, the critical exponents differ substantially from the mean-field predictions.
below 2.5 K. at 25 mK are consistent with a system of fluctuating moments, with a fluctuation rate of 11 MHz. This fluctuation rate is nearly temperature independent

find a sharp increase in magnetic correlations below 10 K and persistent spin dynamics down to 25 mK. Our longitudinal field

the large ionic radii decrease from titanium to germanium, Tb

agreement with the replica symmetry breaking predictions.

dimensional spin glass dynamics. For

n

dimension frustrated materials. A candidate spin liquid, Tb

3

d

unpaired Mn ions below 240 mK for all compositions measured, from

and quintuplet excitations. A magnetic field can be used to tune the energy spectrum of this system, yielding successive triplet and quintuplet condensates at

disorder.

Supported by ERC grant no. 247328 and from MINECO (Spain), contract no. FIS2012-35719-C02

+ 1

, characterized by pinning of topological defects with singularities: vortices, strings, etc. At

\( n = d + 1 \), the presence of nonsingular topological objects, such as kinks and skyrmions, leads to a weak metastability. At

\( n > d + 1 \) topological objects are absent and the behavior of the system is fully reversible, characterized by the exponential decay of correlations in quantitative agreement with the Larkin-Imry-Ma argument. These findings have been confirmed numerically on lattices of up to one billion sites. (Research supported by the DOE Grant DE-FG02-93ER45487.)


8:36AM Y29.00004 Random Fields, Topology, and Glassy States of Matter, EUGENE CHUDNOVSKY.

CUNY-Lehman College — The debate goes on for more than forty years whether weak static random fields destroy the long-range order in condensed matter systems. A recently found answer depends on the topology of the order parameter. The

\( n \)-component order parameter in \( d \) dimensions exhibits glassy behavior at \( n < d + 1 \), characterized by pinning of topological defects with singularities: vortices, strings, etc. At

\( n = d + 1 \), the presence of nonsingular topological objects, such as kinks and skyrmions, leads to a weak metastability. At

\( n > d + 1 \) topological objects are absent and the behavior of the system is fully reversible, characterized by the exponential decay of correlations in quantitative agreement with the Larkin-Imry-Ma argument. These findings have been confirmed numerically on lattices of up to one billion sites. (Research supported by the DOE Grant DE-FG02-93ER45487.)


9:24AM Y29.00006 The cumulative overlap distribution function in spin glasses: mean field vs. three dimensions1. DAVID YLLANES, Syracuse University, ALAIN BILLOIRE, CEA Saclay, ANDREA MAIORANO, ENZO MARINARI, La Sapienza Universita di Roma, VICTOR MARTIN-MAJOR, Universidad Complutense de Madrid — We use a sample-dependent analysis, based on medians and quantiles, to analyze the behavior of the overlap probability distribution in spin glasses. Using analytical and numerical mean-field results for the Sherrington-Kirkpatrick model, as well as data from toy models, we show that this approach is an effective tool to distinguish the low-temperature behavior of replica symmetry breaking systems from that expected in the droplet picture. An application of the method to the three-dimensional Edwards-Anderson models shows agreement with the replica symmetry breaking predictions.

1Supported by ERC grant no. 247328 and from MINECO (Spain), contract no. FIS2012-35719-C02

9:48AM Y29.00008 Ground States of a Disordered Frustrated Quantum Dimer Magnet1. ALEXANDER HRISTOV, MAXWELL SHAPIRO, IAN FISHER, Stanford University, MINSEONG LEE, LINSEY RODENBACH, ASHLEY BERNHEISEL, EUN SANG CHOI, JU-HYUN PARK, Florida State University, LEONARDO CIVALE, Los Alamos National Laboratory, TIM MUNSIE, GRAEME LUKE, McMaster University — We present results of thermodynamic measurements of the site-diluted spin-dimer magnet \( Ba_2(Mn_1-xV_x)O_3 \), including magnetization, torque magnetometry, and AC susceptibility. The parent compound \( Ba_2MnO_3 \) is a frustrated \( S = 1 \) quantum dimer-magnet with a singlet ground state, and triplet and quintuplet excitations. A magnetic field can be used to tune the energy spectrum of this system, yielding successive triplet and quintuplet condensates at low temperatures. Site substitution with \( x = 0 \) breaks Mn-dimers, introducing site disorder into the high-field ordered states. This substitution also introduces unpaired \( S = 1 \) Mn ions, and it has been an open question whether such spin order at low temperatures. Here, we present evidence of the spin freezing of unpaired Mn ions below 240 mK for all compositions measured, from \( x = 0.05 \) to 0.85. We also present the evolution of the high field ordered state with increasing disorder.

1NSF DMR-Award 1205165

10:00AM Y29.00009 Absence of Magnetic Order and Persistent Spin Dynamics in \( Tb_2Ge_2O_7 \). ALANNAH HALLAS, McMaster University, ANGEL AREVALO-LOPEZ, University of Edinburgh, MURRAY WILSON, McMaster University, LIAN LIU, Columbia University, J. PAUL ATTFIELD, University of Edinburgh, YASUTOMO UEMURA, Columbia University, CHRIS WIEBE, University of Winnipeg, GRAEME LUKE, McMaster University — The terbium pyrochlores exhibit many unique magnetic properties, which has generated significant interest in this family of frustrated materials. A candidate spin liquid, \( Tb_2Ti_2O_7 \) fails to order magnetically, despite strong antiferromagnetic correlations. The application of external pressure has been found to produce partial antiferromagnetic order in \( Tb_2Ti_2O_7 \). Recently, we synthesized a new member of this family, \( Tb_2Ge_2O_7 \). Due to the large ionic radii of the transition metals, \( Tb_2Ge_2O_7 \) can be considered a chemical pressure analog of \( Tb_2Ti_2O_7 \). However, neutron scattering measurements revealed an absence of magnetic order in \( Tb_2Ge_2O_7 \) down to 20 mK and dominant ferromagnetic correlations. Now, we have investigated the low temperature magnetism of \( Tb_2Ge_2O_7 \) with muon spin rotation. Our zero field \( \mu \)SR measurements confirm an absence of static order in \( Tb_2Ge_2O_7 \). We find a sharp increase in magnetic correlations below 10 K and persistent spin dynamics down to 25 mK. Our longitudinal field \( \mu \)SR measurements on \( Tb_2Ge_2O_7 \) at 25 mK are consistent with a system of fluctuating moments, with a fluctuation rate of 11 MHz. This fluctuation rate is nearly temperature independent below 2.5 K.
10:12AM Y29.00010 Local probe study of S=1 spin liquid candidate Ba$_3$NiSb$_2$O$_9$. **JEFFREY QUILLIAM**, Département de physique, Université de Sherbrooke, Sherbrooke, QC, Canada. FABRICE BERT, PHILIPPE MENDELS, JEAN-CHRISTOPHE ORAIN, Laboratoire de physique des solides, Université Paris-Sud XI, Orsay, France. ANTHONI MANSEAU, Département de physique, Université de Sherbrooke, Sherbrooke, QC, Canada, CÉLINE DARIE, Institut Néel, Grenoble, France. CHRISTOPHE PAYEN, CATHERINE GUILLOT-DEUDON, Institut des Matériaux Jean Rouxel, Université de Nantes, Nantes, France. — The family of hexagonal perovskites, Ba$_3$M$_2$Sb$_2$O$_9$, has attracted a considerable amount of attention in recent years, with the discovery of several spin liquid candidates. For $M=U$, the material is fairly disordered and likely exhibits a honeycomb-like lattice whereas in other cases the structure consists of triangular planes of spins. Three different structural phases of Ba$_3$NiSb$_2$O$_9$ have been discovered, depending on synthesis pressure [1]. Two of these phases (6HA and 6HB) consist of triangular planes of $S = 1$ moments, and differ primarily by the stacking of these planes. Here, we present muon spin rotation ($\mu$SR) and $^{121}$Sb nuclear magnetic resonance (NMR) results on a high-pressure synthesis of this material, 6HB-Ba$_3$NiSb$_2$O$_9$. Most importantly, we demonstrate that there are no signs of magnetic ordering or spin freezing down to temperatures as low as 20 mK, making this material a plausible spin liquid candidate. Furthermore our NMR results are indicative of gapless excitations, consistent with previous specific heat and magnetic susceptibility results [1].

10:24AM Y29.00011 Giant anisotropic interactions in frustrated quantum magnet BiCu$_2$PO$_6$. **KEMP PLUMB**, Johns Hopkins University. — I will discuss a series of comprehensive inelastic neutron scattering measurements which uncover the full magnetic excitation spectrum in the valence bond ordered compound BiCu$_2$PO$_6$. Owing to its frustrated geometry and potential to realize unique quantum phase transitions in high magnetic fields, BiCu$_2$PO$_6$ has received significant attention in recent literature. However, the true nature of the magnetic Hamiltonian responsible for the high field phenomena has not been known until now. I will present measurements of the spin excitation spectrum in BiCu$_2$PO$_6$ from which the magnetic Hamiltonian is elucidated. The spectrum is unique to the frustrated two-leg ladder geometry in BiCu$_2$PO$_6$ and we have been able to correctly describe the lowest energy excitations within the framework of a bond-operator theory, incorporating anisotropic magnetic exchange interactions which are comparable to the Heisenberg exchange terms. The anisotropic exchange interactions originate from spin orbit coupling and are of an unexpectedly large magnitude for a Cu based magnetic compound, potentially indicating the relevance of Bismuth in the superexchange pathway. BiCu$_2$PO$_6$ is a complex and unique quantum magnet combining frustration and anisotropic exchange; the discovery of such large anisotropic interactions in BiCu$_2$PO$_6$ hints at new routes for incorporating spin anisotropies in 3d transition metal based magnets.

Friday, March 6, 2015 8:00AM - 11:00AM –
Session Y31 GMAG DMP: Focus Session: Spin Chains II: Mostly $S = 1/2$

8:00AM Y31.00001 Local spin dynamics near quantum critical line of spin-1/2 antiferromagnetic Heisenberg XXZ chain with longitudinal magnetic field. **WANG YANG, JIANDA WU, CONGJUN WU**, Univ of California - San Diego. — The spin-1/2 antiferromagnetic quantum XXZ chain is one of the most well-studied integrable model. Although all of its eigenstates and spectrum can be obtained via algebraic Bethe ansatz method, understanding its local dynamics remains a great challenge [1]. In the anisotropic gapped region, while tuning longitudinal field, there is a line of critical fields where the system undergoes quantum phase transitions. Recent experiments on BaCu$_2$V$_8$O$_{16}$ provided some evidences for understanding low-energy spin dynamics near critical line [2]. In this work, we further calculate local spin dynamics in this region in low frequency limit by form factor methods. Our results can be compared with measurements of NMR relaxation rate. [1] J.-S. Caux, H. Konno, M. Sorrell, and R. Weston, Journal of Statistical Mechanics: Theory and Experiment 2012, P01007 (2012) [2] S. Kimura, T. Takeuchi, K. Okunishi, M. Hagiwara, Z. He, K. Kindo, T. Taniyama, and M. Itoh, Physical review letters 100, 057202 (2008).

8:12AM Y31.00002 Spin currents carried by spinons in XXZ Spin Chains: Signatures in Polarized Inelastic Neutron Scattering. **LEONARD PATRICK ENGLISH, HANS-BENJAMIN BRAUN**, University College Dublin, JIRI KULDA, Institute Laue-Langevin, Grenoble. — Quantum spin chains serve as a paradigm for exploring truly quantum phenomena, with spinons being the elementary excitations. Motivated by compounds such as CsCoBr$_3$ and CsCoCl$_3$, we focus on the Ising-like antiferromagnetic Heisenberg XXZ model (spin-1/2). Here we present theoretical results for the total inelastic scattering cross section of spin-polarized neutrons in the presence of an external magnetic field, which is applied transverse to the Ising direction. In particular, we identify the spin current associated with spinons and their corresponding signatures in the neutron scattering cross section. The presence of a transverse magnetic field no longer allows for reliance on $S_{\text{tot}}^z$ as a conserved quantity, which has traditionally been assumed in this context. As a striking consequence, we find that the spinons carry a non-vanishing spin current, even in the limit of infinitesimal fields. Our results are shown to be in good agreement with experimental neutron scattering data on CsCoBr$_3$. 

8:24AM Y31.00003 Finite-temperature scaling at the quantum critical point of the Ising chain in a transverse field. **MANUEL HAEGL**, Neutron Scattering and Magnetism, Laboratory for Solid State Physics, ETH Zurich, 8006 Zurich, Switzerland. DAN HUVONEN, National Institute of Chemical Physics and Biophysics, 12618 Tallinn, Estonia. TATIANA GUIDI, ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, United Kingdom. — Inelastic neutron scattering is used to study the finite-temperature scaling behavior of spin correlations at the quantum critical point in an experimental realization of the one-dimensional Ising model in a transverse field. The target compound is the well-characterized, anisotropic and bond-alternating Heisenberg spin-1 chain material NTENP. The validity and the limitations of the dynamic structure factor scaling are tested, discussed and compared to theoretical predictions. For this purpose neutron data have been collected on the three-axes spectrometers IN14 at ILL and FLEXX at HZB as well as on the time of flight multi-chopper spectrometer LET at ISIS. In addition to the general statement about quantum criticality and universality, present study also reveals new insight into the properties of the spin chain compound NTENP in particular.
Superlattices

ILYA VALMIANSKI, IVAN SCHULLER, University of California-San Diego — This work reports on the structural and magnetic properties of iron-phthalocyanine (FePc) superlattices. FePc has a divalent Fe(II) ion in the center of the molecule that forms quasi one-dimensional (1D) chains when the flat molecules are stacked. These 1D chains exhibit two magnetic regimes: ferromagnetic order below 5K due to inter-chain interactions, and paramagnetic order between 5K and 25K due to short-range intra-chain interactions. H$_2$Pc is a non-magnetic molecule in which, instead of a metal ion, two hydrogen atoms occupy the center of the molecule. We establish a new and more comprehensive phase diagram for this exotic system through the evolution of the magnetic entropy change $\Delta S_M (T, H)$ associated with the magnetocaloric effect. $\Delta S_M$ is measured in a single crystal of Ca$_3$Co$_2$O$_6$ prepared by the flux method and demonstrates the suppression of the SDW modulation by small applied magnetic fields (< 1T). Metamagnetic transitions to a ferrimagnetic up-up-down spin chain arrangement and full ferromagnetic alignment are observed below 25 K. Short-range ordered (SRO) correlations with an antiferromagnetic character grow in volume as the temperature is lowered below 15 K, resulting in a crossover from $\Delta S_M (H) < 0$ to $\Delta S_M (H) > 0$ at 12 K. Our entropy–based analysis reflects current understanding of the role of SDW and SRO phases in Ca$_3$Co$_2$O$_6$, resolves new sub-features of the ferrimagnetic phase, and extends previous results below the onset of slow dynamics (~ 10 K).

1USF authors acknowledge DoE BES under Award # DE-FG02-07ER46438 (magnetic measurements and analysis).

Pressure-induced structural distortions in copper pyrazine dinitrate

KEN-NETH O’NEAL, JUDY CHERIAN, University of Texas, CHRIS LANDEE, MARK TURNBULL, Clark University, ZHENXIAN LIU, Carnegie Institute of Washington, JANICE MUSFELDT, University of Tennessee — The vibrational properties of quasi-one-dimensional Heisenberg antiferromagnet copper pyrazine dinitrate were investigated up to 9 GPa using diamond anvil cell techniques and infrared and Raman spectroscopy. Two structural transitions were discovered, at 0.7 GPa and around 5 GPa. The lower pressure transition involves only the nitrate ligands, revealing enhanced interchain interactions. The higher pressure transition includes modes throughout the spectrum. Importantly, the pyrazine ring-related modes show an overall lowering of symmetry through this transition. Ring buckling under pressure likely reduces the exchange along the chains since the exchange pathway becomes distorted. A smaller $J$ may therefore lower the magnetic field of the quantum critical transition. This tunable exchange interaction could be utilized in other pyrazine bridged molecular systems to bring the quantum critical behavior into experimentally realizable fields.

We thank the National Science Foundation and the Petroleum Research Fund for support of this work.

Wilson ratio of a Tomonaga-Luttinger liquid in the one-dimensional spin-1/2 Heisenberg antiferromagnet CuPzN

CHRISTOPHER AYOYAMA, University of Florida, YOHEI KONO, ISSP, University of Tokyo, CHRISTOPHER AOYAMA, University of Florida, YOHEI KONO, ISSP, University of Tokyo, KRISTEN MARINO, Pennsylvania State University, HAIDONG ZHOU, University of Tennessee, CHISA HOTTA, University of Tokyo, MARK TURNBULL, CHERRY LUCAS, University of Florida, YASUMASA TAKANO, University of Florida — In the Tomonaga-Luttinger liquid (TLL) phase of a one-dimensional antiferromagnet, the Wilson ratio and the TLL parameter, $K$, are one and the same except for a trivial numerical factor. This equivalence allows the determination of $K$ from magnetic susceptibility and specific heat. We have performed accurate magnetcization and specific-heat measurements on the quasi-one-dimensional spin-1/2 Heisenberg antiferromagnet Cu(C$_2$H$_2$N$_2$)(NO$_3$)$_2$, known as CuPzN, at temperatures between 80 mK and 7.5 K and in magnetic fields up to 14.7 T and, from the data in the TLL regime, have obtained $K$ as a function of the magnetic field. The results are in excellent agreement with a prediction based on the Bethe ansatz.

Magnetic properties of the $S = 1/2$ antiferromagnetic spin-chain $\alpha-CuV_2O_7$

GANEETEE GITGEATPONG, Mahidol University, Thailand, YANG ZHAO, NIST Center for Neutron Research, National Institute of Standards and Technology, USA, MAXIM AVDEEV, ROSS PILTZ, Australian Nuclear Science and Technology Organisation, Australia, TAKU SATO, IMRAM, Tohoku University, Japan, KITTIWIT MATAN, Mahidol University, Thailand — Magnetic properties of the $S = 1/2$ antiferromagnetic spin-chain, $\alpha$-CuV$_2$O$_7$, have been studied using magnetization and neutron scattering measurements on powder and single-crystal samples. Magnetic susceptibility reveals a Curie-Weiss temperature of $\Theta = -73.2(9)$ K with a magnetic phase transition at $T_N = 33$ K while the Bonner-Fisher fit to the magnetic susceptibility for $T > T_N$ with magnetic field perpendicular to the crystallographic $a$-axis yields the intra-chain coupling of $|J|/k = 46.0(2)$ K. Small ferrimagnetism below $T_N$ is due to spin-canting caused by Dzyaloshinskii-Moriya interactions. Analysis of the neutron diffraction data reveals that the Cu$^{2+}$ spins are coupled antiferromagnetically along zigzag chains, which run alternately along [011] and [001] directions. The ordered moment of 0.925(3) $\mu_B$ is predominantly along the $a$-axis. Our recent inelastic neutron scattering, which reveals atypical magnetic excitations centered at commensurate wave vectors $(0, \pm 0.25, 0)$ around the magnetic zone center, will also be discussed.

Elastic constants and ultrasound attenuation in the spin-liquid phase of Cs$_2$CuCl$_4$

SIMON STREIB, PETER KOPIETZ, Institut für theoretische Physik, Universität Frankfurt, Germany, PHAM THANH CONG, BERND WOLF, MICHAEL LANG, NATALIJA VAN WELL, FRANZ RITTER, WOLF ASSMUS, Physikalisches Institut, Universität Frankfurt, Germany — The spin excitations in the spin-liquid phase of the anisotropic triangular lattice quantum antiferromagnet Cs$_2$CuCl$_4$ have been shown to propagate dominantly along the crystallographic $b$-axis. To test this dimensional reduction scenario, we have performed ultrasound experiments in the spin-liquid phase of Cs$_2$CuCl$_4$ probing the elastic constant $c_{22}$ and the sound attenuation along the $b$-axis as a function of an external magnetic field along the $a$-axis. We show that our data can be quantitatively explained within the framework of a nearest-neighbor spin-1/2 Heisenberg chain, where ferroms are introduced via the Jordan-Wigner transformation and the spin-phonon interaction arises from the usual exchange-striction mechanism.

Financial support by the DFG via SFB/TRR49 is gratefully acknowledged.

Magnetic Behavior of 1D-Ferromagnetic Fe Chains in FePc/H$_2$Pc Organic Superlattices

CARLOS MONTON, University of California-San Diego, THOMAS GREDIG, California State University-Long Beach, ALI BASARAN, ILYA VALMIANSKI, IVAN SCHULLER, University of California-San Diego — This work reports on the structural and magnetic properties of iron-phthalocyanine (FePc)/metal-free-phthalocyanine (H$_2$Pc) superlattices. FePc has a divalent Fe(II) ion in the center of the molecule that forms quasi one-dimensional (1D) chains when the flat molecules are stacked. These 1D chains exhibit two magnetic regimes: ferromagnetic order below 5K due to inter-chain interactions, and paramagnetic order between 5K and 25K due to short order intra-chain interactions. H$_2$Pc is a non-magnetic molecule in which, instead of a metal ion, two hydrogen atoms occupy the center of the molecule. We have grown FePc/H$_2$Pc superlattices, in which we controlled the alignment of the Fe chains (i.e. perpendicular or parallel to the substrate) by the growth conditions and through the choice of substrate. Additionally we controlled the Fe chain lengths by the thickness of the FePc layer. We have found that reducing the Fe chains length from 70 to 5 atoms increases substantially the coercive field. We will correlate the observed magnetic behavior with structural information obtained from x-ray diffraction.

The research at UCSD was supported by the Office of Basic Energy Science, U.S. Department of Energy, BES-DMS funded by the Department of Energy’s Office of Basic Energy Science, DMR under grant DE FG03 87ER45332.

ABSTRACT WITHDRAWN
10:00AM Y31.00011 Investigation of magnetic structure on (C$_3$H$_{12}$N)CuBr$_3$ system on the basis of DFT study and orbital interaction. CHANGHOON LEE, JISOOK HONG, JI HOON SHIM, Pohang Univ of Sci & Tech, POHANG UNIV OF SCI & TECH TEAM — The (C$_3$H$_{12}$N)CuBr$_3$ compound crystallizes in the monoclinic group $C2/c$. Magnetic susceptibility data down to 1.8 K can be well fitted for the antiferromagnetic spin-1/2 chain, giving the intrachain magnetic coupling constant $J_{inter}$ of $\approx$ $-17$ K. At zero field, (pipH)CuBr$_3$ shows 3D order below $T_S$ = 1.68 K. Calculated by the mean-field theory, the interchain coupling constant $J_{inter}$ = $-0.91$ K is obtained and the ordered magnetic moment is about 0.23 $\mu_B$. However, the interchain interaction should be strong unlike experimental observation. From the analysis of local structure, the $J_{inter}$ spin dimer show the possibility of good orbital overlap via Cu-O...O-Cu path in which angle for Cu-O...O-Cu is 161° indicating strong interchain interaction via Cu-O...O-Cu path. The magnetic structure of (C$_3$H$_{12}$N)CuBr$_3$ system in terms of orbital interaction could anticipated by two-leg spin ladder which such spin ladders interact ferromagnetically to form ladder. In this study, we evaluated spin exchange interactions of (pipH)CuBr$_3$ based on DFT calculations to find the magnetic structure of this system. As a consequence, the $J_{inter}$ interaction is strong and the magnetic structure of this system, indeed, is described by two-leg spin ladder.

1This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education(2013R1A1A2060341).

10:12AM Y31.00012 Magnetic Relaxation and Coercivity of Finite-size Single Chain Magnets. THOMAS GREDIG, MATTHEW BYRNE, Department of Physics and Astronomy, California State University Long Beach, Long Beach, CA 90840, ALESSANDRO VINIGNI, Laboratory for Solid State Physics, ETH Zurich, CH-8093 Zurich, Switzerland — The magnetic coercivity of cusp loops for iron phthalocyanine thin films depends on the iron chain length and the measurement sweep speed below 5 K. The average one-dimensional (1D) iron chain length in samples is controlled during deposition. These 1D iron chains can be tuned over one order of magnitude with the shortest chain having 100 elements. We show that the coercivity strongly increases with the average length of the iron chains, which self-assemble parallel to the substrate surface. Magnetic relaxation and sweep speed data suggest spin dynamics play an important role. Implementing Glauber dynamics with a finite-sized 1D Ising model provides qualitative agreement with experimental data. This suggests that iron phthalocyanine thin films act as single chain magnets and provide a solid test system for tunable finite-sized magnetic chains.

1This research has been supported with the NSF-DMR 0847552 grant.

10:24AM Y31.00013 Orbital ordering and magnetic dimensionalities in the p-orbital spin-1/2 Cs$_2$O$_2$ and Cs$_4$O$_6$, DENIS ARCON, Jozef Stefan Institute — The materials containing magnetic O$_2^-$ anions, i.e., alkali superoxides, AO$_2$ (A = Na, K, Rb, Cs), and alkali sesquioxides, AO$_3$ (A = Rb, Cs), exhibit two key features that make them appealing for investigation of the coupling between lattice, orbital and spin physics as an alternative to the more established d-orbital materials. First, the O$_2^-$ dumbbells can easily reorient down to the low temperatures, thereby modulating the overlaps of p orbitals. Second, as the $S = 1/2$ spin is localized in a pair of p-derived $\pi$ orbitals, their original degeneracy can be removed by the cooperative tilting of O$_2^-$ dumbbells. Here we report on our studies of Cs$_2$O$_2$ and Cs$_4$O$_6$ using $^{133}$Cs nuclear magnetic resonance and electron paramagnetic resonance techniques. In Cs$_2$O$_2$ we find the structural phase transition occurring at 61 K on cooling associated with the freezing out of the O$_2^-$ librations. The transition also includes $\pi^*$ orbital ordering that is responsible for the quasi-one-dimensional low-temperature magnetism. Clear signs of the spin Tomonaga-Luttinger liquid state are found from the spin-lattice relaxation and spin susceptibility data. On the other hand, the mixed valence Cs$_4$O$_6$ shows much more complex phase diagram with several transitions depending on the exact cooling protocol.

10:36AM Y31.00014 Conjugated molecules as amplifiers of anisotropic magneto-resistance in molecular junctions. DAVID RAKHmilevitch, SOUMYAJIT SARKAR, ORA BITTON, LEEOR KRONIK, OREN TAL, Weizmann Institute of Science — The simplest way to manipulate spin transport at the atomic scale is based on the anisotropic magneto-resistance (AMR) effect which refers to the dependence of current through a ferromagnetic element on the direction of its magnetization. However the resulting change in resistance is limited to 15%, making AMR an unlikely candidate for spintronic applications. In this respect, molecules adsorbed on ferromagnetic surfaces, were shown to modify local spin properties and therefore may facilitate in enhancing AMR effect at the atomic scale. We here demonstrate a 210% AMR in a single molecule junction based on a benzene molecule suspended between two nickel (Ni) electrodes. These results are in strike contrast with the AMR for bulk Ni (2%) or atomic Ni junctions (10%) measured on our devices. In addition, we take advantage of the electro-mechanical sensitivity of molecular junctions to show the measured AMR can be effectively tuned by elongating the junction. These results are explained by ab-initio calculations in the context of selective orbital hybridization. Our findings pave the way for simple and highly-effective control of spin transport at the atomic scale, promoting the feasibility of single-molecule spintronics.

10:48AM Y31.00015 Anderson transition in one-dimension using Wegner’s Flow equations. PARAJ BHATTACHARJEE, California Institute of Technology, VICTOR QUITO, State University of Campinas, DAVID PEKKER, University of Pittsburgh, GIL REFAEL, Laboratory of Solid State Physics, ETH Zurich, CH-8093 Zurich, Switzerland — We study the Anderson transition in one-dimensional random single-particle Hamiltonians with long-range hoppings decaying in a power-law. Explicitly, we consider the single particle tight-binding model in the spin representation with disorder both in the fields and hoppings. It has been shown by Mirin et. al. that this model shows an extended-to-localized transition as a function of the power-law exponent with a critical multi-fractal regime when the decay exponent is equal to one. We generalize the flow equation technique, first introduced by Wegner, to the disordered system and use it to study the model and elucidate the character of this transition. This method allows us to efficiently compute the eigenvalues and local observables. We follow, analytically and numerically, the flow of the coupling distributions for the different exponents as a function of the flow-time and look for signatures of the two distinct phases as well as a characterization of the critical point.

Friday, March 6, 2015 8:00AM - 11:00AM —
Session Y32 GMAG DMP: Focus Session: Magnetic Oxide Thin Films and Heterostructures:
Oxide Films 207B - Tula Paudel, University of Nebraska - Lincoln
8:00AM Y32.00001 Novel Magnetic Phenomena in Oxide Thin Films, Interfaces and Heterostructures

THIRUMALAI VENKATESAN, NUSNII-NanoCore, National University of Singapore — Oxide films, heterostructures and interfaces present wonderful opportunities for exploring novel magnetic phenomena. The idea of cationic vacancy induced ferromagnetism was demonstrated by observing ferromagnetism in Ta$_x$Ti$_{1-x}$O$_2$ ($x = 2 - 6\%$). Using XAS, XPS and XMCD, the magnetism was mainly located at the Ti sites and was shown to arise from Ti vacancies as opposed to Ti$^{3+}$. The substrate-film interface was crucial for observing the ferromagnetism, as the required concentration of Ti vacancies could only be maintained close to the interface. With electron transport we were able to see with increasing thickness the emerging role of Kondo scattering (mediated by Ti$^{3+}$) and at larger thickness impurity scattering. The polar LaAlO$_3$/non-polar SrTiO$_3$ interface exhibits a mixture of magnetic phases most likely arising from cationic defects and selective electron occupancy in Ti $t_{2g}$ levels. Using XMCD ferromagnetism was seen at these interfaces even at room temperature. Unlike LaAlO$_3$, polar LaMnO$_3$ is an insulator exhibiting orbital order that has a smaller band gap than SrTiO$_3$. It is a traditional antiferromagnetic material, but when grown on SrTiO$_3$, polar LaMnO$_3$ exhibits ferromagnetism for film thicknesses exceeding 5 unit cells. This is discussed in terms of electronic reconstruction with polar charge transfer to the LaMnO$_3$ side of the interface and also to the surface of the overlayer. Novel magnetic coupling effects are seen in perovskite ferromagnets separated by a polar oxide layer such as LaAlO$_3$ or NdGaO$_3$, whereas non-polar oxides do not show the same effect. The coupling between the ferromagnetic layers oscillates in sign between FM and AFM, depending on the barrier thickness. Such coupling is totally unexpected in the absence of any itinerary electrons, with insulating barriers that are too thick for tunneling. The novel magnetic coupling is shown to be mediated by spin-orbit coupling and also magnetic excitation of defect levels in the polar oxide planes.

8:36AM Y32.00002 Odd-parity magnetoresistance in pyrochlore iridate thin films with broken time-reversal symmetry

TAKAHIRO FUJITA, YUSUKE KOZUKA, MASAKI UCHIDA, Univ of Tokyo, ATSUMI TSUKAZAKI, Tohoku University, TAKA-HISA ARIMÁ, MASASHI KAWASAKI, Univ of Tokyo, DEPARTMENT OF APPLIED PHYSICS AND QUANTUM-PHASE ELECTRONICS CENTER TEAM, INSTITUTE FOR MATERIALS RESEARCH TEAM, PRESTO, JAPAN SCIENCE AND TECHNOLOGY AGENCY (JST) TEAM, DEPARTMENT OF ADVANCED MATERIALS SCIENCE TEAM, RIKEN CENTER FOR EMERGENT MATTER SCIENCE TEAM — Weyl Semimetal phase has a three dimensional Dirac-like band structure, which has been recently predicted to be materialized in lanthanides iridate pyrochlore (La$_2$Ir$_2$O$_7$), accompanied with all-in-all-out spin ordering. Nevertheless, obtaining high quality La$_2$Ir$_2$O$_7$ single crystal has been extremely challenging even in bulk. Here, we report on fabrication and magnetotransport property of Eu$_2$Ir$_2$O$_7$ single crystalline thin films. Our films show clear metal insulator transition at around 100 K. We reveal that one of the two degenerate all-in-all-out domain structures, which are interchangeable with time-reversal operation, can be selectively formed by the polarity of the cooling magnetic field. This domain is robustly sustained against sweep magnetic field of 9 T at 2 K, as evidenced by an unusual odd field dependent term in the magnetoresistance and an anomalous term in the Hall resistance. Our findings pave the way for exploring novel quantum transport predicted at their surfaces/interfaces or magnetic domain walls of the pyrochlore iridates.

8:48AM Y32.00003 The intrinsic magnetic structure and ordering of multiferoic h-LuFeO$_3$ Films

WILLIAM RATCLIFF, STEVEN DISSELER, JULIE BORCHERS, NIST, CHARLES BROOKS, JULIA MUNDY, Cornell University, JAMES CLARKSON, University of California, Berkeley, GREGORY STIEHL, Cornell University, PETER SCHIFFER, University of Illinois at Urbana-Champaign, DAVID MULLER, DARRELL SCHLOM, Cornell University, JARRETT TSYMBAI, PETER DOWBEN, University of Nebraska-Lincoln, Nebraska Center for Materials and Nanoscience, WENBIN WANG, Fudan University, JIAN WANG, Canadian Light Source, EVGENY TSIBIMAL, PETER DOWBEN, University of Nebraska-Lincoln, Nebraska Center for Materials and Nanoscience — We have studied the unoccupied electronic band structure of the hexagonal ferrites h-LuFeO$_3$ and h-YbFeO$_3$ using the absorption spectroscopy obtained with linearly polarized soft X-ray synchrotron radiation. The shapes of the spectra have been analyzed in terms of the splitting of atomic energy levels in various crystal fields corresponding to the local symmetry of the different atomic sites. Significant hybridization between O-2p and various iron and rare earth orbitals (such as Fe-3d, Lu/Yb-5d and Yb-4f) is observed. The photoemission damping is weak in the valence band of LuFeO$_3$, but when grown on SrTiO$_3$, LuFeO$_3$ exhibits ferromagnetism for film thicknesses exceeding 5 unit cells. This is discussed in terms of electronic reconstruction with polar charge transfer to the LaMnO$_3$ side of the interface and also to the surface of the overlayer. Novel magnetic coupling effects are seen in perovskite ferromagnets separated by a polar oxide layer such as LaAlO$_3$ or NdGaO$_3$, whereas non-polar oxides do not show the same effect. The coupling between the ferromagnetic layers oscillates in sign between FM and AFM, depending on the barrier thickness. Such coupling is totally unexpected in the absence of any itinerary electrons, with insulating barriers that are too thick for tunneling. The novel magnetic coupling is shown to be mediated by spin-orbit coupling and also magnetic excitation of defect levels in the polar oxide planes.

9:00AM Y32.00004 X-ray absorption spectroscopy study on h-LuFeO$_3$ and h-YbFeO$_3$ single crystal thin films

XIAOSHAN XU, University of Nebraska-Lincoln, Nebraska Center for Materials and Nanoscience, SHI CAO, TULA PAUDEL, KISHAN SINHA, XUANYUAN JIANG, University of Nebraska-Lincoln, Nebraska Center for Materials and Nanoscience, WENBIN WANG, Fudan University, JIAN WANG, Canadian Light Source, EVGENY TSYMBAL, PETER DOWBEN, University of Nebraska-Lincoln, Nebraska Center for Materials and Nanoscience — We have studied the unoccupied electronic band structure of the hexagonal ferrites h-LuFeO$_3$ and h-YbFeO$_3$ using the absorption spectroscopy obtained with linearly polarized soft X-ray synchrotron radiation. The shapes of the spectra have been analyzed in terms of the splitting of atomic energy levels in various crystal fields corresponding to the local symmetry of the different atomic sites. Significant hybridization between O-2p and various iron and rare earth orbitals (such as Fe-3d, Lu/Yb-5d and Yb-4f) is observed. The spectral weight contributions to the electronic states near the edge of the conduction band are found to consist of Fe-3d, Lu/Yb-5d, and Yb-4f as relatively narrow bands, as well as a wide O-2p band covering much of the measured energy range. The results are consistent with the density functional theory calculation including onsite-Coulomb repulsion corrections in terms of Hubbard U.

9:12AM Y32.00005 Time-resolved x-ray diffraction study of photoinduced strains in h-LuFeO$_3$ single crystal thin film

KISHAN SINHA, XUANYUAN JIANG, Department of Physics and Astronomy, University of Nebraska, Lincoln, Nebraska 68588, USA, XIAO WANG, Department of Physics, Bryn Mawr College, Bryn Mawr, Pennsylvania 19010, USA, ANTHONY DICHIARA, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA, XUEMEI CHENG, Department of Physics, Bryn Mawr College, Bryn Mawr, Pennsylvania 19010, USA, YUELIN LI, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA, XIAOSHAN XU, Department of Physics and Astronomy, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, Nebraska 68588, USA — We have studied the structural response of epitaxially stabilized h-LuFeO$_3$ (0001) thin film to above-band-gap optical excitation (pump) using time-resolved x-ray diffraction (probe) at picosecond time scale. The shift in (004) Bragg peak induced by a 390 nm excitation (30 ps duration) has been studied as a function of pump fluence and pump-probe time delay. The out-of-plane photoinduced lattice strain ($\Delta c/c$) exhibits a non-linear relation with fluence. The relaxation time is on the order of 1 ns. These observations suggest a relaxation mechanism that may be mediated by combined effects of charge recombination and phonon relaxation.
9:24AM Y32.00006 Local control of antiferromagnetic domains in Cr₂O₃[1]. S. ADENWALLA, UDAY SINGH, W. ECHTENKAMP, CH. BINEK, Univ of Nebraska - Lincoln — We have used a Cr₂O₃/Pd/(Co/Pd), exchange biased heterostructure to measure the spatial distribution of anti-ferromagnetic (AFM) domains in magnetoelectric AFM Cr₂O₃. The AFM Cr₂O₃ possesses a residual roughness insensitive surface magnetization below its Néel temperature (Tₙₑₑ 307K). This surface magnetization couples to the ferromagnetic material (Co/Pd) and results in exchange bias. Cooling the Cr₂O₃ from above its Néel temperature in different magnetization states of the ferromagnet results in the formation of AFM domains in Cr₂O₃. The AFM domains in the Cr₂O₃ were mapped by a spatial map of the exchange bias of the ferromagnet for the sample cooled in various remnant conditions of Co/Pd and zero-field cooled Cr₂O₃. The exchange bias, which is high above room temperature, is greatly reduced below the Néel temperature, resulting in a single AFM domain, and then, subsequently writing a reversed AFM domain using the heat from a 6 mW focused laser beam. Scanning the laser beam allows for the writing of any domain pattern with a spatial resolution of 5 μm, limited only by the focusing optics.

1This work is supported by NSF Grant No. 1409622 and MRSEC DMR-0820521.

9:36AM Y32.00007 The role of spin fluctuations in the conductivity of CrO₂[1], KATE HEFFERNAN, D. TALBAYEV, Tulane University, XUEYU ZHANG, A. GUPTA, University of Alabama — Chromium dioxide is a half-metallic ferromagnet with Tₘ = 390K. Below Tₘ, the conductivity of CrO₂ grows by two orders of magnitude and is temperature independent below about 30 K. It is believed that electron scattering by spin fluctuations is responsible for the strong temperature dependence of the conductivity. We performed time-resolved THz spectroscopy (TRTS) and time-resolved magneto-optical Kerr effect (TRMOKE) to study the role of spin fluctuations in electron conduction. A thin film CrO₂ sample was excited by an optical pump pulse. The induced conductivity changes were measured by TRTS and the induced spin response by TRMOKE. A fast and a slow component were observed in both responses. The fast component dominates the TRTS response, while the slow dominates the TRMOKE which we attribute to the spin demagnetization in CrO₂. Since the slow component contributes only a small fraction of the total conductivity change in TRTS, we conclude that spin fluctuations may not play the dominant role in the pump-induced conductivity change. We also observed that the film transmits less THz light after the pump excitation, which corresponds to it becoming more conductive. We will discuss the relationship of our observations to the electronic and optical properties of CrO₂.

1The work at Tulane was supported by the Louisiana Board of Regents through the Board of Regents Support Fund contract number LEQSF(2012-15)-RD-A-23.

9:48AM Y32.00008 Ferromagnetic boundary magnetization properties of epitaxial Cr(2-x)AlₓO₃ thin films. LORENZO FALLARINO, CIC nanoGUNE Consolider, CHRISTIAN BINEK, University of Nebraska - Lincoln, ANDREAS BERGER, CIC nanoGUNE Consolider — The existence of an equilibrium net magnetization at (0001) surfaces is enabled by symmetry constraints for the magnetoelectric antiferromagnet Cr₂O₃. The occurrence of this boundary magnetization (BM) is furthermore roughness insensitive [1]. The BM is hereby fully coupled to the bulk antiferromagnetic order parameter and can be reversed together with it by a combination of E and H fields in bulk materials [2], or solely by magnetic means for single crystal (0001) oriented thin chromia films [3]. In order to understand whether the BM can be extended to alloys containing different oxide materials, we investigated the effect of Al₂O₃ doping onto the structural and magnetic properties of Cr₂O₃. We grew, using a hybrid growth procedure, 100 nm thick high-quality epitaxial Cr(2-x)AlₓO₃(0001) thin films in the concentration range between x = 0 to x = 0.6, preserving the original corundum crystal structure and symmetry. Using SQUID magnetometry, we showed that the critical temperature Tₓ of the NC phase can be tuned by alloying with Al₂O₃ using the BM as a probe to study the magnetic transition. Furthermore, we were able to evaluate the critical exponent and the absolute BM values for different samples. Both properties are consistent with the expected values, corroborating the BM nature of the observed magnetic signals. References: [1] K. D. Belashchenko, Phys. Rev. Lett. 105, 147204 (2010); [2] X. He et al., Nat. Mater. 9,579 (2010); [3] L. Fallarino et al., Appl. Phys. Lett. 104, 022403 (2014)

10:00AM Y32.00009 Electronic and magnetic properties of (1 1 1)-oriented CoCr₂O₄ epitaxial thin film[1], XIAORAN LIU, MICHAEL KAREEV, YANWEI CAO, Department of Physics, University of Arkansas, JIAN LIU, Department of Physics, University of California, Berkeley, SRIMANTA MIDDEY, DEREK MEYERS, Department of Physics, University of Arkansas, JOHN FREELAND, Advanced Photon Source, Argonne National Laboratory, JAK CHAKHALIAN, Department of Physics, University of Arkansas, DEPARTMENT OF PHYSICS, UNIVERSITY OF CALIFORNIA; BERKELEY COLLABORATION, MATERIALS SCIENCE DIVISION, LAWRENCE BERKELEY NATIONAL LABORATORY. — We report on the fabrication of high quality (1 1 1)-oriented ferrimagnetic normal spinel CoCr₂O₄ epitaxial thin films on single crystal Al₂O₃ substrates. The structural, electronic and magnetic properties were characterized by in-situ reflection high energy electron diffraction, atomic force microscopy, X-ray diffraction, X-ray photoemission spectroscopy, SQUID magnetometry and element resolved resonant X-ray magnetic scattering. The comprehensive characterization reveals that no disorder in the cation distribution or multivalency issue is present in the samples. As a result, Kagomé and triangular layers are naturally formed via this specific growth approach. These findings offer a pathway to fabricate two dimensional Kagomé heterostructures with novel quantum many-body phenomena by means of geometrical design.

1J.C. was supported by the DOD-ARO under Grant No. 0402-17291. Work at the Advanced Photon Source, Argonne is supported by the U.S. DOE under Grant No. DEAC02 06CH11357.

10:12AM Y32.00010 Fe₃O₄ thin films: from worse to better than the bulk, L.H. TJENG, X.H. LIU, C.F. CHANG, A.D. RATA, A. KOMAREK, Max Planck Institute for Chemical Physics of Solids, Dresden — Magnetite Fe₃O₄ is one of the most investigated materials from the class of transition metal oxides. It shows a first-order anomaly in the temperature dependence of the electrical conductivity at Tᵥ = 125 K, the famous Verwey transition. However, thin films of Fe₃O₄ show always a lower Tᵥ compared to the bulk material. The transition in films is also much broader than in the bulk. In order to find out the reason, we have performed a systematic investigation of the transport properties in dependence of the oxygen pressure, thickness, and the choice of the substrate. The findings point us the way how to grow films that have very sharp transitions with even higher Tᵥ than the bulk material.

10:24AM Y32.00011 Structural and magnetic properties of epitaxial delafossite CuFeO₂ thin films grown by pulsed laser deposition[1], TESS SENTY, TOYANATH JOSHI, ROBBYN TRAPPEN, JINLING ZHOU, SONG CHEN, UIUC, CHICAGO, IL. — Delafossite CuFeO₂ is a metallic two-dimensional layered compound modeled after the layered graphite structure, which has a magnetic moment at the Cu site and an antiferromagnetic structure. In this work, we report on the growth and low temperature characterization of epitaxial thin films of CuFeO₂ using a pulsed laser deposition system. The films were grown on SrTiO₃(001) substrates at 400°C. The structural quality of the films was confirmed by x-ray diffraction, showing a (00l) orientation, and by atomic force microscopy. The magnetic properties were measured using a SQUID magnetometer, and the magnetic moment was found to be consistent with the theoretical value of 1.8μB per Cu ion. The electrical transport properties were measured using a physical property measurement system, and the Seebeck coefficient was measured to be positive, indicating a p-type semiconductor behavior. The thermal conductivity was measured using a differential scanning calorimeter, and the thermal conductivity was found to be low, consistent with the expected behavior for a two-dimensional material. The films were also found to be metallic, with a high electrical conductivity of 10⁵ S/m at 10 K. Overall, these results demonstrate the potential of CuFeO₂ thin films for applications in low temperature electronics and magnetism.

1This work was supported by a Research Challenge Grant from the West Virginia Higher Education Policy Commission (HEPC.dsr.12.29) and the Microelectronics Advanced Research Corporation (Contract #2013-MA-2382) at WVU. Work at PUC was supported by FONDECyT.
Semiconductor Research Corporation program, sponsored by MARCO and DARPA. The PMA strongly depends on the thickness of the ferromagnetic layers and the interfacial oxidation level of the bilayers. We will also discuss electric field controlled magnetic properties in these systems. This work was supported in part by NSF (ECCS-1310338) and by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation Corporation, sponsored by DARPA.

1. Yubo Cui, Wilhelms Geerts, Fidele Twagirayezu, Department of Physics, Texas State University, San Marcos, TX 78666, Stefan Zollner, Department of Physics, New Mexico State University, Las Cruces, NM 88003 — Recently several electronic devices have achieved significant enhancements that have been attributed to an oxidized NiFe layer. A study on lateral spin valves, was found to have an increased magnetoresistance after leaving it exposed to air. The enhancements were attributed to the partly oxidation of a NiFe layer. Even more recently the turn on voltages of Hematite based water splitting devices was lowered to record low of .61 V with the addition of an amorphous NiFeOx layer. We investigated the optical properties of Ni80Fe20-oxide thin films that were deposited by reactive RF sputtering on quartz and Si/SiO2 substrates. Deposition was performed in an AJA Magnetron System using an Ar gas flow of 8 sccm and an oxygen gas flow of 2 sccm for different substrate temperatures (24-600 degrees Celsius). The optical properties in the visible spectrum and the film thickness were measured using a Woollam M2000 variable angle spectroscopic ellipsometer. Additional measurements were performed with a Woollam IR-VASE from 1.7 to 30 micrometer. The measurement results show the existence of a phonon peak around 382 cm\(^{-1}\) slightly red-shifted from the 390 cm\(^{-1}\) phonon peak of single crystalline NiO. XRD spectra did only reveal X-ray peaks of the rocksalt structure.

Friday, March 6, 2015 8:00AM - 10:48AM
Session Y34 GERA DMP FIAP: Focus Session: Materials for Electrochemical Energy Storage

8:00AM Y34.00001 Advanced 3D Ni(OH)\(_2\)/CNT Gel Composite Electrodes for Supercapacitors\(^1\)
Hanlin Cheng, Hai Minh Duong, National University of Singapore — In order to enhance the performance of supercapacitors, advanced 3D Porous CNT/Ni(OH)\(_2\) gel composite electrodes are developed in this work. Compared with previously reported graphene gel supercapacitors, our electrodes using 1D CNTs have smaller diffusion resistance due to a shorter ion transport path. The developed 3D xerogel composite electrodes demonstrate the success of a careful engineered guest/host materials interface. Initially, the CNT gels are coated on the nickel foam to form a 3D scaffold, which serves as a microscopic electrical conductive network. Then Ni(OH)\(_2\) are incorporated using a traditional electrodeposition method. In this work, two types of the 3D CNT-coated nickel foams are investigated. The gels can be used directly as hydrogels or dried in air to form xerogels. Both hydrogels and xerogels present 3D tangled CNT networks. It shows that the hydrogel composite electrodes with unraveled CNTs, though presenting high capacitances of 1400 F/g at low discharge rate, possess lower capacitances at higher discharge rate and a poor cycling performance of less than 23% retention. In contrast, the xerogel composite electrodes can overcome these limitations in terms of a satisfied discharge performance of 1200 F/g and a good cycling retention more than 85% due to a stronger Ni(OH)\(_2\)/CNT interface. The CNT bundles in the xerogel electrodes formed during the drying process can give a flat surface with small curvature, which facilitate the Ni(OH)\(_2\) nucleation and growth.

8:12AM Y34.00002 Energetic and solvation effects at photoanode-catalyst interfaces: IrO\(_2\)/WO\(_3\)\(^1\)
Yuan Ping, Joint Center for Artificial Photosynthesis, California Institute of Technology and Lawrence Berkeley National Laboratory, William Goddard III, Joint Center for Artificial Photosynthesis, California Institute of Technology. GIULIA GALLI. The University of Chicago — One key challenge in building photo-electrochemical cells to split water is to engineer interfaces between photo-electrodes and catalysts that are stable in harsh pH conditions and permit optimal charge transfer. Iridium oxide is the only known catalyst for oxygen evolution stable in acidic conditions and hence a good candidate to be interfaced with photo-anodes. Using ab initio calculations, we investigated the structural and electronic properties of tungsten trioxide surfaces interfaced with an iridium dioxide thin film. We built a microscopic model of the interface that exhibits a formation energy lower than the surface energy of the most stable IrO\(_2\) surface, in spite of a large lattice mismatch, and we found no impurity states pinning the Fermi level. Both within Density Functional and many body perturbation theory (GW), we found that the two oxides form undesirable Ohmic contacts, when an IrO\(_2\) thin film fully covers WO\(_3\). However, our calculations predicted that if the morphology of the catalyst allows for partial exposure of the two oxides to water, then Schottky barriers may be formed, which favor charge transfer and hence water splitting. This work suggests ways to optimize light-absorber-catalyst interfaces for optimal charge transport.

8:24AM Y34.00003 Connecting the dynamic response of electrodes to their electronic structure \(^1\)
Anton Van Der Ven, Materials Department, University of California Santa Barbara — The electrodes of Li-ion batteries exhibit a wide range of intriguing electronic, thermodynamic and kinetic properties. Most electrode materials undergo a series of phase transformations as a result of drastic changes in Li concentration during each charge and discharge cycle. The mechanisms of these phase transformations remain poorly understood but usually involve a coupling between ionic diffusion, structural changes and interface migration. While phase transformations affect electrodes at the particle level, their mechanisms are ultimately determined by the electronic structure and crystallography of the electrode chemistry. Describing these phase transformations phenomenologically starting from first principles requires suitable coarse-graining strategies and a reliance on statistical mechanical approaches to account for the important role of temperature and entropy. This talk will describe how first-principles statistical mechanical approaches have provided insights about the mechanisms of kinetic processes in a variety of transition metal oxides and sulfides with widely differing crystal structures.
Effects of the dielectric response of solvent molecules filling, DFT+ECs incorporating organic electrolytes, aqueous electrolyte-based asymmetric supercapacitors (ASCs) have been attracting intensive attention recently. In this work, we present an incisive spectroscopic technique for directly probing redox orbits based on bulk electron momentum density measurements via high-resolution X-ray Compton scattering. Application of our method to spinel LiMn2O4 (a lithium ion battery cathode material) is discussed. The orbital involved in lithium insertion and extraction process is mainly the oxygen 2p orbit. Moreover, the manganese 3d states are shown to experience spatial delocalization involving 0.16 electrons per Mn site during the battery operation. Our analysis provides a clear understanding of the fundamental redox process involved in the working of the lithium ion battery. Work supported in part by the US DOE.

Electronic Structure at Electrode/Electrolyte Interfaces in Magnesium based Batteries. JANAKIRAMAN BALACHANDRAN, DONALD SIEGEL, University of Michigan, Ann Arbor — Magnesium is a promising multivalent element for use in next generation electrochemical energy storage systems. However, a wide range of challenges such as low coulombic efficiency, low/varying capacity and cyclability need to be resolved in order to realize Mg based batteries. Many of these issues can be related to interfacial phenomena between the Mg anode and common electrolytes. Ab-initio based computational models of these interfaces can provide insights on the interfacial interactions that can be difficult to probe experimentally. In this work we present ab-initio computations of common electrolyte solvents (THF, DME) in contact with two model electrode surfaces namely — (i) an “SEI-free” electrode based on Mg metal and, (ii) a “passivated” electrode consisting of MgO. We perform GW calculations to predict the reorganization of the molecular orbitals (HOMO/LUMO) upon contact with these surfaces and their alignment with respect to the Fermi energy of the electrodes. These computations are in turn compared with more efficient GGA (PBE) & Hybrid (HSE) functional calculations. The results obtained from these computations enable us to qualitatively describe the stability of these solvent molecules at electrode-electrolyte interfaces.

Mg intercalation mechanism at the Mo6S8 cathode surface proposed by first-principles methods1. LIWEN WAN, DAVID PRENDERGAST, Joint Center for Energy Storage Research, The Molecular Foundry, Lawrence Berkeley National Laboratory — In recent years, great attention has been paid to the development of divalent Mg-ion batteries, which can potentially double the energy density and volumetric capacity compared to monovalent Li-ion batteries. The prototype Mg-ion battery, comprising Mg(anode)/Mg2(AlCl3-BuEt)2/THF(electrolyte)/Mo6S8(cathode), was established in 2000 by Aurbach et al. Despite the remarkable success of this prototype system, we still lack a clear understanding of the fundamental Mg intercalation/deposition mechanism at the electrolyte/electrode interfaces that perhaps results in the observed sluggish Mg transport process. Our previous work has shown that Mg-ions are strongly coordinated in the bulk electrolyte by a combination of counterion, Cl−, and organic aprotic solvent, THF. In this work, we use first-principles methods to study Mg intercalation behavior at the Mo6S8 cathode surface with the presence of solvent molecules. It is found that the image charge, formed on this metallic cathode surface, can effectively weaken the solvent-surface interactions and facilitate Mg intercalation. A detailed Mg intercalation mechanism is proposed and the unique role of Mo6S8 as the cathode material is emphasized.

Asymmetric Supercapacitors with Dominant Pseudocapacitance in Neutral Aqueous Electrolyte. YUANBING MAO, QIANG LI, University of Texas-Pan American — Electrochemical capacitors (ECs) are promising power sources for portable electronics and hybrid electric vehicles. To solve the poor ionic conductivity, intrinsic inflammability and toxicity issues of current ECs incorporating organic electrolytes, aqueous electrolyte-based asymmetric supercapacitors (ASCs) have been attracting intensive attention recently. In this presentation, prototype MnO2-NFs/KCl//CNTs supercapacitor cells in neutral aqueous electrolyte allow rapid charge/discharge kinetics, fast ionic response, and evident pseudocapacitive dominance due to the unique MnO2-NF architecture and novel ASC design. For the first time, the respective contributions of the pseudocapacitance and EDL capacitance to the overall electrochemical performance of ASCs were differentiated with a proof of pseudocapacitive dominance \( \eta_{pseudocap}/\eta_{EC} = 2.5 \). To sum, this study provides a brilliant proof-of-concept design of novel supercapacitors with pseudocapacitive dominance to achieve ultimate energy storage applications with both high energy and power density.

Impact of strong electronic correlations on the phase stability of oxide and phosphate intercalation materials. ERIC ISAACS, CHRIS MARIANETTI, Department of Applied Physics and Applied Mathematics, Columbia University — Li intercalation in certain battery cathode materials such as Li1FePO4 (LFP) occurs via a two-phase (phase separated) process, which significantly impacts the voltage profile and charge/discharge kinetics. The phase separation in LFP is not predicted by density functional theory (DFT), but it is captured by DFT plus Hubbard U (DFT+U) suggesting the significant role of electronic correlations in determining its thermodynamic properties [F. Zhou et al., Phys. Rev. B 69, 201101 (2004)]. In order to understand the impact of such correlations on the phase stability of transition metal oxide and phosphate intercalation materials, here we investigate the formation energies of phase separating LFP, phase stable Li2CoO2, and phase stable Sr2La1-x52TiO2 within DFT+U. We present the relationship between different formation energy contributions and the on-site Coulomb energy. Furthermore, we illustrate how band filling, p-d hybridization, magnetism, and charge and orbital ordering can impact the phase stability of such systems.

1This work is supported as part of the Joint Center for Energy Storage Research (JCESR), an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences.
10:24AM Y34.00011 Structure and interface properties of the electrolyte material Li$_4$P$_2$S$_6$\(^1\)
ZACHARY D. HOOD, Oak Ridge National Lab., CAMERON KATES\(^2\), N. A. W. HOLZWARTH, Wake Forest U. — Li$_4$P$_2$S$_6$ has been identified in several high temperature preparations of lithium thiophosphate electrolytes as a synthesis or decomposition product. Its characteristic P−P bond may be partly responsible for its relative stability. Early structural analyses\(^3\) found the P sites to be disordered. Our previous simulations\(^4\) found a related low energy structure with ordered P sites. We report here a re-examination of the simulation results and new X-ray measurements which indicate that the lowest energy structure of Li$_4$P$_2$S$_6$ is different from that determined in previous analysis. Ionic conductivity and thermal stability are also reported. In addition to examining the bulk electrolyte, we have simulated idealized interfaces of Li$_4$P$_2$S$_6$ and lithium metal representing an electrolyte/anode system.

\(^1\)Supported by NSF grant DMR-1105485.
\(^2\)Currently attending the Pratt School of Engineering at Duke U.
\(^3\)R. Mercier et. al., J. Solid State Chem. 43 151 (1982)
\(^4\)N. A. Holzwarth, J. Power Sources 196 6970 (2011)

10:36AM Y34.00012 Modeling solid electrolyte/electrode interface stability using first principles calculations\(^1\)
NICHOLAS LEPLEY, N. A. W. HOLZWARTH, Wake Forest University — The formation of a stable interface between electrode and electrolyte materials is a necessary property for batteries in general and for Li-ion batteries in particular. We present a framework for understanding and predicting the electrochemical stability of electrode/electrolyte interfaces based on density functional theory calculations. Within this framework, we have extended our previous work\(^2\) to include quantitative results for the solid-solid interface energy of the Li$_4$PS$_4$/Li, Li$_3$PO$_4$/Li, Li$_2$S/Li, Li$_2$O/Li, and Li$_2$PS$_4$/Li$_2$S interfaces. We show that under local equilibrium conditions the interface energy appears to be a good indicator of the stability of the interface. While the results we present are focused on the interface between Li-ion solid electrolytes and Li metal we expect the method to be applicable to other interface systems.

\(^1\)Supported by NSF Grant DMR-1105485

Friday, March 6, 2015 8:00AM - 10:36AM –
Session Y35 DAMOP: Collective Modes and Topological Defects in Bose-Einstein Condensates
210B - Lauren Aycock, Joint Quantum Institute/ Cornell University

8:00AM Y35.00001 Deconstruction of excitations in atomtronic systems using phase reference\(^1\)
MARK EDWARDS, BRENNAN COHELEACH, Georgia Southern University, CHARLES CLARK, Joint Quantum Institute — Laboratory atomtronic systems consisting of a Bose–Einstein–condensed gas with strong horizontal confinement and arbitrary planar potential, such as a ring–plus–disk, are now possible. Perturbing the ring part (e.g., by stirring) can produce excitations such as vortices and solitons. Each excitation uniquely modifies the local condensate phase and these modifications can be probed by overlapping the ring with the unperturbed disk via condensate release. The resulting interference pattern contains signatures of the excitations present at release time. Using the Gross–Pitaevskii equation, we studied whether this interference pattern can be used to determine what excitations were present at release time. We created individual excitations in a ring–plus–disk condensate, released it to see the interference pattern and created a compendium of these patterns. We also studied whether the individual patterns can be superposed and tested the deconstruction procedure by analyzing the interference of a strongly stirred ring by comparing the deconstruction with the condensate state at release time.

\(^1\)Supported by NSF grants PHY–1068761 and ARO Atomtronics MURI

8:12AM Y35.00002 Thermal and quantum fluctuation effects in rotational hysteresis of ring Bose–Einstein condensates\(^1\)
C.W. CLARK, Y.-H. WANG, Joint Quantum Institute, C. HELLER, M. EDWARDS, Georgia Southern University — In a recent experiment\(^2\) a ring Bose–Einstein condensate (BEC) with zero circulation (with winding number $m = 0$) and stirred by a barrier jumped to an $m = 1$ state when stirred faster than a certain critical speed, $\Omega_c^1$. Conversely an $m = 1$ condensate dropped to $m = 0$ when stirred below a critical speed, $\Omega^1_c$, which was lower than $\Omega_c^1$. The hysteresis loop areas, $\Omega^1_c - \Omega^1_c$, disagreed significantly with the predictions of the zero–temperature Gross–Pitaevskii equation. We report the results of simulating this experiment with both the Zaremba–Nikuni–Griffin (ZNG) theory and the Truncated Wigner Approximation (TWA).

\(^1\)Supported by NSF grants PHY–1068761 and ARO Atomtronics MURI

8:24AM Y35.00003 Unusual vortex matter in rotating Bose–Einstein condensates with SU(2) broken symmetry\(^1\)
PEDER GALTELAND, Department of Physics, Norwegian University of Science and Technology, EGOR BABAEEV, Department of Theoretical Physics, The Royal Institute of Technology, ASLE SUDBO, Department of Physics, Norwegian University of Science and Technology — We consider a Ginzburg–Landau model of a rotating two-component Bose–Einstein condensate with SU(2) broken symmetry through the use of numerical Monte Carlo techniques. We include the full spectrum of thermal amplitude- and phase-fluctuations. The model exhibits an unusual state of global phase coherence with no accompanying vortex line lattice. This state is not a counterpart in single-component condensates. The conditions for such a state are experimentally realizable in, e.g., homonuclear mixes of atomic gases in separate hyperfine states, tuned to the SU(2) point with Feshbach resonance techniques.

\(^1\)This work was supported by the Norwegian Research Council and the Norwegian Consortium for High-Performance Computing.
8:36AM Y35.00004 Vortex annihilation and inverse cascades in two dimensional superfluid turbulence, ANDREW LUCAS, PAUL M. CHESLER, Harvard Univ — The dynamics of a dilute mixture of vortices and antivortices in a turbulent two-dimensional superfluid at finite temperature is well described by first order Hall-Vinen-Iordanskii equations, or dissipative point vortex dynamics. These equations are governed by a single dimensionless parameter: the ratio of the strength of drag forces to Magnus forces on vortices. When this parameter is small, we demonstrate using numerical simulations that the resulting superfluid enjoys an inverse energy cascade where small scale stirring leads to large scale vortex clustering. We argue analytically and numerically that the vortex annihilation rate in a laminar flow may be parametrically smaller than the rate in a turbulent flow with an inverse cascade. This suggests a new way to detect inverse cascades in experiments on two-dimensional superfluid turbulence using cold atomic gases, where traditional probes of turbulence such as the energy spectrum are not currently accessible.

8:48AM Y35.00005 Excitation spectrum of a tightly confined spin-2 Bose gas, MATJAZ PAYRITS, RYAN BARNETT, Imperial Coll — We introduce an effective low-energy action for a spin-2 Bose gas in a tight trap in the presence of a quadratic Zeeman field. We derive the excitation spectrum by expanding the action to second order in deviations from the ground state configuration and subjecting it to a functional integral analysis. This is a generalization of standard Bogoliubov theory as it allows for the study of excitations about fragmented states, occurring ubiquitously in spinor Bose gas systems. It is found that the excitations generally consist of mean-field-like states uniformly integrated over rotations about the direction of the magnetic field (or all of SU(3) in the absence of a magnetic field). This parallels the general observation that states breaking fewer symmetries tend to be lower in energy. Though unstable in the thermodynamic limit, these states are stabilized for finite particle numbers, potentially allowing for a convenient means of studying fragmentation experimentally. For the nematic region of the spin-2 phase diagram, we also show that the quadratic Zeeman dependence of the spectrum smoothly approaches the previously obtained discontinuous mean-field dependence.

9:00AM Y35.00006 Probing the Collective Modes of Spherical Shell-Shaped Condensates with Quench Numerics, FRANCES YANG, Smith College, KUEI SUN, The University of Texas at Dallas, KARMELA PADAVIC, SMITHA VISHVESWARA, University of Illinois at Urbana-Champaign, COURTNEY LANNERT, Smith College and the University of Massachusetts at Amherst — We explore the collective modes of Bose-Einstein condensates by numerical solution of the Gross-Pitaevskii equation with an external “bubble trap” potential and the limits of a thin-shell condensate and a filled-spherical condensate.

9:12AM Y35.00007 Microscopic theory of BEC phase transition in a critical region, VITALY KOCHAROVSKY, Texas A&M University, VLADIMIR KOCHAROVSKY, Inst. of Applied Physics of the Russian Academy of Science and Univ. of Nizhny Novgorod, Russia — A microscopic theory, which should connect the asymptotics of the ordered and disordered phases across a critical region, has not been found so far even for anyone of the numerous phase transitions. Here we present such microscopic theory for a phase transition in an interacting Bose gas [Phys. Lett. A 378, n. 49 (2014)]. It allows one to describe formation of a condensate phase from a disordered phase across an entire critical region continuously. We find an exact Hamiltonian for Bose-Einstein condensation (BEC) in a mesoscopic system and derive the exact fundamental equations for the condensate wave function and Green’s functions, which are valid both inside and outside critical region. These equations are governed by a single dimensionless parameter: the ratio of the strength of drag forces to Magnus forces on vortices. We introduce an effective low-energy action for a spin-2 Bose gas in a tight trap in the presence of a quadratic Zeeman field.

9:24AM Y35.00008 Moving solitons in a one-dimensional fermionic superfluid - an exact solution, DMITRY EIFMINK, University of Maryland, VICTOR GALITSKI, Joint Quantum Institute, University of Maryland — A fully analytical theory of a traveling soliton in a one-dimensional fermionic superfluid is developed within the framework of time-dependent self-consistent Bogoliubov-de Gennes equations, which are solved exactly. The soliton manifests itself in a kink-like profile of the superconducting order parameter and hosts a pair of Andreev bound states. They adjust to soliton’s motion and play an important role in its stabilization. A phase jump across the soliton and its energy decrease with soliton’s velocity and vanish at the critical velocity, corresponding to the Landau criterion, where the soliton starts emitting quasiparticles and becomes unstable. The “inertial” and “gravitational” masses of the soliton are calculated and the former is shown to be orders of magnitude larger than the latter. This results in a slow motion of the soliton in a harmonic trap.


9:36AM Y35.00009 3D dimeron as a stable topological object, SHIJIE YANG, YONGKAI LIU, Beijing Normal University — Searching for novel topological objects is always an intriguing task for scientists in various fields. We study a new three-dimensional (3D) topological structure called 3D dimeron in the trapped two-component Bose-Einstein condensates. The 3D dimeron differs to the conventional 3D skyrmion for the condensates hosting two interlocked vortex-rings. We demonstrate that the vortex-rings are connected by a singular string and the complexity constitutes a vortex-molecule. The stability is investigated through numerically evolving the Gross-Pitaevskii equations, giving a coherent Rabi coupling between the two components. Alternatively, we find that the stable 3D dimeron can be naturally generated from a vortex-free Gaussian wave packet via incorporating a synthetic non-Abelian gauge potential into the condensates.

This work is supported by the NSF of China under Grant no. 11374036 and the National 973 program under Grant no. 2012CB821403.

9:48AM Y35.00010 Black–hole lasing action in laboratory Bose–Einstein condensates, YIHSIEH WANG, TED JACOBSON, University of Maryland, MARK EDWARDS, Georgia Southern University, CHARLES W. CLARK, Joint Quantum Institute — A recent experiment infers the the production of Hawking radiation in an analogue black-hole laser, which consists of a Bose-Einstein condensate of about 5,000 $^{87}$Rb atoms in a trap with a translating potential step. In the co-moving reference frame the flow velocity of the condensate exceeds the sound speed in a region confined between two sonic points, the analogue black and white hole horizons. We report simulations of that experiment based on the zero-temperature Gross-Pitaevskii (GP) equation that are consistent with the reported experimental results. The simulations show exponential growth of oscillatory modes trapped between the horizons, with a power spectrum consistent with expectations from the Bogoliubov dispersion relation, which saturates after an initial period. Quantum Hawking radiation occurs spontaneously in the vacuum, but in the presence of a coherent state of phonons it takes on a classical form captured by the zero-temperature GP equation. The growth of the trapped modes results from repeated super-radiant scattering from the black hole horizon, associated with emission of Hawking radiation to the exterior that is not well-resolved in the simulation.

This work is supported by NSF grants PHY-1068761 and PHY-0822671 and the ARO Atomtronics MURI.

3 Supported in part by NSF grants PHY-1068761 and PHY-0822671 and the ARO Atomtronics MURI.
10:00AM Y35.00011 The fate of a gray soliton in a quenched Bose-Einstein condensate. OLEK-SANDR GAMAYUN, Lancaster Univ. YULIA BEZVERSHENKO, Bogolyubov Institute for Theoretical Physics, VADIM CHEIANOV. Leiden University — We investigate the destiny of a gray soliton in a repulsive one-dimensional Bose-Einstein condensate undergoing a sudden quench of the non-linearity parameter. The outcome of the quench is found to depend dramatically on the ratio $\eta$ of the final and initial values of the speed of sound. For integer $\eta$ the soliton splits into exactly $2\eta - 1$ solitons. For non-integer $\eta$ the soliton decays into multiple solitons and Bogoliubov modes. The case of integer $\eta$ is analyzed in detail. The parameters of solitons in the out-state are found explicitly. Our approach exploits the inverse scattering method and can be easily used for the similar quenches in any classical integrable system.

10:12AM Y36.00002 Emission spectrum of atoms in a harmonic trap. POOJA SINGH, YURI ROSTOVTSIV, University of North Texas — We consider an excited atom in a harmonic trap. The evolution of quantum atomic states is theoretically studied under adiabatic approximation. The emission spectra for trapped atoms are calculated. We have show interference effects as well as trapping effect in a trap that has a size larger than the wavelength of radiation.

10:24AM Y35.00013 Conservation of helicity in superfluids. HRIDEISH KEDIA, DUSTIN KLECKNER, University of Chicago, DAVIDE PROMENT, University of East Anglia, WILLIAM T.M. IRVIN, University of Chicago — Helicity arises as a special conserved quantity in ideal fluids, in addition to energy, momentum and angular momentum. As a measure of the knottedness of vortex lines, Helicity provides an important tool for studying a wide variety of physical systems such as plasmas and turbulent fluids. Superfluids flow without resistance just like ideal (Euler) fluids, making it natural to ask whether their knottedness is similarly preserved. We address the conservation of helicity in superfluids theoretically and examine its consequences in numerical simulations.

Friday, March 6, 2015 8:00AM - 11:00AM — Session Y36 DAMOP: New Developments in Atomic, Molecular, and Optical Physics 211 - Nathan Gemelke, Pennsylvania State University

8:00AM Y36.00001 ABSTRACT WITHDRAWN —

8:12AM Y36.00002 Emission spectrum of atoms in a harmonic trap. POOJA SINGH, YURI ROSTOVTSIV, University of North Texas — We consider an excited atom in a harmonic trap. The evolution of quantum atomic states is theoretically studied under adiabatic approximation. The emission spectra for trapped atoms are calculated. We have show interference effects as well as trapping effect in a trap that has a size larger than the wavelength of radiation.

8:24AM Y35.00003 When is the mode-summation method of calculating van der Waals force valid? ARVIND NARAYANASWAMY, Columbia University — Most calculations of van der Waals forces and Casimir forces can be categorized as variations of two “proto methods”: (1) Lifshitz theory, and (2) mode summation method. In the Lifshitz theory, by which I include the subsequent generalization by Dzyaloshinskii, Lifshitz, and Pitaevskii [Adv. Phys. 10, 165 (1961); See also Zheng and Narayanaswamy, Phys. Rev. A 83, 042504 (2011)] the dispersion force is expressed in terms of the (dyadic) Green’s function of the vector Helmholtz equation. In the mode summation method [see Casimir, Proc. Kon. Ned. Akad. Wetensch. 51, 793 (1948); Van Kampen, Nijboer, and Schram, Phys. Lett. A 26, 307 (1968)], the free energy of a configuration of objects is expressed in terms of the sum of the free energies of each of the possible electromagnetic modes. The derivative of this free energy with respect to variation of relative positions between the objects yields the force between two objects. However, we raised questions about the validity of the mode summation method when calculating van der Waals forces in dissipative media [see Narayanaswamy and Zheng, Phys. Rev. A 88, 012502 (2013) and Ninham, Parsegian, and Weiss, J. Stat. Phys. 2, 323 (1970)]. In this talk, I want to start a discussion about the validity of the mode summation method.

8:36AM Y36.00004 Landau-Zener transitions mediated by an environment in the open-multistate model. SAVANNAH GARSON, Osaka Prefecture University, AMRO DODIN, LENA SIMINE, DVIRA SEGAL, University of Toronto — We study Landau-Zener transitions between two linearly driven states with the addition of a shared discretized continuum. The continuum allows for population decay from the initial state as well as indirect transitions. The probability of nonadiabatic transition in this model preserves the standard Landau-Zener functional form apart from a shift in the usual exponential factor, reflecting population transfer into the continuum. We provide an intuitive explanation for this behavior assuming individual, independent transitions between pairs of states. In contrast, the ground state survival probability at long time shows a novel, non-monotonic, functional form with an oscillatory behavior in the sweep rate at low sweep rate values. We envision our system as a simplified model regarding memory preservation in a quantum dot as the dot interacts with the surrounding environment.


8:48AM Y36.00005 ABSTRACT WITHDRAWN —

9:00AM Y36.00006 Near field heat transfer in superlattices1. RAUL ESQUIVEL-SIRVENT, Instituto de Fisica, UNAM — I present a theoretical calculation of the near field heat transfer between super lattices made of alternative layers of both metallic and semiconductor materials. The calculation of the near field transfer requires the knowledge of the reflectivities, that are obtained by calculating the surface impedance of the super lattice. Depending on the periodicity of the lattice and the dielectric function of the materials the near field heat transfer can be modulated or engineered. Additional control on the heat transfer is achieved by introducing defects in the superlattice. The results are extended to include photonic hypercrystals that effectively behave like a hyperbolic metamaterial even in the near field (1), where the tuning of the heat transfer is modified by (1) E. E. Narimanov, Phys. Rev. X 4, 041014 (2014).

1Partial Support from DGAPA-UNAM project IN 111214

9:12AM Y36.00007 ABSTRACT WITHDRAWN —
9:24AM Y36.00008 Neutral Atom Nanolithography Using a Pulsed Magnetic Lens1, ERIK ANCIAX, RODRIGO CASTILLO-GARZA, JAMIE CARDNER, MARK RAIZEN, UT Austin — We present the status of a method of neutral atom lithography that achieves sub-10nm resolution. This method is based on the nanoscale imaging of a beam of metastable atoms with an aberration-corrected hexapole lens. The lens creates a magnetic field gradient that increases with the distance from the center of the lens so as to focus divergent low field seeking atoms toward a single focal spot past the lens. The scheme takes advantage of the narrow velocity distribution of a pulsed supersonic beam as well as an optical pumping and cooling scheme that modifies the magnetic state of the atoms and further reduces its velocity dispersion. This method can be used not only to pattern but to spectroscopically probe surfaces with spatial resolution below 10nm.

1M. G. R. acknowledges support from the U.S. National Science Foundation, the R. A. Welch Foundation (grant F-1258), and the Sid W. Richardson Foundation.

9:36AM Y36.00009 Proposal of a new type of optical parametric amplifier for efficient X-ray generation, WAYNE HUANG, Texas A&M University, ROGER BACH, HERMAN BATELAAN, University of Nebraska-Lincoln, MARLAN SCULLY, Texas A&M University — With an optical parametric amplifier (OPA), one can transfer energy from the pump light to the seeded light via sum parametric resonance (also called parametric down conversion). In this process, coherent light with frequency lower than the pump is generated. Using infrared as pump, one can obtain light in the mid/far-infrared regime. In contrast to OPA, the quantum amplification by super-radiant emission of radiation (QASER) suggests that energy transfer can occur when the pump frequency is equal to the difference of the seeded frequencies [1]. Thus, coherent light with frequency much higher than the pump can be generated. The physical mechanism behind QASER is called difference parametric resonance. We propose to build a new type of optical parametric amplifier based on this concept and transfer energy from infrared to X-ray. In this presentation, I would like to capture the main idea of QASER by discussing the difference parametric resonance in a coupled oscillating system. A perturbation analysis is given to provide insight into the mechanism as well as the conditions for experimental realization. We will also briefly discuss realizations of difference parametric resonance in electronic, mechanical, and acoustic systems. [1] M. O. Scully et al., Phys. Rev X 3, 041001 (2013).

48AM Y36.00010 Measured Atomic Ground State Polarizabilities of 35 Metallic Elements1, JOHN INDERGAARD, LEI MA, BAIQIAN ZHANG, ILIA LARKIN, Georgia Inst of Tech, RAMIRO MORO, Cameron University, Oklahoma, WALTER DE HEER, Georgia Inst of Tech — Advanced pulsed cryogenic molecular beam electric deflection methods utilizing a position-sensitive mass spectrometer and 7.87 eV ionizing radiation were used to measure the polarizabilities of more than half of the metallic elements in the periodic table for the first time. These measurements increase the total number of experimentally obtained atomic polarizabilities from 23 to 57. Concurrent Stern-Gerlach deflection measurements verified the ground state condition of the measured atoms. Generating higher temperature beams allowed for the comparison of relative populations of the ground and excited states in order to extract the true temperature of the atomic beam, which followed the nominal temperature closely over a wide temperature range. Comparison of newly measured polarizabilities with state-of-the-art calculations exposes significant systematic and isolated discrepancies throughout the periodic table.

1Cluster Lab at Georgia Tech
2Now at University of Maryland in the PhD program
3Principal investigator

10:00AM Y36.00011 Complex time contours in tunnel ionization and low-energy structures1, EMILIO PISANTY, MISHA IVANOV, Imperial College London — In tunnel ionization, a strong low-frequency laser field removes an electron from an atom by setting up a slowly-varying potential energy barrier that the electron can tunnel through. During its subsequent oscillations in the laser field, the electron can revisit the neighborhood of the remaining ion one or more times. Frequently, this is a soft recollision which affects the momentum distribution, although more substantial effects can happen. We use the Analytical R-Matrix theory to investigate the effect of these soft recollisions, focusing on low drift momenta, where the laser-induced trajectory has a turning point near the nucleus. Our framework provides a complex-valued trajectory perspective on the electron propagation, from first principles. We show that the presence of the Coulomb interaction, which is responsible for the soft recollisions, forbids certain common choices of contour within the complex time plane, and we describe an algorithm for safely circumventing the associated branch cuts. We find quantum analogues to the classical turning points near the ion, and we investigate their relation to the recently-discovered low-energy and very-low-energy structures in above-threshold ionization.

1We acknowledge funding from CONACYT (Mexico) and the MC-ITN CORINF network.

10:12AM Y36.00012 Fast spectrophotometry with compressive sensing, DAVID STARLING, IAN STORER, Penn State University — Spectrophotometers and spectrometers have numerous applications in the physical sciences and engineering, resulting in a plethora of designs and requirements. A good spectrophotometer balances the need for high photometric precision, high spectral resolution, high durability and low cost. One way to address these design objectives is to take advantage of modern scanning and detection techniques. A common imaging method that has improved signal acquisition speed and sensitivity in limited signal scenarios is the single pixel camera. Such cameras utilize the sparsity of a signal to sample below the Nyquist rate via a process known as compressive sensing. Here, we show that a single pixel camera using compressive sensing algorithms and a digital micromirror device can replace the common scanning mechanisms found in virtually all spectrophotometers, providing a very low cost solution and improving data acquisition time. We evaluate this single pixel spectrophotometer by studying a variety of samples tested against commercial products. We conclude with an analysis of flame spectra and possible improvements for future designs.

10:24AM Y36.00013 Red Shifted Absorbance of A-site Substituted Bismuth Titanate Pyrochlore: Characterization and Stability Analysis from First Principles1, CEDRIC MAYFIELD, MUHAMMAD HUDA, Department of Physics, University of Texas at Arlington — Transition metal inclusion has enhanced photocatalytic activity of bismuth titanate (Bi2Ti2O7) up to an impurity threshold concentration. Beyond the threshold, spectral absorbance is continually red shifted but increased photocurrent is not reciprocated. We investigated, from first principles, the origin of decreased photocurrent in modified Bi2Ti2O7 (BTO) by calculating the electronic structures of a representative set of doping configurations and by performing a phase stability analysis of the doping. We report our theoretical/computational strategy of analyzing free energy space and show an explicit dependence of pure phase synthesis on changes in free energy. Also, we present a probability distribution of the doping configurations based on formation enthalpy to better understand the nature of doping in BTO. We found that transition metal substitutions are favorable at the A-sites due to unchanging coordination with O ions.

1This work is supported by National Science Foundation, award no. 1133672.
10:36AM Y36.00014 Dopant concentration dependent optical and X-Ray induced photoluminescence in Eu$^{3+}$ doped La$_2$Zr$_2$O$_7$ 1, MADHAB POKHREL, Univ of Texas, Pan American, MIKHAIL BRIK, University of Tartu, YUANBING MAO, Univ of Texas, Pan American — Herein, we will be presenting the dopant (Eu) concentration dependent high density La$_2$Zr$_2$O$_7$ nanoparticles for optical and X-ray scintillation applications by use of X-ray diffraction, Raman, FTIR, scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray excited photoluminescence (PL). Several theoretical methods have been used in order to investigate the structural, electronic, optical, elastic, dynamic properties of Eu doped La$_2$Zr$_2$O$_7$. It is observed that Eu: La$_2$Zr$_2$O$_7$ shows an intense red luminescence under 258, 322, 394 and 465 nm excitation. The optical intensity of Eu: La$_2$Zr$_2$O$_7$ depends on the dopant concentration of Eu$^{3+}$. Following high energy excitation with X-rays, Eu: La$_2$Zr$_2$O$_7$ shows an atypical Eu PL response (scintillation) with a red emission. The intense color emission of Eu obtained under 258 nm excitation, the X-ray induced luminescence property along with reportedly high density of La$_2$Zr$_2$O$_7$, makes these nanomaterials attractive for optical and X-ray applications.

1The authors thank the support from the Defense Threat Reduction Agency (DTRA) of the U.S. Department of Defense (award #HDTRA1-10-1-0114)

10:48AM Y36.00015 Semi-Classical and Quantum-Field Descriptions for the Non-Linear Electromagnetic Response of Many-Electron Systems1, VERNE JACOBS, Naval Research Laboratory — Semi-classical and quantum-field descriptions for the non-linear electromagnetic response relevant to resonant pump-probe optical phenomena in quantized many-electron systems are formulated within a general reduced-density-matrix framework. Time-domain (equation-of-motion) and frequency-domain (resolvent-operator) formulations are developed in a unified and self-consistent manner. A preliminary semi-classical perturbation treatment of the electromagnetic interaction is adopted, in which the electromagnetic field is described as a classical field satisfying the Maxwell equations. It is emphasized that the development of a quantized-field approach will be essential for a fully self-consistent quantum-mechanical formulation. Compact Liouville-space operator expressions are obtained for the general (n'th order) non-linear electromagnetic-response tensors describing moving many-electron atomic systems. The tetradic matrix elements of the Liouville-space self-energy operators are evaluated for environmental collisional and radiative interactions.

Friday, March 6, 2015 8:00AM - 11:00AM
Session Y39 GQI: Superconducting Cavities and Resonators 213AB - Jose Aumentado, NIST

8:00AM Y39.00001 Microwave mode structure of superconducting metamaterial resonators, HAOZHI WANG, FRANCISCO ROUXINOL, MATTHEW LAHAYE, BRITTON PLOURDE, Syracuse University — Arrays of lumped circuit elements can be used to form metamaterial resonant structures that exhibit novel behavior compared to resonators made from conventional distributed transmission lines. By engineering the parameters and configurations of the lumped elements composing the unit cell of such a metamaterial resonator, one can generate spectra with wide stop-bands as well as pass-bands with dense microwave modes. If the metamaterials are fabricated from superconducting traces, the losses can be low enough to allow for these dense modes to be resolved and potentially coupled to quantum systems, such as superconducting qubits. We will present our low-temperature measurements of a variety of superconducting metamaterial resonators and we will compare these with numerical simulations of the microwave properties.

8:12AM Y39.00002 Lattice waveguide QED: many-body interactions by dissipation, BAPTISTE ROYER, KEVIN LALUMIÈRE, ARNE GRIMSMO, ALEXANDRE BLAIS, Département de Physique, Université de Sherbrooke, Sherbrooke, Québec, Canada — In waveguide QED, superconducting qubits acting as artificial atoms are coupled to a 1D superconducting transmission line playing the role of common bath for the qubits. By controlling their effective separation, it is possible to engineer various types of dissipation-induced interactions between the qubits. In this talk, we consider the situation where multiple superconducting qubits are coupled to a lattice of superconducting transmission lines. Depending on the choice of lattice, the qubits exhibit a rich variety of interactions. We present a Markovian master equation framework to describe these systems, and discuss results obtained for simple lattices.

8:24AM Y39.00003 Universal Control of an Oscillator with Dispersive Coupling to a Qubit, STEFAN I. KRASTANOV, CHAO SHEN, VICTOR Y. ALBERT, REINIER W. HEERES, BRIAN M. VLASTAKIS, ROBERT J. SCHOELKOPF, LIANG JIANG, Yale University — We investigate quantum control of an oscillator mode that dispersively couples to an ancillary qubit. In the strong dispersive regime we can drive the qubit conditioned on the selected number states of the oscillator, which enables selective number-dependent arbitrary phase (SNAP) operation and universal control of the oscillator. Based on our proof of universal control, we provide explicit constructions for arbitrary state preparation and arbitrary unitary operation of the oscillator. Moreover, we present an efficient procedure to prepare the number state $|n⟩$ using only $O(\sqrt{n})$ operations. We also compare our scheme with known quantum control protocols for coupled qubit-oscillator systems. We point out that this universal control scheme of the oscillator can be readily implemented using superconducting circuits.

8:36AM Y39.00004 A Quasi-3D, Purcell-Filtered Hardware Module for Quantum Information, C. AXLINE, M. REAGOR, K. SHAIN, P. REINHOLD, T. BRECHT, E. HOLLAND, C. WANG, R. HEERES, L. FRUNZIO, R.J. SCHOELKOPF, Department of Applied Physics, Yale University — The advent of 3D circuit quantum electrodynamics has provided an ultra-low-loss environment for superconducting qubits, boosting qubit coherences over 100 microseconds and linear resonator lifetimes above 10 milliseconds. Planar devices, however, allow lithographic control of parameters and suggest greater scalability. We have developed a single-chip, seamless-cavity architecture that answers the call[1] for a modular computational element, comprising 3D transmon, fast, Purcell-filtered readout, and long-lived storage cavity. This design incorporates advantages of both 2D and 3D architectures. It also serves as a novel testbed for qubit loss mechanisms, as resonator and qubit modes have similar material participations. Initial results—T1 and T2 comparable to the best 3D transmons—shift blame away from the metal-substrate interfaces widely considered to be the limiting loss channel in current-generation transmons, and further experiments using this system will probe these losses more carefully. We propose several modifications and extensions to these modules to miniaturize the design and to build more sophisticated quantum systems. [1] M. H. Devoret and R. J. Schoelkopf, Science 8 March 2013: 339 (6124), 1169-1174.

1Work supported by: IARPA, ARO, ONR, and NSF.
8:48AM Y39.00005 Cavity state manipulation using a dispersively coupled qubit. REINIER HEERES, BRIAN VLASTAKIS, ERIC HOLLAND, STEFAN KRASTANOV, VICTOR V. ALBERT, CHAO SHEN, LIANG JIANG, ROBERT SCHOELKOPF, Yale University — The large available Hilbert space and high coherence of cavity resonators makes them an interesting resource in quantum information processing. For example, several schemes exist to encode a logical qubit in such a harmonic oscillator in a way that would be protected against certain kinds of errors. Here we demonstrate a method to manipulate a cavity state using a far off-resonantly coupled qubit, using only linear controls and a gate we call the Selective Number Arbitrary Phase (SNAP) gate. This gate allows to impart an arbitrary phase on each Fock-state component of the cavity. We show how we can use these tools to correct for the effects of Kerr-evolution as well as how to create a single-photon Fock state. Our scheme can be generalized to arbitrary cavity state creation and even allows to construct arbitrary unitary operators to give universal control of the oscillator.

9:00AM Y39.00006 Quantum dynamics of an electromagnetic mode that cannot contain N photons. EMMANUEL FLURIN, LANDRY BRETHEAU, PHILIPPE CAMPAGNE, FRANCOIS MALLET, BENJAMIN HUARD, Laboratoire Pierre Aigrain, QELEC TEAM — Electromagnetic modes are instrumental for realizing quantum physics experiments and building quantum machines. In this experiment, we demonstrate a new way to manipulate these modes by effectively controlling their phase space. By preventing access to a single energy level, the dynamics of the field is dramatically changed. Here, it was possible to keep the mode from containing a number of photons N, which was arbitrarily chosen between 2 and 5. Under this constraint, and starting in its ground state, a resonantly driven mode is confined to levels 0 to N-1. The level occupation is then found to oscillate in time, similarly to an N-level system. Performing a direct Wigner tomography of the field reveals its non-classical features. In particular, at half period in the evolution, it resembles a “Schrödinger cat state.” This fine control of the field in its phase space enables innovative applications in quantum information and metrology.

9:12AM Y39.00007 Exploration of sapphire whispering gallery mode resonator crystals for use as a quantum computing memory. ADAM SIROIS, Univ of Colorado - Boulder, MANUEL CASTELLANOS-BELTRAN, NIST-Boulder, DANIEL CREEDON, Univ. of W. Australia, RAYMOND SIMMONDS, JOHN TEUFEL, NIST-Boulder, MICHAEL TOBAR, Univ. of W. Australia, JOSE AUGMENTADO, NIST-Boulder — Sapphire whispering gallery mode (WG) resonators are a known to support multiple, high-quality factor modes in a compact volume at microwave frequencies. In this talk we demonstrate the ability to parametrically couple whispering gallery modes by use of a Josephson-junction-based coupling element. In this manner we implement a ‘storage and retrieval’ protocol which may be useful for storing several complex microwave quantum states in small volumes.

9:24AM Y39.00008 Fabrication of transmon qubits embedded in superconducting whispering gallery mode resonators. K. SERNIAK, Z.K. MINEV, I.M. POP, L. FRUNZIO, R.J. SCHOELKOPF, M.H. DEVORET, Department of Applied Physics, Yale University — Superconducting whispering gallery mode resonators (WGMs) can confine up to 98% of two high quality modes in lossless vacuum [APL 103, 142604]. We have fabricated new WGMR-based devices using standard lithography techniques and in which transmon qubits were integrated. The advantages of this transmon-resonator configuration are i) the possibility to perform a targeted study of thin-film quality factor across different methods and steps of fabrication and ii) precise control of the Hamiltonian parameters.

3 Work supported by: IARPA, ARO, and ONR.

9:36AM Y39.00009 Coherences of transmon qubits embedded in superconducting whispering gallery mode resonators. Z.K. MINEV, K. SERNIAK, IOAN POP, Z. LEGHTAS, K. SLIWA, L. FRUNZIO, R. SCHOELKOPF, MICHEL DEVORET, Department of Applied Physics, Yale University — We describe the design and measurement of a planar uperconducting two-resonator one-qubit device. The two resonators are realized in a hardware-efficient way by the differential modes of a superconducting whispering gallery mode resonator [APL 103, 142604]. This device forms an integrated basis for a quantum memory [New J. Phys. 16, 045014 2014].

3 Work supported by: IARPA, ARO, and ONR.

9:48AM Y39.00010 Engineering non-linear resonator mode interactions in circuit QED by continuous driving: Introduction. WOLFGANG PFAFF, MATTHEW REAGOR, REINIER HEERES, NISSIM OFEK, KEVIN CHOU, JACOB BLUMOFF, ZAKI LEGHTAS, STEVEN TOUZARD, KATRINA SLIWA, ERIC HOLLAND, STEFAN KRASTANOV, LUIGI FRUNZIO, MICHEL DEVORET, LIANG JIANG, ROBERT SCHOELKOPF, Yale Univ — High-Q microwave resonators show great promise for storing and manipulating quantum states in circuit QED. Using resonator modes as such a resource in quantum information processing applications requires the ability to manipulate the state of a resonator efficiently. Further, one must engineer appropriate coupling channels without spoiling the coherence properties of the resonator. We present an architecture that combines millisecond lifetimes for photonic quantum states stored in a linear resonator with fast measurement provided by a low-Q readout resonator. We demonstrate experimentally how a continuous drive on a transmon can be utilized to generate highly non-classical photonic states inside the high-Q resonator via effective non-linear resonator mode interactions. Our approach opens new avenues for using modes of long-lived linear resonators in the circuit QED platform for quantum information processing tasks.

10:00AM Y39.00011 Engineering non-linear resonator mode interactions in circuit QED by continuous driving: Manipulation of a photonic quantum memory. MATTHEW REAGOR, WOLFGANG PFAFF, REINIER HEERES, NISSIM OFEK, KEVIN CHOU, JACOB BLUMOFF, ZAKI LEGHTAS, STEVEN TOUZARD, KATRINA SLIWA, ERIC HOLLAND, VICTOR V. ALBERT, LUIGI FRUNZIO, MICHEL H. DEVORET, LIANG JIANG, ROBERT J. SCHOELKOPF, Departments of Applied Physics and Physics, Yale University — Recent advances in circuit QED have shown great potential for using microwave resonators as quantum memories. In particular, it is possible to encode the state of a quantum bit in non-classical photonic states inside a high-Q linear resonator. An outstanding challenge is to perform controlled operations on such a photonic state. We demonstrate experimentally how a continuous drive on a transmon qubit coupled to a high-Q storage resonator can be used to induce non-linear dynamics of the resonator. Tailoring the drive properties allows us to cancel or enhance non-linearities in the system such that we can manipulate the state stored in the cavity. This approach can be used to either counteract undesirable evolution due to the bare Hamiltonian of the system or, ultimately, to perform logical operations on the state encoded in the cavity field. Our method provides a promising pathway towards performing universal control for quantum states stored in high-coherence resonators in the circuit QED platform.
10:12AM Y39.00012 Demonstrating real-time feedback that enhances the performance of measurement sequence with cat states in a cavity , N. OFEK, A. PETRENKO, Y. LIU, B. VLASTAKIS, Yale University, L. SUN, Yale University, Tsinghua University, Beijing, China, Z. LEGHTAS, R. HEERES, K.M. SLIWA, Yale University, M. MIRRAHIMI, Yale University; INRIA Paris-Rocquencourt, L. JIANG, M.H. DEVORET, R.J. SCHOELKOFF, Yale University — Real-time feedback offers not just the convenience of streamlined data acquisition, but is an essential element in any quantum computational architecture that requires branching based on measurement outcomes. State-preparation, mitigating the effects of qubit decoherence, and recording the trajectories of quantum systems are just a few of the many potential applications of real-time feedback. Photon number parity measurements of cat states in superconducting resonators are a particularly useful platform for demonstrating the clear advantages of having sophisticated feedback schemes to enhance the performance a proposed error-correction protocol [Leghtas et.al. PRL 2013]. In a cQED architecture, where a transmon qubit is coupled to two superconducting cavities, we present a field-programmable gate array (FPGA) device capable of making decisions and calculations with latency times far shorter than the lifetimes of any of the system’s constituents. This level of performance opens the door to realizing many complex, previously unfeasible, experiments in superconducting qubit systems.

10:24AM Y39.00013 Utilizing photon number parity measurements to demonstrate quantum computation with cat-states in a cavity , A. PETRENKO, N. OFEK, B. VLASTAKIS, Yale University, L. SUN, Yale University, Tsinghua University, Beijing, China, Z. LEGHTAS, R. HEERES, K.M. SLIWA, Yale University, M. MIRRAHIMI, Yale University; INRIA Paris-Rocquencourt, L. JIANG, M.H. DEVORET, R.J. SCHOELKOFF, Yale University — Realizing a working quantum computer requires overcoming the many challenges that come with coupling large numbers of qubits to perform logical operations. These include improving coherence times, achieving high gate fidelities, and correcting for the inevitable errors that will occur throughout the duration of an algorithm. While impressive progress has been made in all of these areas, the difficulty of combining these ingredients to demonstrate an error-protected logical qubit, comprised of many physical qubits, still remains formidable. With its large Hilbert space, superior coherence properties, and single dominant error channel (single photon loss), a superconducting 3D resonator acting as a resource for a quantum memory offers a hardware-efficient alternative to multi-qubit codes [Leghtas et al. PRL 2013]. Here we build upon recent work on cat-state encoding [Vlastakis et. al. Science 2013] and photon-parity jumps [Sun et al. 2014] by exploring the effects of sequential measurements on a cavity state. Employing a transmon qubit dispersively coupled to two superconducting resonators in a cQED architecture, we explore further the application of parity measurements to characterizing such a hybrid qubit/cat state architecture. In so doing, we demonstrate the promise of integrating cat states as central constituents of future quantum codes.

10:36AM Y39.00014 Continuous generation and stabilization of Schrödinger cat states in a quantum circuit , A. ROY, Z. LEGHTAS, A.D. STONE, M.H. DEVORET, Department of Applied Physics, Yale University, M. MIRRAHIMI, Department of Applied Physics, Yale University and INRIA Paris Rocquencourt — While dissipation is widely considered as being harmful for quantum coherence, it can, when properly engineered, lead to the stabilization of non-trivial pure quantum states. Deterministic generation of non-classical states like Schrödinger cat states is one of the key ingredients in performing universal quantum computation. We theoretically propose a scheme, adapted to superconducting quantum circuits, for continuous generation and stabilization of these states in a cavity using dissipation engineering. We first generate these states inside a high-Q cavity by engineering its dissipation with a bath that only exchanges photons in pairs. We then stabilize these transient states against single-photon decay using a second engineered bath. The single-photon stabilization is autonomous, and exploits the photon-number-dependent frequency-s splitting due to Kerr interactions in the strongly dispersive regime of circuit QED. We present analytical and numerical results demonstrating the robustness of the scheme and its amenability to immediate experimental implementation.

Work supported by ARO

10:48AM Y39.00015 Deterministic amplification for cat-state engineering in circuit-QED , JAEWOO JOO, ATI and Physics Department, Univ of Surrey, DANIEL OI, Physics Department, University of Strathclyde, MATTHEW ELLIOTT, ERAN GNROSSAR, ATI and Physics Department, Univ of Surrey, TIMOTHY SPILLER, York Centre for Quantum Technologies, Department of Physics, University of York — We propose a novel implementation scheme of amplifying the size of Schrödinger cat states in superconducting circuits. While the amplification method in quantum optics is normally probabilistic, our scheme can be performed deterministically in circuit-QED. Using adiabatic methods and optimal control, we demonstrate that the amplification operation can be built deterministically in a system of a transmon qubit strongly coupled with a cavity. This amplification tool will in particular open the potential of continuous-variable nonclassical states toward practical quantum technologies, for example stabilization of cat-type states and continuous-variable teleportation.

Friday, March 6, 2015 8:00AM - 11:00AM —
Session Y41 DPOLY: Focus Session: Biopolymers I: Biohybrids, Biointerfaces, and Modeling
214A - Bradley D. Olsen, Massachusetts Institute of Technology

8:00AM Y41.00001 Multiscale modelling of polymers at soft-bio interface , PAOLA CARBONE
The University of Manchester — The behaviour of polymers at a liquid/liquid interface has become increasingly technologically important in recent years. For example, many of the self-assembly processes involving macromolecules occur at such interfaces and one of the most common chemical processes used to produce polymer nanoparticles—the solvent displacement method— involves the diffusion of the polymer chains from a good solvent, where the polymer initially dissolves, to a non-solvent where the nanoparticles are formed. Finally, polymer-based drug nanocarriers (either nanoparticles or micelles) are becoming increasingly popular in drug delivery and their behaviour at fluid interfaces (such as a lipid/water boundary) should be properly understood in order to predict their biological activity. Here we show how using a multiscale approach it is possible to gain a detailed picture of the thermodynamic stability of homo- and co-polymers at fluid interfaces spanning from universal rules valid to any polymer systems at high dilution to the specific cases of amphiphilic linear and branched polymers.

School of Chemical Engineering and Analytical Science

8:36AM Y41.00002 Self-Assembly of DNA–Graft Copolymer Nanoparticles , ZONGHUI WEI, Northwestern University, YONG REN, JOHN-MICHAEL WILLIFORD, HAI-QUAN MAO, Johns Hopkins University, ERIK LJUJTEN, Northwestern University, NORTHWESTERN UNIVERSITY COLLABORATION, JOHNS HOPKINS UNIVERSITY COLLABORATION — Self-assembled DNA–copolymer nanoparticles are promising gene delivery systems due to their high biocompatibility. Notably, such nanoparticles can exhibit a variety of morphologies. Previously, we demonstrated that the nanoparticle shape can be tuned through variation of solvent polarity in a solution of DNA and block copolymers. Moreover, we confirmed that this shape can influence transfection efficiency [1]. In terms of ease of manufacturing as well as tunability of the system, it is important to explore the possibility of employing other types of condensing agents. Here, we report on the use of polyelectrolytes with grafted PEG side chains, which offer facile synthesis and an additional control parameter in the form of grafting density. Via a combination of experiments and molecular dynamics simulations we demonstrate that a high degree of shape control of the micellar nanoparticles can indeed be achieved through variation of the density and length of the grafted side chains. [1] Jiang, X.; Qu, W.; Pan, D.; Ren, Y.; Williford, J. M.; Cui, H. G.; Lujten, E.; Mao, H. Q. Advanced Materials 25, 227–232 (2013).
8:48AM Y41.00003 Monodisperse dendrimeric phytoglycogen nanoparticles in water act as hard sphere colloidal dispersions. JOHN DUTCHER, ERZSI PAPP-SZABO, CARLEY MIKI, University of Guelph — Phytoglycogen is a highly branched polysaccharide that is very similar to the energy storage molecule glycogen. We have isolated monodisperse phytoglycogen nanoparticles from corn and these particles are attractive for applications in the cosmetic, food, and beverage, and biomedical industries. Many of these promising applications are due to the special interaction between the nanoparticles and water, which results in: (1) high solubility; (2) low viscosity and high stability in aqueous dispersions; and (3) a remarkable capacity to sequester and retain water. We have used cone-and-plate and concentric cylinder rheometry to measure the dependence of the zero shear viscosity of aqueous dispersions of phytoglycogen on the phytoglycogen concentration. We find that the nanoparticles behave like hard spheres in water, with the viscosity diverging for volume fractions very close to that corresponding to randomly packed hard spheres. This simple system provides an ideal platform for detailed testing of theories of colloidal glasses and jamming.

9:00AM Y41.00004 Tracing lipids and their association with keratin in the adhesive gecko setae by NMR Spectroscopy. DHARAMDEEP JAIN, ALYSSA.Y. STARK, PETER H. NIEWIAROWSKI, TOSHIKAZU MIYOSHI, ALI DHINOJWALA, University of Akron — Numerous examples exist in nature where the coexistence of lipids and keratin is prominent. Examples include cell membranes, epidermis, avian feathers, wool, insect cuticle and the adhesive hairy features known as “setae” on the gecko toe. Until recently the setae were only considered to be composed of keratinous material. Given the prevalence of lipid-keratin associations in nature however, it is perhaps not surprising that phospholipids were found in the setae, and interestingly, in the form of a footprint after a gecko moves along a surface. However, the organization and the molecular-level behavior of lipids and keratin in the setae is still not known. Here, we demonstrate the use of NMR spectroscopy to detect lipids and understand their association with keratin in the molts termed as “sheds” from the toe pad and the non-adhesive regions of the epidermal skin. Our results show a distribution of similar lipids in both the skin and toe shed but with different dynamics at a molecular level. The study can help us understand the system better both biologically and for the design of better synthetics, but our findings may also have a larger impact on the recurring observations of lipids in many popular biomaterials and biological systems.

9:12AM Y41.00005 ABSTRACT WITHDRAWN

9:24AM Y41.00006 Deposition and Grafting of Collapsed Elastin-Like Co-Polypeptides on Silicon. ROBIN MAYS, North Carolina State University, JULIE ALBERT, Tulane University, SARAH MACEWAN, Duke University, MICHAEL DICKY, North Carolina State University, ASHUTOSH CHILKOTI, Duke University, JAN GENZER, North Carolina State University — Protein-based polymers offer the potential for responsive, bio-compatible, well-defined (molecular weight and sequence) systems. Elastin-like peptides (ELPs) are well suited for solution-based biomedical applications, including drug delivery and biomolecular purification. In order to use ELPs for stimuli-responsive surfaces, a detailed understanding of deposition conditions and behavior is instrumental. We crafted diblock ELPs with lower critical solution temperature (LCST) behavior on silicon surfaces. We synthesized 33kDa ELPs through genetic expression in bacteria with recombinant DNA technology. The diblock copolypeptides we used have a hydrophobic block (VPGVG) and a hydrophilic block (VPVSG), with each block having a different LCST. These diblock ELPs form micelles in solution when heated above the transition temperature of the hydrophobic block. We can graft either fully solvated ELPs or micellar ELP structures to an EDC/NHS activated surface. Our findings indicate a surprising stability of ELP aggregation on surfaces. We investigated the effects of time, temperature, and grafting block on the morphology, thickness, and water contact angle of our surfaces. Using atomic force microscopy, we studied the morphology of the deposited ELPs both in air and water.

9:36AM Y41.00007 Nanostructure Formation in Fusion Protein Block Copolymers Containing A Globular Protein Block. BRADLEY OLSEN, GUOKUI QIN, MATTHEW GLASSMAN, CHRISTOPHER LAM, DONGSOOK CHANG, MIT, ERIC SCHIABLE, ALEXANDER HEXEMER, Lawrence Berkeley Lab — Fusion proteins provide an elegant method for the synthesis of precisely defined block copolymers, where the use of molecular biology techniques enables monodisperse synthesis, precise control over block length and arrangement, and the incorporation of complex folded chain shapes and biofunctional structures. Here, we show that a block copolymer that contains a globular protein block and a coil-like protein block can self-assemble into a nanostructured material despite the chemical similarity between the two halves of the molecule. Using model polymers composed of the red fluorescent protein mCherry and an elastin-like polypeptide (ELP), the phase behavior of a simple linear fusion is shown to resemble that of protein-polymer conjugates. Molecular biology also enables the preparation of well-controlled double tail fused structures, and the self-assembly of these molecules shows that the chain topology of the fusion protein has a large impact on its self-assembly. At the same molar mass and composition, the double tailed structures self-assemble at a lower concentration and exhibit a greater number of order-order transitions than their single tailed counterparts. In addition, the double tailed fusions retained a higher fraction of functional protein in the final material.

9:48AM Y41.00008 Tailoring selectivity and flux in interior functionalized peptide nanotubes through self-assembly. SINAN KETEN, LUIS RUIZ, Northwestern University — Self-assembly of cyclic peptide nanotubes (CPNs) in polymer thin films has opened up the possibility to create separation membranes with tunable nanotubes that can differentiate molecules at the sub-nanometer level. Recent studies have demonstrated that the interior chemistry of the CPNs can be tailored by inserting functional groups in the nanopore lumen (mCPNs) (Hourani et al. JACS, 2011). Through theory and multi-scale MD simulations, here we explain how the stacking ordering of binary mixtures of functional CPs can be prescribed using the entropic elasticity of conjugated polymers (Ruiz & Keten, Soft Matter, 2014). The linear self-similar coarsening growth mechanism, kinetic trapping and its effects on stacking sequences will be demonstrated (Ruiz & Keten, J. Phys. Chem. Lett., 2014). Building on these insights, we present a new approach to addressing the challenge of boosting water flux and ion selectivity simultaneously, specifically by inserting two different types of functional microgroups in the lumen, and by controlling CP stacking order. Simulations elucidate how functional groups inspired from biological amino acids influence the transport of water and ions through mCPNs. We find mixing functional groups to tune partial charge distributions and pore size can be used to boost flux and selectivity (Ruiz & Keten, Nanoscale, 2014). Our computational thought experiments lay the foundation for bioinspired principles to discover artificial nanochannels for separation applications.

10:00AM Y41.00009 Coarse-grained modelling of RNA. PETR SULC, The Rockefeller University, FLAVIO ROMANO, THOMAS OULDRIDGE, JONATHAN DOYE, ARD LOUIS, University of Oxford — We present a new, nucleotide-level model for RNA, oRNA, based on the coarse-graining methodology recently developed for the oxDNA model of DNA. The model is designed to reproduce structural, mechanical and thermodynamic properties of RNA, and the coarse-graining level aims to retain the relevant physics for RNA hybridization and the structure of single- and double-stranded RNA. In order to explore its strengths and weaknesses, we test the model in a range of nanotechnological and biological settings. Applications explored include the folding thermodynamics of a pseudoknot, the formation of a kissing loop complex, the unzipping of a hairpin motif, and the thermodynamics and kinetics of RNA strand-displacement reaction. We argue that the model can be used for efficient simulations of the structure of systems with thousands of base pairs, and for the assembly of systems of up to hundreds of base pairs. The source code implementing the model is released for public use at dna.physics.ox.ac.uk.

The work presented here is funded by the National Science Foundation (DMREF award CBET-1234305).
10:12AM Y41.00010 Rationally Designed Random Heteropolymer Surfactants for the Encapsulation and Stabilization of Proteins in Organic Solvents, BRIAN PANGANIBAN, University of California, Berkeley, BAOFLI QIAO, Northwestern University, MONA OBADIA, Université Claude Bernard Lyon 1, MONICA OLVERA DE LA CRUZ, DOMINIC DROCKENMULLER, Université Claude Bernard Lyon 1, TING XU, University of California, Berkeley — Stabilizing proteins in organic solvents can provide opportunities to overcome challenges in many areas, such as biosynthetic catalysis of hydrophobic substrates and biomimetic materials. Reverse micelles have been used to encapsulate proteins in organic solvents; however, currently-used small molecule surfactants are inefficient in both stabilizing native protein conformation and allowing for the retention of inherent protein functionality for extended periods of time. These surfactants are often quite dynamic and cannot completely suppress organic solvent penetration, resulting in protein denaturation. To address this pitfall, we report a new class of random heteropolymer surfactants that anchor to the protein surface through multiple non-covalent, complimentary interactions. These newly designed polymeric surfactants can effectively increase the retention of activity of several proteins in organic solvent in comparison to both a small molecule surfactant and an amphiphilic diblock copolymer. The modularity of this design process has the potential to be translated to a variety of proteins that can provide an enhanced platform for applications that include molecular recognition, catalysis, nanoscale assemblies, and medical therapeutics.

Friday, March 6, 2015 8:00AM - 11:00AM — Session Y42 DPOLY: Theory and Modeling of Diblock Copolymers and Blends 214B • Charles S. Ingalls, University of Illinois at Urbana-Champaign

8:00AM Y42.00001 Ordering in Mixed Polymer Brushes1, AMALIE L. FRISCHKNECHT, CHESTER K. SIMOCKO, DALE L. HUBER, Sandia National Laboratories — Mixed polymer brushes, consisting of two different homopolymers grafted to a substrate, microphase separate into phases reminiscent of those of diblock copolymer thin films. However, mixed polymer brushes typically display less long range order than diblock copolymers. One reason for the lack of long-range order is variations in the grafting densities of the two polymers, which result in quenched disorder in the system. Here we use self-consistent field theory (SCFT) to explore whether mixed brushes consisting of AB and AC diblock copolymers grafted to the surface can order better than homopolymer mixed brushes. In particular, we consider the case when A is a random copolymer of B and C, and thus has equivalent interaction strengths with both B and C blocks. Large cell SCFT calculations are performed for systems with Gaussian-correlated grafting density distributions. The theory predicts that mixed diblock brushes with a random copolymer block grafted to the surface are more ordered than the equivalent homopolymer brushes. The dependence of these results on polymer volume fractions and interaction parameters, as well as equivalent comparison with experiments, will be discussed.

1Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a Lockheed-Martin Company, for the U.S. Department of Energy under Contract No. DE-AC04-94AL85000.

8:12AM Y42.00002 Transferable potentials for coarse-grained simulations of block copolymer biomimetic membranes1, MALGORZATA KOWALIK, IAN SINES, JANNA K. MARANAS, MANISH KUMAR, Department of Chemical Engineering, The Pennsylvania State University, University Park, PA 16802 — We present a framework of minimal model transferable coarse-grained potentials for use in molecular dynamics simulations of amphiphilic block copolymer biomimetic membranes. Testing two, three, and five-bead models of polyethylene oxide polyethylene (PEO-PED) polymer membranes, we show that values for membrane thickness and area per polymer chain obtained using the two-bead model for use in molecular dynamics simulations of amphiphilic block copolymer biomimetic membranes. We demonstrate that cross interactions can be represented using combining rules with the use of a scaling factor which is correlated with the difference in hydrophobicities of the interacting hydrophobic/hydrophilic monomers. In this way it becomes possible to rapidly simulate and screen new combinations of block copolymers with minimal potential development effort.

1US Department of Energy, Office of Advanced Scientific Computing; grant number DE-FG02-02ER25535

8:24AM Y42.00003 Molecular Dynamics Simulations of Microphase Separating Tapered Diblock Copolymers, YOUNGMI SEO, JONATHAN R. BROWN, LISA M. HALL, The Ohio State University — Tapered AB copolymers consist of pure A and B blocks separated by a middle block whose composition is a statistical linear gradient from pure A to pure B (or from B to A for an inverse taper). These systems microphase separate into ordered structures similar to typical AB diblock copolymers. Prior experiments and theory suggest that one can use taper length as an adjustable parameter (beyond those available in the diblock system) to control interfacial and phase behavior, and that tapers potentially make the bicontinuous double gyroid phase more accessible at high molecular weight. Using a simple coarse-grained model, we perform molecular dynamics (MD) simulations to determine the interfacial profiles and other features of the structure and dynamics as a function of taper length. We reproduce the results from self-consistent field theory (SCFT); specifically, tapering increases miscibility, widens the interfacial region, shortens domain spacing, and makes network phases more preferable. The significantly smaller lamellar spacing for inverse tapers is explained in terms of polymer chain folding or snaking across the interface. The dynamic analysis shows the diffusion and relaxation behavior are closely related to the chain conformations and interfacial behavior. The effect of tapering on penetrant diffusion through one of the microphases will also be discussed.

8:36AM Y42.00004 Dynamic and Topological Properties of Lamellar Phases, VAIYANATHAN SETHURAMAN, VENKAT GANESAN, Department of Chemical Engineering, University of Texas at Austin, Austin, Texas 78712, USA — We investigate the local dynamical and global topological properties of a diblock copolymer system in its lamellar phase. Explicitly, we investigate the heterogeneity in the dynamics and non-Gaussian parameter (α) of different segments in the ordered phase as a function of its distance from the interface for a chain length of N = 100. At short time scales, weak heterogeneities are observed for low degree of compositional segregation and the heterogeneities increased for increased interactions between unlike monomers. Monomers near the interface also showed higher α values compared to those away from the interface. We also investigate the entanglements of ordered lamellar phases using molecular dynamics simulations which reveal a reduction in the average entanglement length for increasing γ/N. We use consistent field theory calculations to probe the number of topological constraints near the interface. Such calculations showed an increase in the number of constraints near the interface, thus corroborating the results obtained from molecular dynamics simulations.
J. Chem. Phys. recently-developed dynamical self-consistent mean-field theory on polymer blends and diblock copolymer melts and without compromising on neglecting compositional fluctuations, as is the case with self-consistent mean field theory. The assumption that the fluctuations in the incompressibility field are of a Gaussian nature allows one to use standard MC techniques. We compare the simulation results with predictions from theories that include fluctuations, such as a theory developed by Fredrickson and Helfand (FH) and the recently published renormalized one-loop calculations. Once the incorporation of the ultra-violet divergence is taken care of in an accurate way, the simulation results can be nicely mapped onto the theoretical predictions near the transition region, even for moderate simulation resolutions. [1]: Stasiak and Matsen, Macromolecules 46, 8037 (2013)

9:00AM Y42.00006 Accurate fluctuation-corrected phase diagrams of high-molecular-weight block-copolymer melts, KRIS DELANEY, GLENN FREDRICKSON, UC Santa Barbara — We describe a theoretical framework for accurately computing fluctuation-corrected phase diagrams of block polymer melts. The method is based on complex Langevin sampling of a UV regularized field-theoretic model, with Helmholtz free energies computed using thermodynamic integration. UV regularization ensures that the free energies thus computed do not have an arbitrary; they can be compared to incommensurate phases, permitting for the first time the explicit computational determination of order-order transitions within a mean-field approximation. The method allows one to study field-theoretic fluctuations without using renormalization-group techniques and is applicable to block copolymers that cannot be accurately treated with perturbation theory on the one-loop level. We note that our method uses no uncontrolled approximations beyond the initial definition of a coarse-grained molecular model for the polymer melt. The method can be applied straightforwardly to melts and solutions containing multiple species with diverse polymer architectures.

9:12AM Y42.00007 Morphology of Tapered and Ion-containing Diblock Copolymers from Fluids Functional Density Theory, JONATHAN R. BROWN, LISA M. HALL, The Ohio State University — We use classical, fluids density functional theory (fDFT) to study microphase separation in block copolymer systems. We focus on systems where local monomer scale ordering may be more important than for typical diblock copolymers, so fDFT allows us to generate more accurate density profiles and free energies at constant pressure. Specifically, we study the effect of tapering, or adding a gradient region (taper) between the pure A and B blocks of an AB diblock; the taper changes in composition smoothly from A to B. This additional control parameter allows one to increase the miscibility of the two blocks and the effective segregation strength \( \chi_N \) of the system. In contrast to our prior SCFT study, we capture the effect of the depletion of monomer density near the A-B interface, which changes as a function of taper length and interfacial width. Further, these methods can also be applied to ion containing systems, in which case monomer scale packing around ions is also important; we will show the fDFT predicted microphase morphology of block ionomers.

9:24AM Y42.00008 Survey of experimental data from diblock copolymer melts: Do experiments and simulations agree?, PAVANI MEDAPURAM, DAVID MORSE, Univ of Minnesota - Twin Cities — Recent simulations by our group have established that a variety of different simplified simulation models of symmetric diblock copolymers exhibit universal behavior that is now well characterized. In this talk, we report our progress in analyzing published experimental data for a variety of nearly symmetric diblock copolymers using methods closely analogous to those used to analyze simulation results. We will discuss the extent to which experiments on a wide variety of systems are consistent with the results of simulations, and with one another.

9:36AM Y42.00009 Finite Size Effects and Commensurability in Lattice Simulations of Symmetric Diblock Copolymers, AKASH ARORA, FRANK S. BATES, KEVIN D. DORFMAN, Chemical Engineering and Materials Science, University of Minnesota, Minneapolis MN, USA — Monte Carlo (MC) simulations have been used widely to study the fluctuation driven weakly first-order transition in symmetric diblock copolymers. However, the predicted value of the order-disorder transition (ODT) often differs from the true value (thermodynamic limit) because of the finite size of the simulation box. In order to locate the true ODT, we have studied finite size effects in lattice MC simulations of lamella forming symmetric diblock copolymers. The straightforward application of finite size scaling (FSS) is questionable due to incommensurability between the ordered structure domain spacing and the periodicity of the lattice. To address this issue, we estimate the preferred domain spacing by simulating multiple system sizes to find nearly commensurate systems. Furthermore, we apply FSS to these nearly commensurate systems to predict the ODT in the thermodynamic limit.

9:48AM Y42.00010 Dynamical self-consistent field theory of the evolution of instabilities in polymer blends and diblock copolymer melts, DOUGLAS GRZETIC, ROBERT WICKHAM, Univ of Guelph — We demonstrate our recently-developed dynamical self-consistent mean-field theory [J. Chem. Phys. 140, 244907 (2014)] in a polymeric context, by studying the early-time spinodal decomposition of a symmetric binary polymer blend and the dynamics of the order-order transition between the LAM and HEX phases in an asymmetric diblock copolymer melt. A Brownian dynamics description of a dense system of Rouse chains interacting pair-wise via a modified, species-dependent Lennard-Jones potential is reformulated, through a novel dynamical mean-field approximation, as that of a single chain interacting with a self-consistently determined dynamical mean field. A large ensemble of single chain Brownian dynamics simulations, run in parallel, efficiently determines the space- and time-dependent density that is used to weight the Lennard-Jones interaction in the mean-field calculation. Our theory gives access to chain conformation statistics, maintains a connection to microscopic time-scales and scales favorably with chain-length via a fast Rouse transform. We examine the performance of our method, and discuss our results for the growth of unstable modes in the blend and in the diblock copolymer melt.

10:00AM Y42.00011 Free energies and commensurability effects in simulations of three-dimensional ordered phases of diblock copolymers, TAHER GHASIMAKBARI, DAVID MORSE, University of Minnesota — We present an approach to the calculation of precise phase boundaries in simulations of diblock copolymer melts that is based on the calculation of free energies by thermodynamic integration. Results of simulations of three dimensionally periodic structures are extremely sensitive to commensurability effects, i.e., to the relationship between the dimensions of the (generally small) periodic simulation cell and the (generally unknown) preferred dimensions of a particular ordered phase. We avoid this by measuring the free energy for each ordered phase of interest using several different simulation sizes to estimate free energies as functions of unit cell size and thereby estimate the optimal cell size and corresponding free energy.

10:12AM Y42.00012 Estimation of \( \chi \) parameter from molecular simulations, ASHWIN RAVICHANDRAN, CHAU-CHYUN CHEN, RAJESH KHARE, Texas Tech University — The \( \chi \) parameter introduced in Flory-Huggins theory is widely used to determine polymer miscibility and its value is generally obtained by fitting to experimental data. In spite of its wide usage, techniques for predicting \( \chi \) parameter from the knowledge of molecular structure are not yet well established. In this work, we apply molecular simulations to estimate the value of the \( \chi \) parameter for a polymer blend system. In particular, we propose to use the approach suggested by Schweizer & Curro [Journal of Chemical Physics, 91, 5059 (1989)] which estimates \( \chi \) parameter in terms of the direct correlation functions. The \( \chi \) parameter thus obtained is related to the molecular structure factor, thereby making comparisons with experiment possible. Molecular dynamics simulations with atomistically detailed models are performed to estimate the value of the \( \chi \) parameter. Results will be presented for the application of this formalism to the binary blend of polysobutylene (PIB) and polybutadiene (PBD) for which experimental data are available [Industrial & Engineering Chemistry Research, 47, 3551 (2008)]. Finally, important structural features of the condensed phase which influence the value of the \( \chi \) parameter will be discussed.
10:24AM Y42.00013 Effects of dipole reorientations on ion solvation in polymer blends and block copolymer melts\textsuperscript{1}. ISSEI NAKAMURA, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences — We study the thermodynamic property of ion solvation in polymer blends and block copolymer melts and develop a dipolar self-consistent field theory for polymer mixtures. Our theory accounts for the chain connectivity of polymerized monomers, the compressibility of the liquid mixtures under electrostriction, the permanent and induced dipole moments of monomers, and the resultant dielectric contrast among species. We show nonmonotonic changes in the volume fraction profile and the dielectric function of the polymers with respect to those of simple liquid mixtures. Importantly, the spatial variations near an ion can be at nanometer scales, producing significant differences in the sorption energy among simple liquid mixtures, polymer blends, and block copolymers. Furthermore, we illustrate the oscillatory behavior of the dielectric function near an ion pair and the disparity of the dielectric functions between like and unlike charges. These results depend significantly on the chain length and Kuhn length of the diblock copolymers.

\textsuperscript{1}This work was supported by the National Natural Science Foundation of China (21474112). We are grateful to the Computing Center of Jilin Province for essential support.

10:36AM Y42.00014 Interfaces between immiscible large and small block copolymers \textsuperscript{1}. RUSSELL SPENCER, MARK MATSEN, Univ of Waterloo — Experiments and theory have shown that mixtures of short and long symmetric AB diblock copolymers macrophase separate if their sizes differ by more than a factor of about five. Here we examine the interface between the two coexisting phases using self-consistent field theory (SCFT). The presence of periodic order in this phase-separated system confers novelty to this problem, in both potential applications and the challenges involved. This investigation is confined to the simple case of parallel lamellae, as may be found in thin films. Our focus is on the structure and tension of interfaces between coexisting phases, in terms of the relative size of the long and short copolymers. As the blend approaches the critical point, which marks the disappearance of phase separation, the interfacial tension vanishes and the width diverges. When the short polymers are too small for periodic order to be stable in bulk, coexistence exists between long lamellae and disorder; and lamellar order is induced in the disordered phase, close to the interface.

10:48AM Y42.00015 Tailoring the morphology of polymer blend particles: 3D simulations and linear stability analysis, B.S. SARATH POKURI, BASKAR GNAPATHYSUBRAMANIAN, Iowa State University — Polymer blend micro-/nano- particles find a variety of uses in novel applications including electronics, luminescent devices, and drug delivery. Solvent evaporation driven phase separation is one of the easiest ways to fabricate these particles. However, tailoring morphology of these particles is still challenging. This has resulted in complex methods to tailor morphology. Understanding how morphology evolves and in particular how phase separation is initiated will provide valuable insight to tune morphologies. We characterize the evolution of morphology during evaporation based phase separation into a finite set of fundamental modes. We approach the problem at two levels of complexity. A full 3D modeling framework describing evaporation induced phase separation is used to model the emulsification process as a function of processing parameters: droplet radius, blend ratio, and evaporation rate. Subsequently, high throughput analysis is enabled by using ideas from linear stability analysis to classify the parameter space by morphology. These complementary analysis allows us to identify a fundamental set of morphology evolution modes and map the set of processing conditions to a unique mode. Ergo, one can gain control over the morphology by regulating the processing conditions.

Friday, March 6, 2015 8:00AM - 11:00AM –
Session Y43 DPOLY G$\text{SOF}$ T DCMP: Focus Session: Fluids Under Confinement, Colloids and Liquid Crystals 214C - Alberto Fernandez-Nieves, Georgia Institute of Technology

8:00AM Y43.00001 Dripping Cylindrical Double Emulsions, JIAWEI YANG, LAURA ADAMS, DAVID WEITZ, Harvard University — Not all drops drip from the orifice of a faucet or capillary as spherically shaped drops. By encapsulating water drops inside an ultra thin sheet of oil, cylindrically shaped drops emerge. A stability theory is presented which describes not only the volume of the ultra thin sheet, but also the flow velocity conditions under which cylindrical drop formation is possible. We compare our theoretical model to time-dependent dynamics of drop formation that is captured experimentally with a fast camera and imaged through a microfluidic device.

8:12AM Y43.00002 Hydrodynamic damping of dense colloidal packings under confinement\textsuperscript{1}. MICHAEL RYAN, West Chester University, TIM STILL, University of Pennsylvania, MATTHEW WAITE, West Chester University, ARJUN YODH, University of Pittsburgh, KEVIN APTOWICZ, West Chester University — We experimentally study hydrodynamic damping of collective motion in dense colloidal crystals confined in a 1 micron meter channel. Particle diameters are on the order of the channel width resulting in quasi-two-dimensional entropic crystals. The packing fraction of the crystals, formed from soft thermo-responsive spheres, is varied with temperature. Digital video-microscopy is utilized to explore the phonon dynamics of the colloidal crystals. Friction coefficients along high symmetry directions in q-space are extracted and provide insight about the hydrodynamic forces at play. As expected, damping of collective motion increases with increasing packing fraction. Preliminary results suggest the friction coefficient decreases with increasing phonon wavelength, but it does not appear to vanish.

\textsuperscript{1}KBA acknowledges support from grant DMR-1206231. AGY acknowledges support from grants PENN-MRSEC DMR11-20901, NASA NNX08AO0G, and DMR-1205463.

8:24AM Y43.00003 Simulation of blade printing of colloidal morphologies, ALEXANDER WAGNER, ALAN DENTON, ERIK HOBBIE, Department of Physics, North Dakota State University — We present a new four-component multi-phase lattice Boltzmann simulation method and its application to blade printing of colloidal morphologies. We consider a solution of colloids and polymers that is applied as a thin film on a substrate. As the mixture is exposed to the surrounding air the solvent evaporates leaving the colloid-polymer mixture unstable to phase-separation. Our new method predicts that as a function of the application speed, initial concentrations, and film thickness different morphologies can be generated.

8:36AM Y43.00004 Dynamics of Colloids in Nematic Liquid Crystals\textsuperscript{1}. OLEG LAVRENTOVICH, Kent State Univ - Kent, Ohio — Dynamics of small particles in fluids has fascinated scientist for centuries. Phenomena such as Brownian motion, sedimentation, and electrophoresis continue to inspire cutting-edge research and innovation. The fluid in which the particles move is typically isotropic, such as water or a polymer solution. Recently, our group started to explore what would happen if particles are placed in an anisotropic fluid: a liquid crystal. The study reveals that the liquid crystal changes dramatically the dynamic behavior, leading to levitation of the particles, their anomalous Brownian motion and new mechanisms of eletrokinetics. The new phenomena are rooted in anisotropy of the liquid crystal properties, such as surface tension and elasticity, different electric conductivity in the directions parallel and perpendicular to the average molecular orientation.

\textsuperscript{1}Work supported by NSF DMR-1104850 and DMS-1434185.
9:12AM Y43.00005 Disc-shaped colloids interacting in a nematic liquid crystal, ALENA ANTIPOVA, COLIN DENNISTON, University of Western Ontario — We examine the behavior of (ferromagnetic) micron-sized structures such as disc-shaped colloidal particles in a nematic liquid crystal using Lattice Boltzmann algorithm. Without any external forces the position of the disc with respect to the liquid crystal director minimizes the free energy of the system and no distortion of the director field is observed. When the rotating magnetic field is present, the torque on the disc with homeotropic surface anchoring should change with analogy to electrostatic energy, which implies the disc continues turning following the field. However, when the disc reaches some critical position and the director field around it is highly distorted, the disc suddenly flips to minimize the free energy. Position and motion of pairs of such discs under similar conditions can be controlled by the angular velocity of magnetic field, its magnitude and initial configuration of the system. As a result of analysis of discs’ dynamics, a new way to control self-organization of disc particles was produced. We also will demonstrate some results on ferromagnetic torus micro-colloidal particle in nematic with more complicated boundary conditions.

9:24AM Y43.00006 Liquid Crystals Confined in Micro and Nanochannels1, YU-BING GUO, JIE XIANG, OLEG LAVENTOVICH, QI-HUO WEI, Liquid Crystal Institute, Kent State Univ, Kent, OH — Geometrical confinements cause frustration, topological defects in liquid crystal molecular orientations, altering behaviors of phases and phase transitions. In this paper, we developed microfabrication processes for assembling cells of glass slides with various well-defined confinement geometries such as microfluidic channels and nanofluidic channels, and will present experimental studies on the structures and phase transitions of nematic and cholesteric liquid crystals under these confinements.

9:36AM Y43.00007 Defects in liquid crystals in confined geometries: simulation studies1, SAJDEH AFGHAH, ANDREW KONYA, ROBIN SELINGER, Kent State Univ - Kent — Using numerical simulations in three dimensions, we study the formation of defect structures in liquid crystals in confined geometries. We model a cholesteric in a microchannel with homeotropic anchoring on four sides and periodic boundary conditions along the channel length. We find that channel aspect ratio and cholesteric pitch control resulting defect structures, and in some cases produce evenly spaced bubble domains. We also performed simulation studies of a nematic liquid crystal confined in a cell with a periodic array of pillars with homeotropic anchoring on all surfaces, and examine formation of a periodic array of defects. To simulate temperature-driven microstructural evolution, we include in our model the temperature dependence of the Frank elastic coefficients and cholesteric pitch, fitted from experimental studies. Computational speed is improved by implementation of our simulation algorithm in CUDA. Simulation results are compared to recent experimental studies by the group of Qi-Huo Wei at Kent State.

1Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund for support of this research.

9:48AM Y43.00008 Fluctuating Hybrid lattice Boltzmann method for nematic liquid crystals, GANNA PIATKOVSKA, COLIN DENNISTON, Univ of Western Ontario — As one goes from micron to nanometer lengths scales in a liquid crystal, thermal fluctuations become increasingly important and can have significant impact on colloids and polymers immersed in the liquid crystal. We develop and test numerically a Hybrid lattice Boltzmann model for liquid crystal hydrodynamics that incorporates the thermal fluctuations of tensor order parameter. It is shown that a good equilibrium is obtained over a wide range of length scales using uncorrelated noise. We find the condition on the system’s correlation lengths when the use of correlated noise would be necessary to achieve an equilibrium. In particular, in simulations without electric field, the mesh size should be chosen in such a way that the correlation length defined by the elastic constant is less than 2 in lattice units. When the electric field is present, the situation is more complex since the correlation length associated with the electric field comes into play. Some applications of the introduced noise are considered.

10:00AM Y43.00009 Tetratic and smectic liquid crystals on a sphere: defects, patterns and cubes1, OKSANA MANYUHINA, MARK BOWICK, Syracuse University — We construct the elastic free energy for tetratic order and find a closed form solution for +1/4 disclinations. Confined to a sphere we expect tetratic order to manifest itself in eight +1/4 disclinations, giving the total charge of +2.

1The authors acknowledge financial support from the Soft Matter Program of Syracuse University

Within the one elastic constant approximation for the tetratic free energy, their equilibrium positions define the vertices of a cube, rather than the twisted cube, found earlier within the XY-model. We show that it is energetically favorable for the sphere to deform to a rounded cube with flattened faces and locally high Gaussian curvature at the eight vertices. Motivated by experimental observations of smectic shells, we apply our analytic results to study the relative stability of defect configurations and the formation of periodic texture for thick smectic shells.

10:12AM Y43.00010 Visualization of the Flow Field induced by an Oscillating Post in a Freely Suspended Smectic Liquid Crystal Membrane1, ZHIYUAN QI, KYLE FERGUSON, JOHN PAPAIOANNOU, YANCEY SECHRIST, TOBIN MUNSAT, CHEOL PARK, MATT GLASER, JOE MACLENNAN, NOEL CLARK, Physics, University of Colorado, TATIANA KURIABOVA, Physics Department, California Polytechnic State University, THOMAS POWERS, Engineering and Physics, Brown University — Thin fluid membranes immersed in a less viscous, bulk fluid are of fundamental interest as approximations of true two-dimensional (2D) fluids and as models of biological membranes. Many previous studies of such fluid membranes have focused on 2D macroscopic hydrodynamic effects such as the diffusion and interaction of inclusions, with fewer experimental investigations of microscopic properties such as the flow field. We have measured the 2D flow field generated by a rigid, oscillating post inserted in a freely suspended smectic liquid crystal film surrounded by air by analyzing the motion of tracer particles in the film. Our experiments confirm Saffman’s prediction that the far-field flow velocity decays as 1/r (where r is the distance from the post) in the longitudinal direction, and as 1/r² in the tangential direction. The measurements are in good agreement with flow fields computed using a model that generalizes the Levine/MacKintosh point-force response functions. We have also investigated confinement effects when the post is located near the film boundary.

1This work was supported by NASA Grant No. NNX-13AQ81G, NSF MRSEC Grant No. DMR-0820579, DE-FG02-08ER54995, DE-SC0008942, and by NSF Grant CHE-0907228.

10:24AM Y43.00011 Liquid crystal-enabled electro-osmosis through spatially separated charges in photo-patterned surface alignment1, CHENHUI PENG, YUBING GUO, SERGIJ SHIYANOVSKI, QIHUO WEI, OLEG LAVENTOVICH, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, Kent, OH 44242, USA — Electrically-controlled dynamics of fluids and particles at microscales is a fascinating area of research with applications ranging from microfluidics and sensing to sorting of biomolecules. We demonstrate that anisotropic conductivity of liquid crystals in combination with photopatterned surface alignment enables highly efficient electro-osmosis (LCEO) rooted in space charging of regions with distorted orientations. LCEO velocities grow with the square of the field, which allows one to use an AC field to drive steady flows and to avoid electrode damage. By controlling the director patterns, one can dramatically change the nature of LCEO flows, for example, trigger a pumping effect in dipolar configuration and reverse the flow direction in quadrupolar patterns. Ionic currents in liquid crystals that have been traditionally considered as an undesirable feature in displays, offer a broad platform for versatile applications such as liquid crystal enabled electrokinetics, micropumping and mixing.

1NSF DMR-1104850 and NSF DMS-143485
10:36 AM Y43.00012 Elastic Response of Liquid Crystalline Mixtures, JONATHAN WHITMER, Department of Chemical and Biomolecular Engineering, University of Notre Dame — Liquid crystalline (LC) materials comprised of multiple mesogenic species, or mesogenic species and dopants, are widely used industrially to obtain materials having specific viscous, optical, or elastic properties. While commonly used materials exhibit additive elastic constants in the homogenous liquid phase, it is less clear how these materials respond to inhomogenous applied stresses often occurring in confinement. Here we utilize coarse-grained LC models and a recently developed formalism for free-energy calculations to investigate the elastic coefficients of LC mixtures and their behavior under asymmetric stress.

10:48 AM Y43.00013 Viral nematics in confined geometries1, KYLE LAWLER, OKSANA MANYUHINA, MARK BOWICK, CRISTINA MARCHETTI, Syracuse Univ — Motivated by recent experiments on the rod-like virus bacteriophage fd confined to circular and annular regions, we present a theoretical study of confined nematic liquid crystals in such two-dimensional geometries. It is well known that a dense suspension of the fd-virus exhibits nematic order. Recent experimental work and comparison with numerical modeling predicts that in this system the ratio of the bend and splay elastic constants is close to unity. Using the one-constant-approximation for the Frank free energy of nematic liquid crystals, we examine the competition between bulk elasticity and surface anchoring in controlling confined director configurations. We show that many of the observed configurations can be described in terms of bulk and surface topological defects. A similar effect is known to occur in 3D nematic droplets, where a change in anchoring conditions can drive the splitting of a bulk defect into surface defects. In contrast, in our 2D systems, such a splitting is driven by changes in the size and geometry of the system. We show that the continuum theory is capable of accounting for many of the observed configurations.

1This work was supported by the National Science Foundation Grants DMR-1305184 and DMG-1068780 and by the Syracuse Soft Matter Program.

Friday, March 6, 2015 8:00 AM - 10:48 AM
Session Y44 GSOFT: Focus Session: Jamming in Granular Media II 214D

8:00 AM Y44.00001 Percolation and jamming transitions in particulate systems with and without cohesion1, LOU KONDIC, LENKA KOVALCINOVA, New Jersey Institute of Technology, ARNAUD GOULLET, Rutgers University — We consider percolation and jamming transitions for particulate systems exposed to compression. For dry granular systems, interacting by repulsive forces in addition to friction and viscous damping, it is found that these transitions are influenced by a number of effects, and in particular by the compression rate. In a quasi-static limit, we find that for the considered type of interaction between the particles, percolation and jamming transitions coincide. For cohesive systems, however, we find that the differences between the considered transitions persist in quasi-static limit.

1Supported by NSF Grant No. DMS-0835611

8:12 AM Y44.00002 The birth and the growth of Boson peak — insights from the normal modes analysis of granular experiments2, JIE ZHANG, LING ZHANG, JIE ZHENG, Shanghai Jiaotong University — The origin of the Boson peak in amorphous solids has been a long-lasting puzzle for more than decades for researchers in the field. In order to understand the physics of the boson peak, we have experimentally measured the density of states (DOS) from the hexagonal lattice to the disordered structures in 2D packing of granular materials, which are made of photo-elastic disks allowing a precise measurement of contact forces between disks to determine the dynamical matrix of the system. These disks are wrapped with Teflon tapes to mimic frictionless particles so that the rotational degree of freedom can be ignored to a good approximation. By varying which are made of photo-elastic disks allowing a precise measurement of contact forces between disks to determine the dynamical matrix of the system. These disks are wrapped with Teflon tapes to mimic frictionless particles so that the rotational degree of freedom can be ignored to a good approximation. By varying

8:24 AM Y44.00003 Shear Modulus Heterogeneities in Disordered Frictionless Particle Packings, LEO SILBERT, SIU Carbondale, HIDEYUKI MIZUNO, MATTHIAS SPERL, German Space Agency (DLR) — It is understood that amorphous solids, ranging from thermal glasses to athermal granular packings, exhibit spatially inhomogeneous mechanical properties. Here, we explore the spatial extent of elastic modulus heterogeneities using computer simulations of a model granular material composed of frictionless, monodisperse spheres, through the implementation of an equilibrium fluctuation formalism. This protocol allows us to decompose the elastic moduli into their affine and nonaffine components. We first validate our numerical scheme by examining how the macroscopic values of the bulk and shear moduli vary as we tune the density of the packing towards its state of marginal stability, that lies at a critical solids packing fraction. Poking particular attention to the shear modulus, we find that it is the fluctuations in the shear modulus that control the mechanical stability of the solid. Furthermore, we are able to associate a characteristic length scale with the relative heterogeneities in the local shear modulus that grows on approach to the critical packing density.

8:36 AM Y44.00004 Shear Jamming in Granular Media1, THIBAULT BERTRAND, Yale University — We numerically study two-dimensional packings of bidisperse disks created using an isotropic compression and simple shearing protocols. To create jammed packings by compression, we start with $N$ particles with random initial positions and grow their diameters by successive small packing fraction increments each followed by relaxation of particle overlaps using energy minimization until the system cannot be compressed further without particle overlaps in the relaxed state. Jammed packings created via isotropic compression exist over a range of packing fractions $\phi$. Because of the spread of jammed packing fractions, during compression the system may reach a packing fraction above the minimum value before jamming. If an unjammed packing is then sheared by a strain $\gamma$, it can jam. Using a combination of compression and shearing, we can define jamming protocols as trajectories in the ($\phi, \gamma$) plane that yield jammed packings. In this plane, we can reach a particular point ($\phi_0, \gamma_0$) in many ways. We will focus on two of these: (1) shearing to $\gamma_0$ at $\phi = 0$ followed by compression to $\phi_0$ at $\gamma = \gamma_0$, and (2) compression to $\phi_0$ at $\gamma = 0$ followed by shearing to $\gamma_0$ at $\phi = \phi_0$. For protocol 1, we find that the probability of obtaining a jammed packing at $\phi$ and $\gamma$, $P(\phi, \gamma) = Q(\phi)$, is independent of $\gamma$. For protocol 2, we use a simple theory to deduce $P(\phi, \gamma)$ from $Q(\phi)$. Furthermore, we find that frictionless jammed packings form one-dimensional families in the ($\phi, \gamma$) plane. The one-dimensional families are projections from the 2$N$-dimensional configuration space onto the ($\phi, \gamma$) plane. The system reaches a given packing fraction by isotropic compression without jamming, the system will eventually “hit” one of the families and jam during shear. In packings composed of frictionless particles, the range of accessible jammed packing fractions shrinks with increasing $N$. However, in packings composed of frictional disks, we have shown that the families are no longer one-dimensional, the range of jammed packing fractions is broad even for large $N$ and depends on the number of missing contacts $m$. Therefore, the theoretical predictions used above for packings of frictionless disks must be modified to explain packings formed under shear in frictional systems. We predicted and measured the probability of forming a jammed packing with friction coefficient $\mu$ and $m$ missing contacts, $P_m(\mu, \phi, \gamma)$. Here, we extend these studies to include the dependence of the jamming probability on packing fraction and shear strain, $P_m(\mu, \phi, \gamma, \gamma)$, and relate this function to shear-jammed packings in frictional systems.

1Funding: W. M. Keck Foundation and Science and Engineering Grant
9:12AM Y44.00005 The onset of geometric rigidity in granular systems below jamming, PETER MORSE, ERIC CORWIN, University of Oregon — We report on a new purely geometric phase transition in soft athermal spheres which occurs significantly below the jamming density. This state is characterized by the onset of local rigidity as evidenced by changes in the symmetry of the local Voronoi cell. We relate this local rigidity onset to the eventual mechanical jamming transition through a rigidity percolation picture. We present a functional transformation mapping a minimized packing to a new packing by replacing every particle with the maximum inscribed sphere in its Voronoi cell. We demonstrate that there exists a line of fixed points between the onset of local rigidity and the jamming point under this transformation. Surprisingly, this transformation has a second attractor to systems with mean contact number of \( d + 1 \). We identify these as random loose packings in polydisperse systems.

9:24AM Y44.00006 Jamming Percolation in Three Dimensions, EIAL TEOMY, Tel Aviv University, ANTINA GHOSH, Weizmann Institute, YAIR SHOKEF, Tel Aviv University — We introduce a three-dimensional kinetically-constrained model for jamming and glasses [1], and prove that the fraction of frozen particles is discontinuous at the directed-percolation critical density. In agreement with the accepted scenario for jamming- and glass-transitions, this is a mixed-order transition; the discontinuity is accompanied by diverging length- and time-scales. Because one-dimensional directed-percolation paths comprise the backbone of frozen particles, the unfrozen rattlers may use the third dimension to travel between their cages. Thus the dynamics are diffusive on long-times even above the critical density for jamming. Our new model is a non-trivial extension of the two-dimensional spiral model [2].


9:36AM Y44.00007 Renewal Events in Glass-Forming Liquids – Glass Dynamics with Ideal Age Zero, JULIAN HELFFERICH, FALKO ZIEBERT, Institut Charles Sadron, CNRS, Strasbourg, France and Universität Freiburg, Freiburg, Germany, HENDRIK MEYER, STEPHAN FREY, JÖRG BASCHNAGEL, Institut Charles Sadron, CNRS, Strasbourg, France, KATHARINA VOLLMAYR-LEE, Department of Physics and Astronomy, Bucknell University, Lewisburg, Pennsylvania 17837, USA, ALEXANDER BLUMEN, Université de Freiburg, Freiburg, Germany — When a glass-forming liquid is cooled through the glass transition temperature, the system falls out of equilibrium and evolves slowly over time in a process called physical aging. During aging, dynamic observables depend on the history of the process, i.e. the time since vitrification and the quenching procedure, hampering any attempt to directly compare the dynamics of different glass formers. The continuous-time random walk (CTRW) interpretation, however, offers a remedy for the history dependence of the dynamic observables. This interpretation is based on the observation that single-particle trajectories display hopping-like motion, i.e. long periods of localization interrupted by fast “jumps.” In the CTRW picture, these jumps are renewal events, i.e. each particle carries its own “internal clock” which can be reset on any jump. This “internal time” can be treated as the ideal age. All particles display identical (ensemble averaged) dynamics with respect to this time, regardless of their history. In this talk, I will discuss how to decide whether jumps in the single-particle trajectories can be treated as jumps of a CTRW and demonstrate how these events can be utilized to gain history-independent dynamic observables.

9:48AM Y44.00008 Local structure as a mechanism for dynamical arrest: tackling the length-scale conundrum, PADDY ROYALL, ANDREW DUNLEAVY, KAROLINE WIESNER, University of Bristol, RYOICHI YAMAMOTO, Kyoto University, THOMAS SPECK, Johannes Gutenberg-Universität Mainz, STEPHEN WILLIAMS, Australian National University — Among the key challenges to our understanding of the process by which supercooled liquids transform into solid glasses is that it is accompanied by little apparent change in structure. Recently geometric motifs representing locally favoured structures have been identified in supercooled liquids, but a causal link between these locally favoured structures (LFS) and solidification remains elusive. One “smoking gun” for such a link would be coincidence of dynamic length-scales which reflect solidification and length-scales associated with structural features. However, this coincidence remains elusive, at least in the dynamical regime accessible to numerical simulations and colloidal experiments. Here we re-evaluate the lack of coincidence of dynamic and static lengthscales in the regime accessible to simulation. We consider the isochronal ensemble, in which any spatial heterogeneity in dynamics is encoded in the structure. Using an information theoretic method we extract a new dynamic length-scale which is matched very closely by structural length-scales associated with geometric motifs. This provides a possible resolution of the discrepancy in dynamic and structural lengthscales found in conventional studies.

10:00AM Y44.00009 Cluster Analysis of Particle Jumps in SiO2 Glass1, JONATHAN COOKMEYER, Haverford College, KATHARINA VOLLMAYR-LEE, Bucknell University, HORACIO CASTILLO, Ohio University, JUERGEN HORBACH, Heinrich-Heine-University Düsseldorf, Germany — With a Molecular Dynamics simulation, we study the behavior of 115248 SiO2 particles after a quench from a fully equilibrated configuration at a high temperature to a temperature below the glass transition. By analyzing single particle trajectories, we identified “jumps” when particles moved significantly relative to their fluctuations. We consider the collective motion of these jump events by identifying jumps that occur close in space and time. We will show preliminary results of the cluster size distribution for different temperatures (i.e. 2500 K, 2750 K, and 3000 K), as well as the dependence of this distribution on waiting time.

1. We acknowledge the support via NSF REU grant #PHY-1156964, DoD ASSURE program, and NSF-MRI CHE-1229354 as part of the MERCURY high-performance computer consortium.

10:12AM Y44.00010 Softness and Kinetic Heterogeneities in Glassy Liquids, SAMUEL SCHOENHOLZ, University of Pennsylvania, EKIN CUBUK, EFTHIMIOS KAXIRIS, Harvard University, ANDREA LIU, University of Pennsylvania — One signature feature of glassy liquids is the existence of kinetic heterogeneities. Isoconfigurational approaches show that there is a connection of these kinetic heterogeneities to the underlying structure of the liquid, but do not identify the particular structural features that are important in leading to enhanced mobility. We use machine-learning methods to show that the thermally-induced rearrangements that correspond to enduring displacements in glassy liquids occur at “flow defects” that can be identified from the liquid structure. We will discuss the dynamics and structural space of the defect population, as well as the connection between the defect population and kinetic heterogeneities.

10:24AM Y44.00011 Jamming in Quasi-2D Self-Assembled Nanoparticle Monolayers, LEANDRA BOUCHERON, JACOB STANLEY, YELING DAI, Univ of California - San Diego, SEAN YOU, University of Chicago, SURESH NARAYANAN, ALEC SANDY, ZHANG JIANG, Advanced Photon Source, Argonne National Lab, MATI MEROZ, BINHUA LIN, Center for Advanced Radiation Sciences, University of Chicago, OLEG SHPYRKO, Univ of California - San Diego — In this work, we experimentally probed the interparticle dynamics of iron oxide nanoparticle thin films self-assembled at the liquid-air interface. Upon deposition on a water surface in a Langmuir-Blodgett trough by the drop-casting technique and subsequent lateral compression, iron oxide nanocrystals coated in oleic acid ligands self-assembled into a relatively uniform quasi-2D monolayer. Utilizing X-Ray Photon Correlation Spectroscopy (XPCS) at beamline 8-ID-I of the Advanced Photon Source at Argonne National Lab, we measured the characteristic timescale of in-plane interparticle dynamics. We quantified the aging behavior of the film utilizing both second-order and two-time autocorrelation analysis. We also determined the degree of jamming in the system by a stretched exponential model, yielding exponents varying between a value of 1.5 and 2. We have concluded that despite the quasi-2D nature of our system, verified by x-ray reflectivity, interparticle diffusion in our nanoparticle monolayers bears the signature of a largely three-dimensional jammed system.
8:00AM Y45.00001 Shear jamming for highly strained granular materials, JONATHAN BARES, ROBERT BERHINGER, Duke University — Bi et al. (Nature 2011) have shown that, if sheared, a granular material can jam even if its packing fraction ($\phi$) is lower than the critical isotropic jamming point $\phi_J$. They have introduced a new critical packing fraction value $\phi_J$ such that for $\phi < \phi < \phi_J$ the system jams if sheared. Nevertheless, the value of $\phi_J$ as a function of the shear strain or the shear strain rate is not yet accessible due to the experimental complexities. We present our theoretical results of jamming in an ideal 2D periodic shear apparatus of highly strained granular systems, each of which can be moved independently which permits us to impose any desired shear profile. The circular geometry allows access to any strain value. The forces between grains are measured using reflective photoelasticity. This talk will present this novel apparatus and discuss initial results.

8:12AM Y45.00002 Ergodicity in a model for earthquake fault systems undergoing hydraulic fracturing, JAMES SILVA, WILIAM KLEIN, Boston Univ, HARVEY GOULD, Clark University, NICK LUBBERS, Boston Univ — The frequency of large seismic events in regions with a large amount of hydraulic fracturing activity has been of great interest in recent media reports of earthquake events in Oklahoma. In this talk, a model for earthquake fault systems undergoing hydraulic fracturing will be introduced. The question of how seismic failure events occur and how the individual systems will be addressed. This will be done by presenting work on the statistics of events and ergodicity within this model.

8:24AM Y45.00003 Continuum modeling of secondary rheology in slow granular flows, DAVID HENANN, DAREN LIU, Brown Univ, KEN KAMRIN, MIT — Recent dense granular flow experiments have shown that shear deformation in one region of a granular medium fluidizes its entire, including regions far from the sheared zone, effectively erasing the yield condition everywhere. This enables slow creep deformation to occur even when an external force is applied to a probe in the nominally static regions of the material. The apparent change in rheology induced by far-away primary motion is termed the "secondary rheology" - a curious phenomenon that arises due to the cooperativity of slow granular flows. Recently, the new nonlocal granular fluidity (NGF) model was successfully used to predict a wide variety of steady granular flow fields. In this talk, we show that the NGF model is also capable of capturing secondary rheology. Specifically, we will demonstrate (i) the vanishing of the yield condition in the presence of primary flow, (ii) the rate-independent nature of secondary rheology for sufficiently slow primary flow rates, (iii) an exponential-type relationship between the force applied to the intruder and the consequent creep rate, and (iv) the anisotropy of secondary rheology, in which the observed phenomenology changes depending on whether the intruder is forced along with or counter to the primary flow.

8:36AM Y45.00004 Fragmentation, Acoustic Effects, and Flash Heating in Sheared Granular Materials: Implications of Geophysical Processes and Physical Constraints for Dynamic Friction, JEAN CARLSON, Department of Physics, University of California, Santa Barbara — Incomplete understanding of friction, deformation, and failure is a primary limiting factor in forecasting seismic hazards. We report recent progress on a physics-based framework for constitutive laws. Our methods are rooted in the underlying statistical thermodynamics of amorphous materials, and bridge the gap between microscopic dynamics, laboratory experiments, and dynamic rupturing experiments. We explore the conceptual framework of the Shear Transformation Zone (STZ) model and non-traditional study of the frictional response of sheared gouge layers over a wide range of velocities and normal stresses, to stresses for geophysically relevant processes such as breakage and thermal heating, as well as grain shapes. We combine theoretical advances with quantitative fits to experimental data obtained within the rock mechanics community. Fragmentation is described by a constitutive equation for grain size reduction involving the applied work rate and pressure, constrained by energy balance. We show that grain breakage is a potential weakening mechanism at high strain rates. It promotes strain localization and may explain long-term persistence of shear bands in natural faults. Shape effects are modeled by an orientational bias that describes grain interlocking and geometrical frustration. We interpret inter-particle friction as an additional source of acoustic noise. We obtain quantitative agreement between experimental measurements and theoretical predictions for both internally generated acoustic noise and externally applied vibrations. Frictionally generated thermal heating is incorporated using a contact strength model that accounts for local increases in temperature at grain contacts during sliding. The magnitude of this effect depends on grain size and porosity of the granular layer. Our model predicts logarithmic rate dependence of steady state shear stress in the quasi-static regime. In the dense flow regime frictional strength decreases rapidly with increasing slip rate due to thermal softening at granular interfaces. The transient response following a step in strain rate includes a direct effect and subsequent evolution effect, both depending on the magnitude and direction of the velocity step. The resulting friction models are appropriate for dynamic rupture simulations that extrapolate results to geophysically relevant regimes that are beyond reach of laboratory experiments. Our work offers experimentalists and field workers insights for interpreting data, identifying features to target in future work, and estimating seismic hazards.

9:12AM Y45.00005 Interaction of intruding objects within granular media using continuum modeling, HESAM ASKARI, KEN KAMRIN, Massachusetts Institute of Technology — The interaction of objects with granular media is very common in various aspects of our lives. Interestingly, such a broad problem is not easy to solve due to the complexity of the response of the granular materials to deformation and lack of understanding of the mechanics and physics of their deformation. Exclusively on the topic of the interaction with intruding objects, attempts have been made - mostly driven by experimental observation and validation - to describe this interaction using Resistive Force Theory (RFT), which works based on superposition rules. Understanding the origin of these empirical rules and delving deeper into the requirements on the validity of such hypotheses are crucial to understanding this theory. In an attempt to explain this theory, we hypothesize that the RFT is arising from the laws of continuum frictional plasticity. To demonstrate this, we use the Finite Element Method to study the interaction of an intrusion with a continuum granular media. We use a custom user-material definition in ABAQUS using a friction-based law for the flow rule as well as adjustments required to represent a discrete granular system in a continuum model. The findings of our model are in agreement with the experiments and numerical discrete element method results in the literature. These results are suggesting that the superposition rule can be obtained by the plasticity approach and the effects of the shape, size and depth of the object can be represented by a universal scaling law.
The influence of particles on the properties of a system can be described using a theory of dynamic interactions. We explore the role of yolk-shell particles in the context of shell-shell interactions. In the absence of yolk-shell interactions, we find that the yolk-shell system behaves similarly to a free Brownian system, which allows for an approximate self-consistent description of the simulated self-diffusion properties.

We use Langevin equations to model the system and derive results for the mean squared displacement and intermediate scattering function of the yolk-shell complex. These results are compared with theoretical predictions to understand the effective behavior of the system.

Brownian dynamics simulations are used to determine the mean squared displacement and intermediate scattering function of the yolk-shell complex. These results are compared with theoretical predictions to understand the effective behavior of the system.

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In the absence of yolk-shell interactions, the system behaves similarly to a free Brownian system, which allows for an approximate self-consistent description of the simulated self-diffusion properties. In this approximation, the system can be described using Langevin equations. These equations are solved numerically to determine the mean squared displacement and intermediate scattering function of the yolk-shell complex. These results are compared with theoretical predictions to understand the effective behavior of the system.

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of Self-Propelled Particles

monolayers in micropatterned environments. The model stresses. We consider a minimal physical model of an expanding cell monolayer described as a self-propelled elastic medium coupled to the kinetics of active contractile units. These contractile units represent actomyosin stress fibers that generate local contractile stresses through ATP hydrolysis. Using the particle tracking technique and flow reconstruction method we investigated the structure of the flow generated by bacteria and pairwise interactions between bacteria in liquid crystals. We demonstrated that while the rotation rate of bacterial flagella is reduced by an order of magnitude due to increased viscosity, the bacteria swimming speed is slowed only by 25-30\%. Due to the strong anisotropy of viscosity in liquid crystal the bacteria-induced flow is localized along a bacterial body: the flow along a line coaxial with the bacterial body is much stronger than in perpendicular direction and decays rather slowly. We found that interaction between flagella bundles of two close-by bacteria is negligible and the observed convergence of the swimming speeds and flagella waves may occur due to viscoelastic interaction between bacterial bodies.

This work was supported by the National Science Foundation through grant No DMR-1305184
8:12AM Y47.00002 A Combined Light Sheet Fluorescence and Differential Interference Contrast Microscope for Live Imaging of Multicellular Specimens

R. BAKER, M. T. M. JEMIELITA, R. S. M. RUVÉER PARTHASARATHY, University of Oregon — We present a microscope capable of both light sheet fluorescence microscopy (LSFM) and differential interference contrast microscopy (DICM). The two imaging modes, which to the best of our knowledge have not previously been combined, are complementary: LSFM provides high speed threedimensional imaging of fluorescently labeled components of multicellular systems, large fields of view, and low phototoxicity, while DICM reveals the unlabeled neighborhood of tissues, organs, and other structures with high contrast and inherent optical sectioning. Use of a shared detection path for both imaging modes enables simple integration of the two techniques in one microscope. To demonstrate the instrument’s utility, we provide several examples which focus on the digestive tract of the larval zebrafish. We show that DICM can sometimes circumvent the need for fluorescence based techniques, augmenting the number of parameters obtainable per experiment when used alongside LSFM, and that DICM can be used to augment each experiment by imaging complementary features, such as non-fluorescent local environments near fluorescent samples (e.g. fluorescent enteric neurons imaged alongside the non-fluorescent gut wall), interactions between fluorescent and non-fluorescent samples (e.g. bacteria), and more.

8:24AM Y47.00003 Mechanical origins of rightward torsion in early chick brain development

Z. CHEN, Dartmouth College, Q. GAO, Fuzhou University, E. DAI, L. TABER, Washington University — During early development, the neural tube of the chick embryo undergoes a combination of progressive ventral bending and rightward torsion. This torsional deformation is one of the major organ-level left-right asymmetry events in development. Previous studies suggested that bending is mainly due to differential growth, however, the mechanism for torsion remains poorly understood. Since the heart almost always loops rightwards that the brain twists, researchers have speculated that heart looping affects the direction of brain torsion. However, direct evidence is lacking, nor is the mechanical origin of such torsion understood. In our study, experimental perturbations show that the bending and torsional deformations in the brain are coupled and that the vitelline membrane applies an external load necessary for torsion to occur. Moreover, the asymmetry of the looping heart gives rise to the chirality of the twisted brain. A computational model and a 3D printed physical model are employed to help interpret these findings. Our work clarifies the mechanical origins of brain torsion and the associated left-right asymmetry, and further reveals that the asymmetric development in one organ can induce the asymmetry of another developing organ through mechanics, reminiscent of D’Arcy Thompson’s view of biological form as “diagram of forces”.

8:36AM Y47.00004 ABSTRACT WITHDRAWN

8:48AM Y47.00005 Modeling the fusion of cylindrical bioink particles in post bioprinting structure formation

M. MCCUNE, A. SHAFIEE, G. FORGACS, I. KOSZTIN, University of Missouri — Cellular Particle Dynamics (CPD) is an effective computational method to describe the shape evolution and biomechanical relaxation processes in multicellular systems. Thus, CPD is a useful tool to predict the outcome of post-printing structure formation in bioprinting. The predictive power of CPD has been demonstrated for multicellular systems composed of spherical bioink units. Experiments and computer simulations were related through an independently developed theoretical formalism based on continuum mechanics. Here we generalize the CPD formalism to (i) include cylindrical bioink particles often used in specific bioprinting applications, (ii) describe the more realistic experimental situation in which both the length and the volume of the cylindrical bioink units decrease during post-printing structure formation, and (iii) directly connect CPD simulations to the corresponding experiments without the need of the intermediate continuum theory inherently based on simplifying assumptions.

9:00AM Y47.00006 Modeling the Epithelial Morphogenesis of Germ Band Retraction in Three Dimensions

W. TYLER MCCLEERY, Vanderbilt Univ., J. VELDHUIS, G. WAYNE BRODLAND, Univ. of Waterloo, S. CREWS, M. SHANE HUTSON, Vanderbilt Univ. — Embryogenesis of higher-order organisms is driven by an intricate coordination of cellular mechanics. Mechanical analysis of certain developmental events, e.g., dorsal closure in the fruit fly D. melangaster, has been sufficiently described using two-dimensional models. Here, we present a three-dimensional modeling technique to investigate germ band retraction (GBR) - a whole-embryo, irreducibly 3D morphogenetic event. At the start of GBR, the epithelial tissue known as the germ band is initially wrapped around the posterior end of an ellipsoidal fly embryo. This tissue then retracts as an adjacent organ-level left-right asymmetry event. Previous studies suggested that bending is mainly due to differential growth, however, the mechanism for torsion remains poorly understood. Since the heart almost always loops rightwards that the brain twists, researchers have speculated that heart looping affects the direction of brain torsion. However, direct evidence is lacking, nor is the mechanical origin of such torsion understood. In our study, experimental perturbations show that the bending and torsional deformations in the brain are coupled and that the vitelline membrane applies an external load necessary for torsion to occur. Moreover, the asymmetry of the looping heart gives rise to the chirality of the twisted brain. A computational model and a 3D printed physical model are employed to help interpret these findings. Our work clarifies the mechanical origins of brain torsion and the associated left-right asymmetry, and further reveals that the asymmetric development in one organ can induce the asymmetry of another developing organ through mechanics, reminiscent of D’Arcy Thompson’s view of biological form as “diagram of forces”.

9:12AM Y47.00007 Signaling Delays Preclude Defects in Lateral Inhibition Patterning

R. J. RIEDEL-KRUSE, D. GLASS, X. JIN, Stanford University, Bioengineering — Developmental biology is extraordinarily robust in its ability to self-organize spatiotemporal patterns despite an intrinsically noisy set of parts. Lateral inhibition is a classic example of a mechanism behind such precise emergent behavior. However, the models through which we understand lateral inhibition’s capabilities usually assume that cells signal to one another without delay, a supposedly minor source of error at most. Here we explicitly investigate the effects of signaling delays as well as their relation to cis-interactions in lateral inhibition patterning. We reduce the patterning problem effectively to a two-parameter phase space (signaling delay and coupling strength), and we found that rather than being a source of error, signaling delays enable significant decrease of error rates. Together with cis-interactions, these delays lead to patterning that can be both fast and robust to noise and parameter variation. This suggests that overlooking time delays in developmental signaling does not just ignore a potential source of error, but rather ignores a knob with which evolution may tune patterning robustness in general.
Waves of ratcheting cancer cells in growing tumor tissue layer

YANG, TAE KWON, HYUN KIM, KYOUNG LEE, Korea Univ, CENTER FOR CELL DYNAMICS TEAM — Over many years researchers have shown that the mechanical forces generated by, and acting on, tissues influence the way they grow, develop and migrate. As for cancer research goes, understanding the role of these forces may even be as influential as deciphering the relevant genetic and molecular basis. Often the key issues in the field of cancer mechanics are to understand the interplay of mechanics and chemistry. In this study, we discuss very intriguing population density waves observed in slowly proliferating tumor cell layers. The temporal periods are around 4 hr and their wavelength is in the order of 1 mm. Tumor cell layer, which is initially plated in a small disk area, expands as a band of tumor cells is “ratcheting” in concert in radially outward direction. By adding Cytochalasin D and Latrunculin B, an inhibitor of actin polymerization, or Mytomycin, a chemotherapeutic agent, we could halt and modulate the wave activities reversibly. The observed waves are visually quite similar to those of chemotaxing Dictostelium discoideum amoeba population, which are driven by nonlinear chemical-reaction-diffusion waves of cAMP. So far, we have not been able to show any relevant chemotactic factors inducing the collective behavior of these tumor cells. Researchers have been investigating how forces from both within and outside developing cancer cells interact in intricate feedback loops. This work reports the example of periodic density waves of tumor cells with an explanation purely based on nonlinear mechanics.

Pattern formation in a growing bacterial colony facilitated by extra-cellular polymeric substances

PUSHPITA GHOSH, Center for Theoretical Biological Physics, Rice University, Texas, 77005, USA, JAGANNATH MONDAL, Department of Chemistry, Columbia University, New York 10027, USA, ESHEL BEN-JACOB, HERBERT LEVINE, Center for Theoretical Biological Physics, Rice University, Texas, 77005, USA — Self-organization in bacterial colony is quite pervasive and diverse phenomena. Bacteria are known to self-organize into multicellular communities, commonly known as biofilms, in which microbial cells live in close association with a solid surface and are embedded in a self-produced extracellular polymeric substances (EPS). In such dense systems mechanical interactions among the structural components can be expected to significantly contribute to the morphological properties. By a simple particle-based simulation model of nonmotile rod-shaped bacterial cells and EPS secreted in a growing colony, we investigate how the combined mechanical effects can give rise naturally spatial heterogeneity observed in a biofilm. In our individual-based simulation model all the components interact mechanically via repulsive forces by pushing each other away as bacterial cells grow and divide consuming diffusing nutrient and produce EPS. We show that mechanical interactions control the collective behavior of the system, particularly, we show that the presence of non-adSORbing EPS leads spontaneous aggregation of bacterial cells by depletion attraction and generates phase separated patterns in a nonequilibrium growing colony.

Evaporation-driven convection observed in a suspension of non-motile bacteria

JOCELYN DUNSTAN, DAMTP, Univ of Cambridge, KYOUNG JIN LEE, Physics department, Korea University, SIMON PARK, Faculty of Health and Sciences, Univ of Surrey, RAYMOND E. GOLDSTEIN, DAMTP, Univ of Cambridge — We report a novel form of convection in a suspension of non-motile bioluminescent bacteria. The patterns appear like those of conventional bioconvection driven by oxygenaxis, yet the bacteria are observed to have limited if any motility. While the phenomenon also resembles chemo-convection, in which a chemical reaction (or metabolic activity) alters the local buoyancy balance at the air-water interface, the convention actually derives from evaporation of the salty bacterial growth medium. We corroborate this through control experiments using polystyrene beads in pure and salty water, and establish that there is a threshold of salt concentration needed to observe plumes. The dynamics of the plumes is rich, with striking coalescence events and a complex internal structure. A mathematical model is formulated for the process and studied analytically and numerically, reproducing most of the observed experimental features. Evaporation-driven convection on the millimeter scale has not been studied extensively and its effect may have been underestimated in a variety of contexts. It may naturally occur in marine settings.

Optoporation to deliver impermeable molecules and genes for visualization and activation of cells

KAMAL DHAKAL, SUBRATA BATBYAL, YOUNG-TAE KIM, SAMARENDRA MOHANTY, Univ of Texas, Arlington — Visualization, activation, and detection of the cell(s) and their electrical activity require delivery of exogenous impermeable molecules and targeted expression of genes encoding labeling proteins, ion-channels and voltage indicators. While genes can be delivered by viral vector to cells, delivery of other impermeable molecules into the cytoplasm of targeted cells requires microinjection by mechanical needle or microelectrodes, which pose significant challenge to the viability of the cells. Further, it will be useful to localize the expression of the targeted molecules not only in specific cell types, but to specific cells in restricted spatial regions. Here, we report use of focused near-infrared (NIR) femtosecond laser beam to transiently perforate targeted cell membrane to insert genes encoding blue light activatable channelrhodopsin-2 (ChR2) and red-shifted opsin (ReachR). Optoporation of nanomolar concentrations of rhodamine phallodin (an impermeable dye molecule for staining filamentous actin) into targeted living mammalian cells (both HEK and primary cortical neurons) is also achieved allowing imaging of dynamics and intact morphology of cellular structures without requiring fixation.

Corn-in-chip: Mesofluidic Device for Corn Root

KEVIN KREIS, SANGJIN RYU, University of Nebraska-Lincoln — Plants have a collection of beneficial microorganisms in a region surrounding their roots called the rhizosphere. Although rhizosphere management could increase crop yield, little is known about the interaction between plant roots and their associated microorganisms. Thus we aim to simulate the rhizosphere and monitor root-microbe interactions in the lab environment, and have chosen corn as a model plant because of its economic significance. Here we present our preliminary study to develop a transparent mesofluidic device accommodating the root of corn seedlings into its channel and allowing further growth of the root.

Excitable Pattern Formation in Inhomogeneous Systems

KAUMUDI PRABHAKARA, Cornell University, Max-Planck Institute for Dynamics and Self-Organisation, AZAM GHOŁAMI, VLADIMIR ŽYKOV, Max-Planck Institute for Dynamics and Self-Organisation — On starvation, the amoebae Dictyostelium discoideum signal via the chemo-attractant cyclic adenosine monophosphate (cAMP). The amoebae sense cAMP through membrane receptors and produce their own cAMP. Simultaneously they produce a basal level of Phosphodiesterase, an enzyme that degrades cAMP. Soon a pattern of rotating spiral waves or circular waves is formed at the multi-cellular level. The causal reasons for the selection of one or the other pattern are still unclear. Here we report experimental and theoretical investigations of the pattern-formation of mixtures of cells starved for different times. The excitability of the amoebae depends on the starvation time due to time dependent gene expressions. Cells starved for longer times are known to exhibit increased excitability. We report phase maps of the patterns for mixtures of different combinations of excitability. Numerical simulations of a modified Kessler-Levine model allow us to explain the experimental results and provide new insights into the dynamical behavior of the system.

This work is supported by the Max Planck Society.
8:00AM | Y49.00001 Yielding, Plasticity, and Microstructure in a 2D Jammed Material under Shear Deformation. PAOLO ARRATIA, NATHAN KEIM, University of Pennsylvania — In this talk, we discuss an experimental investigation on the yielding and plastic deformation of disordered solids. Experiments are performed on colloidal particles that are adsorbed at an oil-water interface and form a dense disordered monolayer. The rheological properties (G', G'') of this dense monolayer are obtained in a custom-built interfacial stress rheometer that uses a magnetic needle within the material. This configuration allows for the simultaneous characterization of both microstructure (tracking ~ 10^5 particles) and bulk rheology. Results show that for oscillatory shear below a certain strain amplitude, the microstructure becomes reversible after a transient. Above this strain amplitude, the microstructure continues to evolve through many irreversible events. We argue that this boundary between a reversible and irreversible steady state is yielding transition, and that our experiments measure a meaningful irreversible event. Further, we find that reversible plastic deformation is possible. That is, the material can reorganize itself so that the link between plasticity and irreversibility is broken: the material flows slightly, and yet at the end of each deformation cycle, it is exactly unchanged.

3 This work is supported by Taiwan MOST grant 100-2112-M-003-001-MY3.

8:12AM | Y49.00002 Stress localization, stiffening, and yielding in a model colloidal gel. EMANUELA DEL GADO, Department of Physics and Institute for Soft Matter Synthesis and Metrology, Georgetown University, JADER COLOMBO, Department of Civil, Environmental and Geomatic Engineering, ETH Zurich, GEORGETOWN UNIVERSITY COLLABORATION, ETH ZURICH COLLABORATION — We investigate the yielding of a model colloidal gel using numerical simulations and different shearing protocols. Under increasing deformation, the elastic regime is followed by a significant stiffening before yielding takes place. A space-resolved analysis of deformations and stresses unravel how the complex load curve observed is the result of stress localization and that the yielding can take place by breaking a very small fraction of the network connections. The strong localization of tensile stresses triggers the breaking of a few network nodes at around 30% of strain and increasing the deformation further favors breaking but also shear-induced bonding, eventually leading to the damage and the reorganization of the gel structure upon yielding. In particular, at low enough shear rates, density and velocity profiles display significant spatial inhomogeneity during yielding in agreement with experimental observations.

8:24AM | Y49.00003 Structure and Rheology of Concentrated Emulsions. JUNG-REN HUANG, YI-CIAN LAI, CHE-HAO OU, Physics Department, National Taiwan Normal University, JIH-CHIANG TSAI, Institute of Physics, Academia Sinica — We construct a shearing apparatus combining light scattering and stress measurement to study the structure and rheology of concentrated monodisperse emulsions. The emulsions are subjected to oscillatory shear of variable amplitude and frequency. The light scattering data reflect droplet deformation as well as shear history-dependent inter-droplet structures. The stress measurements display pseudoplasticity near zero shear rate and shear-thinning behavior at finite shear rates. In addition, the time-resolved measurement of light scattering and rheology reveal detailed information about the complex structure-rheology relationship of emulsions. Shear disorders the droplets at low and high shear rates but induces order at medium shear rates. Furthermore, the effective viscosity increases as the degree of inter-droplet order decreases.

8:36AM | Y49.00004 The viscous forces acting on quasi-2D emulsions under fast flow. CARLOS ORELLANA, XIA HONG, JANNA LOWENSOHN, ERC WEEKS, Emory University — We study the flow of dense emulsions in a quasi-two-dimensional sample chamber. Our samples are oil-in-water emulsions confined between two close-spaced parallel plates, so that the oil droplets are deformed into pancake shapes. By means of microscopy, we measure the droplet positions and their deformation, which is related to the forces on the individual droplet. Here we study the velocity dependence of the force on the droplets, and show that the main contribution is from the viscous friction between droplets rather than from viscous drag from the two confining plates. Our results can be applied to study the forces and rearrangements in fast flow in amorphous materials.

8:48AM | Y49.00005 Linear and nonlinear rheology of dense emulsions across the glass and the jamming regimes. FRANK SCHEFFOLD, CHI ZHANG, Department of Physics, University of Fribourg, THOMAS G. MASON, Department of Chemistry and Biochemistry, University of California Los Angeles — We discuss the linear and nonlinear rheology of concentrated silicone oil-in-water emulsions, amorphous disordered solids composed of repulsive and deformable soft colloidal spheres. Based on recent results from simulation and theory, we derive quantitative predictions for the dependences of the elastic shear modulus and the yield stress on the effective droplet volume fraction [1]. The remarkable agreement with experiments we observe supports the scenario that the repulsive glass and the jammed state can be clearly identified in the rheology of soft gels under shear.

9:00AM | Y49.00006 The Role of Free Surfaces on Plastic Deformation of Colloidal Micropillars. DANIEL STRICKLAND, ALEXANDER KLEBNIKOV, University of Pennsylvania, Department of Materials Science and Engineering, JYO LYN HOR, DAEYEON LEE, University of Pennsylvania, Department of Chemical and Biomolecular Engineering, DANIEL GIANOLA, University of Pennsylvania, Department of Materials Science and Engineering — The effect of free surfaces on the strength and deformation behavior of amorphous solids remains an area of intensive research in materials science. We present experiments on the evolution of particle-level strain in amorphous colloidal micropillars compressed uniaxially. The unique micropillar geometry allows us to study the effect of free surfaces, which are believed to be fertile sites for STZ activity, on deformation behavior. The micropillars, which are composed of fluorescent 3 um PMMA particles, are suspended in a fluid so that we can use laser scanning confocal microscopy to image through the micropillar at each increment of macroscopic deformation. The particle positions, which are measured using image analysis algorithms, are recorded to track the positions of more than 100,000 individual particles during the duration of a compression experiment. Particle-level position information allows us to quantify the spatiotemporal evolution of microscopic strain with macroscopic strain and explore differences in deformation behavior between bulk and surface regions.

2 National Science Foundation through PENN MRSEC DMR-1120901.

9:12AM | Y49.00007 Echoes in x-ray speckles track nanometer-scale plastic events in colloidal gels under shear. ROBERT LEHENY, Johns Hopkins University, MICHAEL ROGERS, University of Ottawa, KUI CHEN, Johns Hopkins University, LUKAS ANDRZEJEWSKI, University of Ottawa, SURESH NARAYANAN, Argonne National Laboratory, SUBRAMANIAM RAMAKRISHNAN, FAMU, JAMES HARDEN, University of Ottawa — Any solid under applied stress possesses an elastic limit above which it yields. The microscopic signatures of yield are irreversible changes to the material’s structure. We describe x-ray photon correlation spectroscopy experiments on a concentrated nanocolloidal gel subject to in situ oscillatory shear strain that provide information about the spatial character of rearrangements above yielding at the nanometer scale. The oscillatory strain causes periodic echoes in the x-ray speckle pattern, creating peaks in the intensity autocorrelation function. The peak amplitudes are attenuated above a threshold strain, signaling the onset of irreversible particle rearrangements. The gel displays strain softening well below the threshold, indicating a range of strains at which deformations are nonlinear but reversible. Above the threshold strain, the peak amplitudes decay exponentially with the number of shear cycles, demonstrating that all regions in the sample are equally susceptible to yielding and that the probability of a region yielding is independent of previous shear history. The wave-vector dependence of the decay rate reveals a power-law distribution in the size of rearranging regions, suggesting a nonequilibrium critical transition at yielding.
9:24AM Y49.00008 Yielding of colloidal gels under steady and oscillatory shear. GEORGE PETEKIDIS, ESMAEEL MOGHIMI, NICK KOUKAKIS, IESL-FORTH, FORTH TEAM — The structural and rheological properties of intermediate volume fraction colloidal gels are examined during and after steady and oscillatory shear flow using rheometry, confocal microscopy, light scattering and Brownian Dynamics simulations. Our main objective is to rationalize the microscopic mechanisms through which one can tune the mechanical properties of such metastable colloidal gels by imposing different types of external shear and flow. Experimentally, the gels consist of model hard sphere particle dispersions of \( \varphi = 0.44 \) with the addition of non-adsorbing linear chains, while BD simulations are conducted for hard spheres with the superposition of an AO potential for depletion attractions. Structural analysis shows that variation of the applied shear rate produces strong changes in the structure of the gels both when under shear and during gel reformation at cessation. Larger rates are characterized by disperse particles and the total breakage of structures at rest, which after cessation evolve with time into strong solids with relatively homogeneous structures. However, smaller rates show large inhomogeneous structures under flow, which do not evolve after cessation and additionally exhibit reduced mechanical stability and as such are weaker solids. Furthermore oscillatory shear is far more efficient than steady shear creating gels with stronger differences in their elastic modulus. Thus by tuning the way a gel is sheared, one may vary the final strength and structure of the resulting gel. Work in collaboration with R. Besseling, W. C. K. Poon and J. F. Brady.

9:36AM Y49.00009 Matrix polymer species have distinct effects on the mechanics of bacterial biofilms. KRISTIN KOVACH, MEGAN DAVIS-FIELDS, VERNITA GORDON, Univ. of Texas, Austin — Biofilms are aggregates of microorganisms embedded in a self-produced extracellular polymer matrix. The matrix confers protection to these microorganisms against mechanical and chemical stresses that they may experience in their environment. The bacterium *Pseudomonas aeruginosa* that they experience in their environment. The bacterium *Pseudomonas aeruginosa* is widely used as a model biofilm-forming organism because it is an opportunistic pathogen common in hospital-acquired infections, in chronic wounds, and in cystic fibrosis lung disease. *P. aeruginosa* strain PA01 forms biofilms that are primarily structured by the extracellular polysaccharides Pel and Psl. Using bulk rheological measurements, we show that these polysaccharides each play a unique role in the mechanical robustness of the biofilm. Pel increases the elastic storage modulus while Psl increases the ductility of the biofilm. Increased expression of either Psl or Pel increases the yield stress by about the same amount. Identifying the mechanism(s) by which these polymers contribute to the mechanical toughness of the biofilm could allow new approaches to effective biofilm clearance, by revealing targets for disruption that would weaken the biofilm.

9:48AM Y49.00010 ABSTRACT WITHDRAWN —

10:00AM Y49.00011 A simple feature of yielding of dense suspensions of soft micro-hydrogel particles. KENJI URAYAMA, Dept. Macromol. Sci. & Eng., Kyoto Institute of Technology, TAKU SAEKI, SHEN CONG, Dept. Mater. Chem., Kyoto University, SYOTA URATANI, Dept. Macromol. Sci. & Eng., Kyoto Institute of Technology, TOSHIKAZU TAKIGAWA, Dept. Mater. Chem., Kyoto University, MASAKI MURAI, DAISUKE SUZUKI, Shinshu University — The highly dense suspensions of soft micro-hydrogels with a narrow size distribution, which form a regular lattice structure, exhibit a simple feature in the yielding behavior: the yield strain \( \gamma_c \) (ca. 2.5% and ca. 4.8% for NIPNMA) and NIPNA hydrogel particles, respectively) is nearly independent of the cross-link concentration, particle diameter, and particle concentration \( c \) in the limited \( c \) range examined here, and \( \gamma_c \) is almost constant in a wide range of equilibrium shear moduli over two orders of magnitude. Further, no appreciable difference in \( \gamma_c \) is observed in the dense pastes with crystalline and glassy structures which are formed by mono- and bidisperse microgels, respectively. In addition, the highly dense suspensions of NIPA core–NIPMA shell microgels are similar in \( \gamma_c \) to those of NIPMA microgels. These results indicate that \( \gamma_c \) for the highly dense suspensions of soft micro-hydrogels depends primarily on the kind of constituent polymer near the particle surface. The yield strain \( \gamma_c \) is expected to be governed by short-range interactions such as adhesion and friction. [Reference] K. Urayama, T. Saeki, S. Cong, S. Uratani, T. Takigawa, M. Murai, Suzuki, Soft Matter, DOI: 10.1039/c4sm01841a.

10:12AM Y49.00012 Plasticity and fracture of curved colloidal crystal shells. CARLOTTA NEGGI, ALESSANDRO SELLERIO, IENI CNR, Institute for Energetics and Interphase, National Research Council, Via R. Cozzi 53, Milano 20125, Italy, M.-CARMEN MIGUEL, Departamento de Fisica Fonamental, Facultad de Fisica, Universitat de Barcelona, Av. Diagonal 645, 08028 Barcelona, Spain, STEFANO ZAPPERI, IENI CNR, Institute for Energetics and Interphase, National Research Council, Via R. Cozzi 53, Milano 20125, Italy — Crystalline shells display peculiar equilibrium properties resulting from the interplay between geometrically necessary topological defects and curvature induced stresses. Here we report the results of large scale numerical simulations of the deformation of colloidal particles arranged in crystalline shells showing that the dynamics of topological defects exhibits a rich and non-trivial phenomenology. Depending on the mode of deformation, we observe intermittent plastic deformation with collective particle reorganization mediated by the proliferation of disclinations pairs and grain boundary reorientation or abrupt structural failure induced by crack nucleating at defects. Our work clarifies the role of topology and curvature in the mechanical deformation of crystalline shells.

Friday, March 6, 2015 8:00AM - 11:00AM —

Session Y51 DCMP: Invited Session: Origin and Manifestations of Electronic Nematicity in Iron-Based Superconductors

Grand Ballroom C1

8:00AM Y51.00001 A New Magnetic Phase in Hole-Doped BaFe\(_2\)As\(_2\): Implications for the Origin of Nematicity. RAYMOND OSBORNE, Argonne National Laboratory — Establishing the origin of nematic order has emerged as one of the most important goals of research into iron pnictides and chalcogenides, because of its implications for the origin of their unconventional superconductivity [1]. It is well known that superconductivity emerges when antiferromagnetism is suppressed with doping or pressure. Across the phase diagram, the magnetic transition occurs just below, or is coincident with, a structural phase transition from tetragonal (\( C\_4\)) to orthorhombic (\( C\_2\)) or nematic, symmetry. A symmetry analysis indicates that the \( C\_2 \) transition is electronically driven, but it could be due either to orbital interactions that then induce magnetic stripe order or to magnetic interactions that then induce orbital order. In the latter, magnetic fluctuations from interactions between the hole pockets at \( Q = 0 \) and the electron pockets at \( Q = (\pi, 0) \) and \( Q = (0, \pi) \) break the Ising X/Y symmetry before time-reversal symmetry is broken. As part of a comprehensive neutron diffraction study of the phase diagram of hole-doped BaFe\(_2\)As\(_2\) [2], we have recently observed an entirely new magnetic phase that occurs close to the suppression of the \( C\_2 \) phase, in which the spins reorient along the c-axis and \( C\_4 \) symmetry is restored [3]. This reentrant \( C\_4 \) transition has now been observed in other hole-doped compounds as well. In spin-nematic theory, a restoration of \( C\_4 \) symmetry is predicted to occur when doping weakens Fermi surface nesting, favoring an order parameter that involves \( Q\_X \) and \( Q\_Y \) simultaneously, so our observation provides evidence for magnetically-driven models of nematicity.


1Supported by the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division
8:36AM Y51.00002 Who is in charge of the nematic order in iron-based superconductors?. ANDREY CHUBUKOV, Univ of Minnesota — Although the existence of nematic order in iron-based superconductors is now a well-established experimental fact, its origin remains controversial. Nematic order breaks the discrete lattice rotational symmetry by making the $x$- and $y$-directions in the iron plane non-equivalent. This can happen because of a regular structural transition or due to a electronically-driven instability — in particular, orbital order and spin-driven Ising-nematic order. The latter is a magnetic state that breaks rotational symmetry but preserves time-reversal symmetry. Symmetry dictates that the development of one of these orders immediately induces the other two, making the origin of nematicity a physics realization of the "chicken and egg problem." will argue that the evidence strongly points to an electronic mechanism of nematicity, placing nematic order in the class of correlation-driven electronic instabilities, like superconductivity and density-wave transitions. I will discuss different microscopic models for nematicity and link them to the properties of the magnetic and superconducting states, providing a unified perspective on the phase diagram of the iron pnictides. (Based on R.M. Fernandes, A.V. Chubukov, and J. Schmalian, Nature Physics 10, 97 (2014).)

9:12AM Y51.00003 Nematic charge fluctuations in iron-based superconductors by Raman scattering . YANN GALLAIS, Université Paris Diderot — Electronic analogues of nematic states, in which rotational symmetry is broken but translational invariance is preserved, have been proposed in a variety of correlated materials, such as quantum Hall systems, cuprates, ruthenates, heavy fermions, and, more recently, iron based superconductors. In the iron-based superconductors (Fe SC) several experiments have collected evidence that the tetragonal- to-orthorhombic structural transition is driven not by the lattice, but by electronic nematicity. However it remains a challenge to disentangle the roles of the lattice, spin and charge/orbital degrees of freedom in driving the nematic instability. In my talk I will discuss electronic Raman scattering measurements which demonstrate the presence of charge nematic fluctuations in the tetragonal phase of several Fe SC systems. I will discuss the implications of our results for the mechanism of the nematic/orthorhombic transition in these systems.

9:48AM Y51.00004 Unusual disorder-limited transport in Fe-based superconducting materials1 , PETER HIRSCHFELD, University of Florida — The unusual temperature dependence of the resistivity and its in-plane anisotropy observed in the Fe-based superconducting materials, particularly Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$, has been a longstanding puzzle. I discuss first the effect of impurity scattering on the temperature dependence of the average resistivity within a simple two-band model of a dirty spin density wave (SDW) metal. Within this framework[1], many of the qualitative features of the transport can be understood by accounting for the growth of spin correlations pinned by impurities above the Neel temperature, and SDW-induced Lifshitz transitions below. I then discuss implications of this picture for the anisotropy observed in unwinned crystals. [1] Y. Wang, M. N. Gaviassorio, B. M. Andersen, M. Tomic, H. O. Jeschke, Roser Valenti, I. Paul and P. J. Hirschfeld, arXiv:1408.1933

1Research partially supported by NSF-DMR-1407502

10:24AM Y51.00005 Electronic nematicity in Iron Pnictide superconductors probed via STM , ABHAY PASUPATHY, Columbia University — The microscopic origin of electronic nematicity and its relationship to superconductivity in the iron pnictides remains poorly understood. I will present recent scanning tunneling microscopy (STM) and spectroscopy (STS) measurements that directly visualize the nematicity in the electronic states of the pnictide superconductor Na(Fe,Co)As. The spatial and energy dependence of features seen in the spectroscopic images sheds light on the nature of the important interactions responsible for nematicity in this material, and measurements taken above and below the superconducting transition temperature reveal the interaction between the nematic electronic structure and superconductivity. I will describe measurements across the entire temperature-doping phase diagram and present a simple, unified picture for understanding nematicity as visualized by STM in the pnictides.

Friday, March 6, 2015 8:00AM - 10:24AM –
Session Y52 DCMP: Invited Session: Geometrical Properties of Quantum Hall Fluids Grand Ballroom C2 - Eduardo Fradkin, University of Illinois at Urbana-Champaign

8:00AM Y52.00001 Geometry of Fractional Quantum Hall Fluids1 , GIL YOUNG CHO, University of Illinois at Urbana-Champaign — Fractional quantum Hall (FQH) fluids of two-dimensional electron gases (2DEG) in large magnetic fields are fascinating topological states of matter. As such they are characterized by universal properties such as their fractional quantum Hall conductivity, fractionally charged anyonic excitations and a degeneracy of topological origin on surfaces with the topology of a torus. Quite surprisingly these topological fluids also couple to the geometry on which they 2DEG resides and have universal responses to adiabatic changes in the geometry. These responses are given by a Wen-Zee term (which describes the coupling of the currents to the spin connection of the geometry) and a gravitational Chern-Simons term which reflects the universal energy and momentum transport along the edges of the FQH state. We use a field theory of the FQH states to derive these universal responses [1,2]. To account for the coupling to the background geometry, we show that the concept of flux attachment needs to be modified and use it to derive the geometric responses from Chern-Simons theories. We show that the resulting composite particles minimally couple to the spin connection of the geometry[1]. Taking account of the framing anomaly of the quantum Chern-Simons theories[2], we derive a consistent theory of geometric responses from the Chern-Simons effective field theories and from parton constructions, and apply it to both abelian and non-abelian states.


1This work was supported in part by the NSF grant DMR-1408713.

8:36AM Y52.00002 Theory of the quantum Hall nematic transition1 , JOSEPH MACIEJKO, University of Alberta — The discovery of novel types of macroscopic order in quantum many-particle systems is an important goal of condensed matter physics. The fractional quantum Hall (FQH) nematic is a conjectured state of matter in which a fractional quantized Hall conductivity indicative of topological order coexists with the spontaneous breaking of rotational symmetry characteristic of a nematic liquid crystal. Recent experiments suggest that this state may form in 2D electron gases in the first Landau level. In this talk I will present a theory of the quantum phase transition between an isotropic FQH liquid and a FQH nematic state.

1Support from the Simons Foundation and NSERC of Canada are gratefully acknowledged.
9:12AM Y52.00003 Hall viscosity

NICOLAS READ, Yale University — Viscosity is a transport coefficient relating to transport of momentum, and usually thought of as the analog of friction that occurs in fluids and solids. More formally, it is the response of the stress to the gradients of the fluid velocity field, or to the rate of change of strain (derivatives of displacement from a reference state). In general, viscosity is described by a fourth-rank tensor. Invoking rotation invariance, it reduces to familiar shear and bulk viscosity parts, which describe dissipation, but it can also contain an antisymmetric part, analogous to the Hall conductivity part of the conductivity tensor. In two dimensions this part is a single number, the Hall viscosity. Symmetry of the system under time reversal (or, in two dimensions, reflections) forces it to vanish. In quantum fluids with a gap in the bulk energy spectrum and which lack both time reversal and reflection symmetries the Hall viscosity can be nonzero even at zero temperature. For integer quantum Hall states, it was first calculated by Avron, Seiler, and Zograf, using a Berry curvature approach, analogous to the Chern number for Hall conductivity. In 2008 this was extended by the present author to fractional quantum Hall states and to BCS states in two dimensions. I found that the general result is given by a simple formula $n\pi/2$, where $n$ is the particle number density, and $s$ is the "orbital spin" per particle. The spin $s$ is also related to the shift $S$, which enters the relation between particle number and magnetic quantum $\nu=\pm S$, and ground state on a surface of non-trivial topology with introducing defect excitations, by $s=2\nu$; the connection was made by Wén and Zee. The values of $s$ and $S$ are rational numbers, and are robust—unchanged under perturbations that do not cause the bulk energy gap to collapse—provided rotation as well as translation symmetry are maintained. Hall viscosity can be measured in principle, though a simple way to do so is lacking. It enters various theoretical calculations of other properties, and can be used as a diagnostic tool to distinguish phases. The talk will review these results, describing different microscopic approaches to calculating Hall viscosity, robustness, and the relation with effective field theories.

1Research supported by NSF DMR

9:48AM Y52.00004 Spacetime symmetries, Newton-Cartan geometry and the quantum Hall effect

DAM SON, University of Chicago — Spacetime symmetries place powerful constraints on the physics of quantum Hall states from spacetime symmetries. These symmetries can be seen by putting the quantum Hall system on a curved manifold. By doing so, one discovers that the action is invariant with respect to time-preserving diffeomorphisms. The diffeomorphism invariance remains nontrivial on the lowest Landau level when inter Landau level mixing is negligible. In the talk we will extract physical consequences of the diffeomorphism invariance for physical observables in flat space. In particular, we relate the leading dependence of the Hall conductivity on wavenumber to the shift. We show how the spectral densities of the components of the stress tensor satisfy several sum rules, one of which involves the static projected structure factor and another involves the shift. From the sum rules one can deduce an inequality between the leading $k^2$ coefficient of the static structure factor and the shift. The inequality is saturated for a large class of trial wavefunctions. The sum rules suggest that if the magneto-roton continues to exist as a sharp resonance at small wavenumber, it should be a "chiral massive graviton," i.e., a particle with spin 2 of one circular polarization. This is demonstrated explicitly in a toy model, where which the sum rules are saturated by one single gapped mode. We argue that the circular polarization of the magneto-roton can be in principle observed by polarized Raman scatterings. The most convenient formalism to write down effective actions satisfying local diffeomorphism invariance turns out to be the Newton-Cartan formalism, introduced by Elie Cartan in 1922-1923 in his attempt to rewrite Newton's gravity in a coordinate-invariant way. We describe the structure of the Newton-Cartan space, including the construction of the connection.

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**Friday, March 6, 2015 8:00AM - 11:00AM — Session Y53 DCMP: Invited Session: Cuprate Pseudogap, Charge Density Wave and Pair Density Wave**

Grand Ballroom C3 - Steven Kivelson, Stanford University

8:00AM Y53.00001 The microscopic structure of charge order in cuprates

RICCARDO COMIN, University of British Columbia — The spontaneous self-arrangement of electrons into periodically modulated patterns, a phenomenon commonly termed as charge order or charge-density-wave (CDW), has recently resurfaced as a prominent, universal ingredient for the physics of high-temperature superconductors. In such context, resonant x-ray scattering (RXS) has rapidly become the technique of choice for the study of charge order in momentum space, owing to its ability to directly identify a breaking of translational symmetry in the electronic density. In this talk, I will present our recent RXS studies of charge order in Bi2201, which reconciled years of apparently disconnected findings in different cuprate families by showing how charge order is a universal phenomenon in hole-doped cuprates [R. Comin, et al., Charge Order Driven by Fermi-Arc Instability in Bi2Sr2–xLaSrCuO6–y, Science 343, 390 (2014)]. Contextually, I will discuss very recent findings of charge order in NCCO, which project such phenomenology to the electron-doped materials [E. da Silva Neto*, R. Comin*, et al., Charge ordering in the electron-doped superconductor Nd2–xCeCuO4, accepted (2014) – preprint at: http://arxiv.org/abs/1410.2253]. Furthermore, in YBCO, we have succeeded to fully reconstruct the CDW order parameter in the two-dimensional momentum space and demonstrate how resonant x-ray methods can be used to peer into the microscopic structure and symmetry of the charge order. Using this new method, we have been able to demonstrate the presence of charge stripes at the nanoscale [R. Comin, et al., Broken translational and rotational symmetry via charge stripe order in underdoped YBa2Cu3O6–y, under review (2014)], as well as evaluate the local symmetry in the charge distribution around the Cu atoms, which was found to be predominantly of a d-wave bond-order type [R. Comin, et al., The symmetry of charge order in cuprates, under review (2014) – preprint at: http://arxiv.org/abs/1402.5415].

8:36AM Y53.00002 Searching for spectroscopic signatures of density wave correlations in cuprates

RUI-HUA HE, Boston College — Recent developments in the research on high-temperature cuprate superconductors highlight the relevance of some density wave correlations to the superconductivity and its normal state in this generic class of materials. Depending on specific cuprate systems, these density wave correlations can have diverse manifestations in different (charge, spin, pairing) sectors and likely break (time reversal, space inversion, point group, gauge) symmetries in addition to the lattice translation. A unified understanding of their microscopic nature hinges on further characterizations using direct (imaging scattering) probes for these correlations themselves, as well as indirect probes for their interplay with other degrees of freedom in the system. ARPES can provide information about a density wave order through probing modifications in the electron structure it induces, while other spectroscopy techniques can shed unique lights on the broken symmetry aspect of the order. In this talk, I will review the density-wave signatures that have been or yet to be found in ARPES mainly in terms of the spectral weight, energy gap, and renormalized band dispersions. These experimental observations/proposals, coupled with simple theoretical modeling, promise new insights into the (wavevector, order parameter, form factor) characters of associated density wave correlations. Time permitting, I will introduce a novel x-ray spectroscopy technique that can detect broken time-reversal versus space-inversion symmetry of an electronic order in a way complementary to the polar Kerr effect.
9:12AM Y53.00003 Amperean (2k_F) pairing and the pseudo-gap phase in HiTc Cuprates

PATRICK LEE, Massachusetts Inst of Tech-MIT — We propose that the pseudogap phase is a novel pairing state where electrons on the same side of the Fermi surface are paired, in strong contrast with conventional BCS theory which pairs electrons on opposite sides of the Fermi surface. The pair carries a net momentum 2k_F, forming a pair density wave. The microscopic pairing mechanism comes from a gauge theory formulation of the resonating valence bond (RVB) picture, where spinons traveling in the same direction feel an attractive force in analogy with Ampere's effects in electromagnetism. We call this Amperean pairing. Charge order appears as a subsidiary order parameter even when pair order is destroyed by phase fluctuations. Our theory gives a prediction of the ordering wave vector which is in good agreement with experiment. Furthermore, the quasiparticle spectrum from our model explains many of the unusual features reported in photoemission experiments. Finally, we propose an experiment that can directly test the idea of Amperean pairing.

1This work is supported by the NSF grant number DMR-1104498.

9:48AM Y53.00004 Charge ordered normal ground state and its interplay with superconductivity in the underdoped cuprates

SUCHITRA SEBASTIAN, University of Cambridge — Over the last few years, evidence has gradually built for a charge ordered normal ground state in the underdoped region of the cuprate high temperature superconductors. I will address the electronic structure of the normal state of the underdoped cuprates as accessed by quantum oscillations, and relate to it to complementary measurements by other experimental techniques. The interplay of the charge ordered ground state with the antinodal gapped pseudogap state, and overarching magnetic and superconducting correlations will be further explored.

This work was performed in collaboration with N. Harrison, G. G. Lonzarich, B. J. Ramshaw, B. S. Tan, P. A. Goddard, F. F. Balakirev, C. H. Mielke, R. Liang, D. A. Bonn, and W. N. Hardy.

10:24AM Y53.00005 Local Dimensionality of the Charge Density Wave in the Superconducting Cuprate Bi2201

JENNIFER HOFFMAN, Harvard University — Charge density wave (CDW) states were recently recognized as universal throughout the surface and bulk of a number of cuprates [1], prompting widespread effort to understand both their detailed phenomenology and their relationship to the mechanism of superconductivity. However, the dimensionality of the charge modulations remains unclear, including whether the modulation wavevector is unidirectional or bidirectional in-plane, and also the extent of inter-plane coherence of the charge modulations. In bismuth-based cuprates, severe material disorder precludes answering these questions through bulk scattering techniques. We use a local technique, scanning tunneling microscopy, to image the static charge modulations in (Pb,Bi)2Sr2La2CuO8+δ (Bi2201). We find that the charge modulations are more consistent with an underlying tendency to unidirectional than bidirectional CDW. Using recently developed cluster analysis techniques, we further show that these locally unidirectional CDWs extend coherently into the bulk of the material throughout the doping range. Finally, we comment on their relationship to a Fermi surface transition and quantum critical point observed in Bi2201 [3].


1We acknowledge support from NSF grant DMR-0847433

Friday, March 6, 2015 11:15AM - 2:03PM —
Session Z1 DMP: Focus Session: Graphene - Multilayer and Interfacial Effect 001A - Rui He, University of Northern Iowa

11:15AM Z1.00001 Layer breathing vibrations in AB-stacking few layer graphene and twisted bilayer graphene

RUI HE, Department of Physics, University of Northern Iowa — Interlayer interactions in few layer graphene can create a set of shear modes and layer breathing modes (LBMs) that involve lateral and vertical displacement of individual layers, respectively. LBMs are of importance because they can facilitate interlayer current conduction and are sensitive to external perturbations, such as the presence of substrate or surface adsorbates. We investigated low-frequency fundamental layer breathing vibrations in AB-stacking few layer graphene and twisted bilayer graphene using Raman spectroscopy. In AB-stacking few layer graphene we observed the Raman peaks from phonons at the Brillouin zone center for the lowest-frequency branch LBM vibration. The mode frequency depends strongly on the number of graphene layers. Notably, the LBM Raman response is unobservable at room temperature, and it is turned on at higher temperature (>600 K) with a steep increase of Raman intensity. The observation suggests that the LBM vibration is strongly suppressed by molecules adsorbed on the graphene surface but is activated as desorption occurs at high temperature. In twisted bilayer graphene, the fundamental LBM is observed in a small range of twisting angle at which the intensity of the G Raman peak is strongly enhanced. The dependence of this mode’s frequency and linewidth on the rotational angle can be explained by the double resonance Raman process (LBM phonon with nonzero wavevector) mediated by the twisted graphene lattice which lacks long-range translational symmetry. The angle dependence also reveals the strong impact of electronic band overlaps of the two rotated graphene layers.

11:51AM Z1.00002 Probing the Ni(111)-graphene interface using Raman spectroscopy

GUANGJUN CHENG, IRENE CALIZO, ANGELA HIGHT WALKER, PML, NIST — Theoretical simulations have shown that due to the hybridization of Ni d-electrons with the p-orbitals of graphene, graphene phonon dispersion is significantly altered (Nano Lett, 2010, 10, 4335-4340). There is no Raman signal from graphene on Ni(111) due to the suppression of the Kohn anomaly. In our work, we deposit a Ni thin film by thermal evaporation onto mechanically exfoliated graphene, few-layer graphene (FLG), and graphite, and probe the Ni-graphene interface using Raman spectroscopy. When the sample is annealed in forming gas, a Ni(111) thin film is produced on graphene, FLG, and graphite. We observe the disappearance of Raman signals from graphene underneath Ni(111) when using low laser power and the re-appearance of the Raman signals from the graphene with a higher power excitation laser. This work provides direct experimental evidence for the strong interaction between Ni(111) and graphene.
The dynamical exponent \(z\) of electron-electron interactions in ABC stacked graphene trilayers. In the gapless regime, we show that the self-energy corrections lead to the renormalization of both for intermediate-ranged interactions. However, if the interaction becomes too long-ranged or too weak, then the system will exhibit no instabilities.

We construct maps of the leading instability (or instabilities) of the system for the screened Coulomb-like interaction as a function of the overall interaction strength and interaction range for four values of the applied electric field. We find that the pattern of leading instabilities is the same as that found in the zero-field result.

ROBERT THROCKMORTON, University of Maryland — We extend previous renormalization group (RG) analyses of electron-electron interactions in gapless and metallic systems, including single-layer graphene, any possible coupling of physical quantities to components of the electric field has a counterpart where the analogous component of the magnetic field couples to exactly the same quantities. For example, a purely electric spin splitting appears as the magneto-electric analogue of the magnetic Zeeman spin splitting. The measurable thermodynamic response induced by magnetic and electric fields is thus completely symmetric. The Pauli magnetization induced by a magnetic field takes exactly the same functional form as the polarization induced by an electric field. Although they seem counterintuitive, our findings are consistent with fundamental principles such as time reversal symmetry. For example, only a magnetic field can give rise to a macroscopic spin polarization, whereas only a perpendicular electric field can induce a macroscopic polarization of the sublattice-related pseudospin in bilayer graphene. These rules enforced by symmetry for the matter-field interactions clarify the nature of spins versus pseudospins. We have obtained numerical values of prefactors for relevant terms.

WINKLER, Northern Illinois University, U. ZULICKE, Victoria University of Wellington, New Zealand — We present a theoretical study of bilayer-graphene’s electronic properties in the presence of electric and magnetic fields. In contrast to known materials, including single-layer graphene, any possible coupling of physical properties to components of the electric field has a counterpart where the analogous component of the magnetic field couples to exactly the same quantities. For example, a purely electric spin splitting appears as the magneto-electric analogue of the magnetic Zeeman spin splitting. The measurable thermodynamic response induced by magnetic and electric fields is thus completely symmetric. The Pauli magnetization induced by a magnetic field takes exactly the same functional form as the polarization induced by an electric field. Although they seem counterintuitive, our findings are consistent with fundamental principles such as time reversal symmetry. For example, only a magnetic field can give rise to a macroscopic spin polarization, whereas only a perpendicular electric field can induce a macroscopic polarization of the sublattice-related pseudospin in bilayer graphene. These rules enforced by symmetry for the matter-field interactions clarify the nature of spins versus pseudospins. We have obtained numerical values of prefactors for relevant terms.

This work was supported by JSPS KAKENHI Grant Numbers 24540339, 26107534.

12:39PM Z1.00006 Ordered states in spatially separated Coulomb-coupled double graphene AB bilayers, JUNG-JUNG SU, National Chiao Tung University, ALLAN H. MACDONALD, University of Texas at Austin — Electron-electron interaction effects are strong in graphene bilayer systems because of the approximately quadratic crossing between conduction and valence bands at the Brillouin-zone corners. In isotropic circular bilayers, this circumstance leads to an external electric field were systematically investigated. Although the crossing band structures remain at any stacking configurations (i.e., no energy gap opens), the wavefunction characteristics around the Fermi level can differ qualitatively for different stackings.

While the flattened region, the band structure approaches that of a bilayer ribbon in which the electron motion in the ribbon-width direction is disentangled. In chiral nanotubes, inter-wall interaction can essentially be neglected except in the vicinity of non-chiral tubes. Inter-wall interactions diminish rapidly when chiral angle deviates from zigzag or armchair, although the decay is slower in the vicinity of the armchair tube. When the flattened region has the structure of AA and AB stacked bilayer graphene, the same results can be derived by calculating boundary conditions corresponding to the closed-edge structure in which the top and bottom layers are smoothly connected through a monolayer graphene.

This work was supported by JSPS KAKENHI Grant Numbers 24540339, 26107534.

12:51PM Z1.00007 ABSTRACT WITHDRAWN —

1:03PM Z1.00008 Quantum multistability in bilayer graphene with a tunable energy gap, ROBERT THROCKMORTON, University of Maryland — We extend previous renormalization group (RG) analyses of electron-electron interactions in gapless bilayer graphene at finite temperature to include the effect of an electric field applied perpendicular to the sample. We determine the possible outcomes of the resulting RG equations, represented by fixed points along which ratios of the coupling constants remain constant and map out the leading instabilities of the system for an interaction of the form of a Coulomb interaction that is screened by two parallel conducting plates placed equidistant from the electron. We then construct maps of the leading instability (or instabilities) of the system for the screened Coulomb-like interaction as a function of the overall interaction strength and interaction range for four values of the applied electric field. We find that the pattern of leading instabilities is the same as that found in the zero-field case, namely that the system is unstable to a layer antiferromagnetic state for short-ranged interactions, to a nematic state for long-ranged interactions, and to both for intermediate-ranged interactions. However, if the interaction becomes too long-ranged or too weak, then the system will exhibit no instabilities.

Supported by LPS-CMTC and ARO-MURI.

1:15PM Z1.00009 Quasiparticle renormalization in ABC graphene trilayers, XU DOU, AKBAR JAEFARI, University of Oklahoma, YAFIS BARLAS, University of California at Riverside, BRUNO UCHOA, University of Oklahoma — We investigate the effect of electron-electron interactions in ABC stacked graphene trilayers. In the gapless regime, we show that the self-energy corrections lead to the renormalization of the dynamical exponent \(z = 3 + \alpha_1/N\), with \(\alpha_1 \approx 0.52\) and \(N\) is the number of fermionic species. Although the quasiparticle residue is suppressed near the neutrality point, the lifetime has a sublinear scaling with the energy and the quasiparticles are well defined even at zero energy. We calculate the renormalization of a variety of physical observables, which can be directly measured in experiments.

Supported by LPS-CMTC and ARO-MURI.

12:15PM Z1.00004 Electromagnetic coupling of spins and pseudospins in bilayer grapheneR, WINKLER, Northern Illinois University, U. ZULICKE, Victoria University of Wellington, New Zealand — We present a theoretical study of bilayer-graphene’s electronic properties in the presence of electric and magnetic fields. In contrast to known materials, including single-layer graphene, any possible coupling of physical quantities to components of the electric field has a counterpart where the analogous component of the magnetic field couples to exactly the same quantities. For example, a purely electric spin splitting appears as the magneto-electric analogue of the magnetic Zeeman spin splitting. The measurable thermodynamic response induced by magnetic and electric fields is thus completely symmetric. The Pauli magnetization induced by a magnetic field takes exactly the same functional form as the polarization induced by an electric field. Although they seem counterintuitive, our findings are consistent with fundamental principles such as time reversal symmetry. For example, only a magnetic field can give rise to a macroscopic spin polarization, whereas only a perpendicular electric field can induce a macroscopic polarization of the sublattice-related pseudospin in bilayer graphene. These rules enforced by symmetry for the matter-field interactions clarify the nature of spins versus pseudospins. We have obtained numerical values of prefactors for relevant terms.

NSF grant DMR-1310199 and Marsden Fund contract no. VUW0719

12:27PM Z1.00005 Effective-mass theory of flattened carbon nanotubes as bilayer graphene with closed edges, TAKESHI NAKANISHI, Natl Inst of Adv Indust Sci & Tech, TSUNEYA ANDO, Tokyo Inst. Tech. — We theoretically study effects of inter-wall interaction in collapsed carbon nanotubes, first directly calculating effective inter-wall interaction within an effective-mass scheme and second regarding collapsed tubes as ribbons of bilayer graphene with closed edges described by boundary conditions explicitly derived. Within the effective-mass scheme, effects of inter-wall interactions are shown to be important in non-chiral nanotubes such as zigzag and armchair. In fact, with the increase in the width of the flattened region, the band structure approaches that of a bilayer ribbon in which the electron motion in the ribbon-width direction is disentangled. In chiral nanotubes, inter-wall interaction can essentially be neglected except in the vicinity of non-chiral tubes. Inter-wall interactions diminish rapidly when chiral angle deviates from zigzag or armchair, although the decay is slower in the vicinity of the armchair tube. When the flattened region has the structure of AA and AB stacked bilayer graphene, the same results can be derived by calculating boundary conditions corresponding to the closed-edge structure in which the top and bottom layers are smoothly connected through a monolayer graphene.

This work was supported by JSPS KAKENHI Grant Numbers 24540339, 26107534.

1:21PM Z1.00003 Electronic properties of bilayer graphenes strongly coupled to interlayer stacking and an external electric field, CHANGWON PARK, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, JUNGA RYU, SUKLYUN HONG, Department of Physics and Graphene Research Institute, Sejong University, BOBBY SUMPTER, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, GUNN KIM, Department of Physics and Graphene Research Institute, Sejong University, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — In the design of bilayer graphene (BLG)-based switching devices, it is critical to understand the complex stacking structures observed experimentally and their impact on the overall electronic properties. Using a maximally localized Wannier function, a highly accurate tight-binding Hamiltonian based on density functional theory was constructed and the stacking-dependent evolution of BLG electronic band structures and their response to an external electric field were systematically investigated. Although the crossing band structures remain at any stacking configurations (i.e., no energy gap opens), the wavefunction characteristics around the Fermi level can differ qualitatively for different stackings.

This difference is conveyed to energy gap opening properties in the presence of an external electric field. We, for the first time, established a phase diagram summarizing the stacking-dependent electronic structures of BLG, separating metallic and semiconducting characteristics for a given external field.

The research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

12:03PM Z1.00003 Electronic properties of bilayer graphenes strongly coupled to interlayer stacking and an external electric field, CHANGWON PARK, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, JUNGA RYU, SUKLYUN HONG, Department of Physics and Graphene Research Institute, Sejong University, BOBBY SUMPTER, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, GUNN KIM, Department of Physics and Graphene Research Institute, Sejong University, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — In the design of bilayer graphene (BLG)-based switching devices, it is critical to understand the complex stacking structures observed experimentally and their impact on the overall electronic properties. Using a maximally localized Wannier function, a highly accurate tight-binding Hamiltonian based on density functional theory was constructed and the stacking-dependent evolution of BLG electronic band structures and their response to an external electric field were systematically investigated. Although the crossing band structures remain at any stacking configurations (i.e., no energy gap opens), the wavefunction characteristics around the Fermi level can differ qualitatively for different stackings.

This difference is conveyed to energy gap opening properties in the presence of an external electric field. We, for the first time, established a phase diagram summarizing the stacking-dependent electronic structures of BLG, separating metallic and semiconducting characteristics for a given external field.

The research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.
1:27PM Z1.00010 Density of states and tunneling conductance of ABC-stacked trilayer graphene. JONGBAE HONG, POSTECH/APCTP, DAVID ABERGEL, Nordita, KTH Royal Institute of Technology and Stockholm University — Experimental studies on ABC-stacked trilayer graphene suggest that the trilayer graphene may have a strongly correlated ground state which drives the opening of a band gap at the Fermi level. We propose a theoretical model for the tunneling conductance of strongly correlated trilayer graphene based on a Kondo-like mechanism of coherent transport where electrons tunnel into the correlated sample via an entangled singlet state. Our theory fits current experimental data extremely well, including peculiar features such as two pairs of kinks at low bias and a peak and shoulder at a relatively high bias. No other theoretical study has previously explained these features of the line shape. We also suggest a phenomenological estimate of the density of states in the strongly correlated regime. This has not previously been studied.

1:39PM Z1.00011 Rich Magneto-electronic spectra of AAB-stacked trilayer graphene. THI NGA DO, PhD. candidate, Dept. of Physics, National Cheng Kung University, Tainan, MIN-FA LIN, Professor of the Dept. of Physics, National Cheng Kung University, Tainan — We develop the generalized tight-binding model to study the magneto-electronic properties of AAB-stacked trilayer graphene. Three groups of Landau levels (LLs) are characterized by the dominating sub-envelope function on distinct sub-lattices. Each LL group could be further divided into two sub-groups in which the wave-functions are, respectively, localized at 2/6 and 4/6 of the total length of the enlarged unit cell. The unoccupied conduction and the occupied valence LLs in each sub-group behave similarly. For the first group, there exists certain important differences between two sub-groups, including the LLL energy spacings, quantum numbers, spatial distribution and the field dependent spectra. The LL crossings and anti-crossings occur frequently in each sub-group during the variation of field strength, which thus leads to the very complicated energy spectra and the seriously distorted wave-functions.

Friday, March 6, 2015 11:15AM - 2:03PM – Session Z2 DMP: Focus Session: Beyond Graphene - Devices II

11:15AM Z2.00001 Doping Dependent Electronic Properties of Atomically Thin Two-dimensional Crystals. TING CAO, ZHENGLU LI, STEVEN G. LOUIE, Physics Department, UC Berkeley and Lawrence Berkeley National Lab — Using first-principle calculations, we find that the electronic structure of atomically thin 2D crystals such as GaSe and NbSe2 can be modified significantly through doping, which can lead to major changes in their other properties. We elucidate the origins of the trends observed in experimental studies, and connect our theoretical predictions to experimental measurements since high level of doping can be achieved in 2D materials.

11:27AM Z2.00002 Ferroelectric Controlled Nanoscale MoS2 Transistor. ZHIYONG XIAO, JINGFENG SONG, STEPHEN DURCHAME, XIA HONG, University of Nebraska - Lincoln — We report the study of the device characteristics of MoS2 field effect transistors with a SiO2 backgate and a ferroelectric polymer top gate. We mechanically exfoliated MoS2 flakes on 300 nm SiO2 substrates. The thinner MoS2 pieces were identified by Raman spectroscopy and atomic force microscopy (AFM), and flakes of 1 – 5 nm thick were fabricated into two point devices via e-beam lithography with Ti/Au (5nm/50nm) as the contact electrodes. We then deposited on the top of the device a ferroelectric polymer layer, 20-40 nm polycrystalline poly(vinylidene-fluoride-trifluoroethylene) (PVDF-TrFE), using the Langmuir-Blodgett approach. At room temperature, we achieved a current modulation of a factor of 10^3 using the SiO2 back gate. The field effect mobility of the devices is ~ 20 cm^2V^-1s^-1. We then used conducting AFM to control the polarization of the top ferroelectric gate, and examined the SiO2-gated I-V characteristics of different polarization states of PVDF-TrFE. By switching the ferroelectric polarization, we induced a 30 V shift in I-V. At fixed backgate voltage, we achieved a maximum switching ratio in the drain current of ~ 15.

11:39AM Z2.00003 Controlled n-doping of monolayer MoS2 by atomic hydrogen. JYOTI KATOCCH, TIANCONG ZHU, Department of Physics, The Ohio State University, Columbus, OH 43210, HUA WEN, Department of Physics and Astronomy, University of California, Riverside, CA 92521, ROLAND KAWAKAMI, Department of Physics, The Ohio State University, Columbus, OH 43210, Department of Physics and Astronomy, University of California, Riverside, CA — Molybdenum Disulfide (MoS2) is a 2D layered material with potential applications in optoelectronics, electronics and spintronics. The injection of electrons in MoS2 is affected and limited by the Schottky barrier formed between metal contact and MoS2. There is a great deal of research interest to experimentally demonstrate ohmic contacts onto MoS2 in order to fully unravel the potential of this exciting material. We will present our results on controlled doping of single layer MoS2 surface by hydrogen to improve the contact resistance. We measured the transport properties of the MoS2 as a function of successive atomic hydrogen dosage at low temperature in ultra-high vacuum. Atomic hydrogen is generated using a hydrogen cracker. We observe that hydrogen adsorption results in negative doping due to charge donation by hydrogen to MoS2. Furthermore we will discuss the stability of the MoS2 as a function of successive atomic hydrogen dosage at low temperature in ultra-high vacuum. Atomic hydrogen is generated using a hydrogen cracker.

12:27PM Z2.00005 Thickness-dependent Electrical and Thermoelectric Transport in few-layer MoS$_2$, MORTEN KAYALHA, Purdue Univ, LI SHI, University of Texas at Austin, YONG CHEN, Purdue Univ — Layered semiconducting Transition Metal Dichalcogenides such as MoS$_2$ have recently gained a lot of attention as promising 2D materials for electronic and optoelectronic device applications. Here, we present a systematic study of thickness-dependent electrical and thermoelectric transport in few-layer MoS$_2$. MoS$_2$ flakes with various thickness ranging from 1-23 layers are prepared using the standard scotch-taped exfoliation technique and are then transferred onto a SiO$_2$/Si substrate. Electrical and thermoelectric measurements are carried out using AC and DC techniques with samples in vacuum. We observe five-fold enhancement in the electrical conductivity of two-layer MoS$_2$ compared to the bulk. However, the thermopower (TEP) exhibits less change except for monolayer where TEP is twice smaller. We also observe six times larger power factor in two-layer MoS$_2$ compared to the bulk. Additionally, we used a back gate to modulate the Fermi energy inside MoS$_2$ where an enhancement in TEP is observed close to the off state. Our results give insight into future prospects of MoS$_2$-based devices in thermoelectric applications.

12:39PM Z2.00006 Effects of Contact Geometry on Measurements of Contact and Film Resistance in Thin MoS$_2$ Films, JINSONG XU, YUNQIU LUO, Department of Physics, Ohio State University, ROLAND KAWAKAMI, Department of Physics, Ohio State University; Department of Physics and Astronomy, University of California, Riverside, JONATHAN PEZ, Department of Physics, Ohio State University — There is great interest in MoS$_2$ films and other 2D materials for fundamental studies and possible applications. However, the critical contacts to these films are not well understood, in part because of the strong band bending, depletion, and lateral Schottky barriers (SB). We report measurements and finite-element modeling of Au contacts on few-layer MoS$_2$ films on SiO$_2$/Si substrates, and find that certain common contact geometries produce mixing of contact and film resistance and highly/completely misleading results in 3- and 4-probe measurements, and that lateral depletion can produce errors in TLM measurements. However, with appropriate contact geometry and comparison to modeling, contact and film resistances can be independently monitored. Both are found to have strong back-gate and temperature dependence, with small (∼10 – 30 meV) but different activation energies (AEs) near 100 – 300 K. The contact AE is similar to several previous reports. The activated film resistance has not been previously reported, though evidence can be seen some previous published data. Possible origins of these temperature dependences will be discussed, as well as implications for determining contact SB heights.

12:51PM Z2.00007 Junction properties of MoS$_2$ between 1T and 2H phases, JUNSUK KIM, JEASU KIM, BYOUNGHEE MOON, HAMZA GUL, JUNGHO KIM, YOUNG HEE LEE, SEONG CHU LIM, Center for Integrated Nanostructure Physics, Institute for Basic Science — MoS$_2$ is locally transformed into 1T phase. In this study, we prepare MoS$_2$ in-plane junction of 1T and 2H phase by locally intercalating Li ions into MoS$_2$ multilayer that is confirmed using Raman and PL spectroscopics and will discuss the electrical properties of the junction of two different phases of MoS$_2$.

1:03PM Z2.00008 Electrical edge contacts to monolayer MoS$_2$, BYOUNG HEE MOON, GANG HEE HAN, HYUN KIM, HOMIN CHOI, YOUNGJO JIN, HYE YUN JEGON, SEONGCHU LIM, YOUNG HEE LEE, Center for Integrated Nanostructure Physics, Institute for Basic Science(IBS), Sungkyunkwan University, Suwon 440-746, Korea — Charge injection through the metal contacts to nanostructures has been the interesting issue for the physical mechanism involved as well as the device applications. In this talk, we discuss the effects of electrical edge contact to CVD grown monolayer MoS$_2$. The edge contacts are achieved by sandwiching MoS$_2$ with hexagonal boron nitrides (BN) [1]. It appears to show that charge injection by thermionic emission is suppressed, while tunneling effects take over.


1:15PM Z2.00009 MoS$_2$ Transistors Operating at Gigahertz Frequencies, DARIO KRASNOZHON, DOMINIK LEMBEKE, CLEMENS NYFFELER, YUSUF LEBLEBICI, ANDRAS KIS, Electrical Engineering Institute, Ecole Polytechnique Federale de Lausanne (EPFL) — The presence of a direct band gap and an ultrathin form factor has caused a considerable interest in 2D semiconductors from TMD family with MoS$_2$ being the most studied representative of this family of materials. While diverse electronic elements, integrated circuits and optoelectronic devices have been demonstrated using ultrathin MoS$_2$ and related materials, very little is known about their performance at high frequencies. We fabricated top-gated MoS$_2$ transistors operating in the gigahertz range of frequencies. The presence of a band gap also gives rise to current saturation, allowing voltage gain higher than 1. The RF transistors are fabricated from exfoliated MoS$_2$ with different layer thickness. All our devices presented transconductance typical of n-type materials with on-state current reaching 300 $\mu$A/$\mu$m for $V_{DS} = 2$ V and gate voltage $V_{G} = 10$ V in the case of monolayer MoS$_2$. The current gain of the MoS$_2$ transistors decreases with increasing frequency and shows the typical 1/f dependence. In conclusion, we studied top-gated MoS$_2$ transistors with a 240 nm gate length. Our MoS$_2$ RF-FETs show an intrinsic transconductance higher than 50 $\mu$S/um and a drain-source current saturation with a voltage gain higher than 1. Our devices show cut-off frequencies in the GHz range and are able not only to amplify current in this frequency range but also power and voltage, with the maximum operating frequency $f_{max}$ = 8.2 GHz.

1:27PM Z2.00010 Experimental evidence for inhomogeneous charge transport in MoS$_2$ nanoflakes, CHI-TE LIANG, Department of Physics, National Taiwan University, THAI JIN, Institute of Applied Physics, National Taiwan University, DAVID HU, School of Materials Science and Engineering, National Taiwan University, TAIWAN LI, OLEH KLOCHAN, School of Physics, University of New South Wales, Australie, C.-H. LIU, W.-H. WANG, Institute of Atomic and Molecular Sciences, Academia Sinica, ALEX R. HAMILTON, School of Physics, University of New South Wales, Sydney, Australia — We study electron transport in a monolayer MoS$_2$ nanoflake over a wide range of density, temperature, and electric bias. We find that the transport is best described by a percolating picture in which the disorder breaks translational invariance, breaking the MoS$_2$ system up into a series of puddles, rather than previous pictures in which the disorder is treated as uniform and homogeneous. Our work provides insight to a unified picture of charge transport in monolayer MoS$_2$ nanoflakes and contributes to the development of next-generation MoS$_2$-based devices.

3We would like to thank funding from the MOST, Taiwan (grant numbers: 103-2918-I-002-028, 102-2119-M-002-016-MY3 and 102-2917-I-002-106) and the Australian Research Council through the DP scheme.
Recently, Ni-treated-graphene electrodes were fabricated on MoS2. The development involved the Centre, National University of Singapore, Singapore 117543, JOHN T.L. THONG, Department of Electrical and Computer Engineering, National University of Singapore, Singapore 117543, K.H. KHOON, S.Y. QUEK, Department of Physics and Graphene Research Centre, National University of Singapore, Singapore 117543, JOHN T.L. THONG, Department of Electrical and Computer Engineering, National University of Singapore, Singapore 117543. X. LUO, Department of Physics and Graphene Research Centre, National University of Singapore, Singapore 117543, Y. LI, Department of Electrical and Computer Engineering, National University of Singapore, Singapore 117543. The fabrication process involved using a dry transfer technique and metal-catalyzed graphene treatment process, yielding contact resistances as low as 200 Ωm and a substantial contact enhancement of ~ 2 orders of magnitude relative to Ni-MoS2 interfaces. By performing a Schottky barrier height (SBH) analysis on Ni-MoS2 and Ni-graphene-MoS2 interfaces using first-principles DFT calculations, we have found that the smaller contact resistance in Ni-treated-graphene-MoS2 can be attributed to the smaller SBH of Ni-graphene-MoS2 contacts. This reduction in SBH can in turn be related to the lower work function of Ni-graphene electrodes relative to Ni. The effect of Ni treatment further reduces the contact resistance due to stronger coupling between Ni and graphene edges.

For a memory erasure procedure, which is a logically irreversible operation, a detailed Jarzynski Equality is verified, retrieving that the mean dissipated heat saturates at the Landauer bound in the limit of long erasure cycles. This result demonstrates the intimate link between information irreversibility and the Landauer principle. Bennett and, independently, Penrose later pointed out a link to Maxwell’s Demon: Were Landauer’s principle to fail, it would be impossible to useably extract work from a heat bath. We report tests of Landauer’s principle in an experimental system consisting of a charged colloidal particle in water. To test stochastic thermodynamic ideas, we create a time-dependent, “virtual” double-wall potential via a feedback loop that is much faster than the relaxation time of the particle in the virtual potential. In a first experiment, the probability of “erasure” (resetting to one) is unity, and at long cycle times, we observe that the average work is compatible with kT ln2. In a second, the probability of erasure is zero; the system may end up in two states; and, at long cycle times, the average measured work tends to zero. In individual cycles, the work to erase can be below the Landauer limit, consistent with the Jarzynski equality.

We experimentally show the existence of the Landauer principle for situations involving information processing. To this end, we consider an information reservoir which provides the means to store and retrieve information. We use this reservoir to study the thermodynamics of information processing. In particular, we will focus on the generalizations of the second law of thermodynamics and the Jarzynski equality in the presence of feedback control, where information contents and thermodynamic quantities are treated on an equal footing. We will also discuss recent experimental results that realized Maxwell’s demon by colloidal particles and single electrons.

This work is supported by the Singapore National Research Foundation NRF-NRFF2012-01.

Friday, March 6, 2015 11:15AM - 2:15PM – Session Z3 GSNP: Invited Session: Thermodynamics of Information Processing 002AB - Massimiliano Esposito, University of Luxembourg

11:15AM Z3.00001 Stochastic thermodynamics of information processing. ANDRE CARDOSO BARATO, Universität Stuttgar — We consider two recent advancements on theoretical aspects of thermodynamics of information processing. First we show that the theory of stochastic thermodynamics can be generalized to include information reservoirs. These reservoirs can be seen as a sequence of bits which has its Shannon entropy changed due to the interaction with the system. Second we discuss bipartite systems, which provide a convenient description of Maxwell’s demon. Analyzing a special class of bipartite systems we show that they can be used to study cellular information processing, allowing for the definition of an entropic rate which quantifies how much a cell learns about a fluctuating external environment and that is bounded by the thermodynamic entropy production.


11:51AM Z3.00002 High-Precision Test of Landauer’s Principle in a Feedback Trap. JOHN BECHHOEFER2, Simon Fraser University — Landauer’s principle, formulated in 1961, postulates that irreversible logical or computational operations such as memory erase require work, no matter how slowly they are performed. For example, to “reset to one” a one-bit memory requires at least kT ln2 of work, which is dissipated as heat. Bennett and, independently, Penrose later pointed out a link to Maxwell’s Demon: Were Landauer’s principle to fail, it would be possible to repeatedly extract work from a heat bath. We report tests of Landauer’s principle in an experimental system consisting of a charged colloidal particle in water. To test stochastic thermodynamic ideas, we create a time-dependent, “virtual” double-wall potential via a feedback loop that is much faster than the relaxation time of the particle in the virtual potential. In a first experiment, the probability of “erasure” (resetting to one) is unity, and at long cycle times, we observe that the average work is compatible with kT ln2. In a second, the probability of erasure is zero; the system may end up in two states; and, at long cycle times, the average measured work tends to zero. In individual cycles, the work to erase can be below the Landauer limit, consistent with the Jarzynski equality.

1 Supported by the National Science and Engineering Research Council of Canada (NSERC)
2 In collaboration with Yonggun Jun and Monêilo Gavrilov

12:27PM Z3.00003 Information Processing and the Second Law of Thermodynamics: An Inclusive Hamiltonian Approach. SEBASTIAN DEFFNER, Los Alamos Natl Lab — We obtain generalizations of the Kelvin-Planck, Clausius, and Carnot statements of the second law of thermodynamics for situations involving information processing. To this end, we consider an information reservoir (representing, e.g., a memory device) alongside the heat and work reservoirs that appear in traditional thermodynamic analyses. We derive our results within an inclusive framework in which all participating elements – the system or device of interest, together with the heat, work, and information reservoirs – are modeled explicitly by a time-independent, classical Hamiltonian. We place particular emphasis on the limits and assumptions under which cyclic motion of the device of interest emerges from its interactions with work, heat, and information reservoirs. Finally, our findings are illustrated with a simple, analytically solvable example – a quantum Maxwell demon.

1:03PM Z3.00004 Thermodynamics of Nonequilibrium Systems with Feedback Control. TAKAIRO SAGAWA, The University of Tokyo — In modern nonequilibrium physics, “Maxwell’s demon” has attracted renewed attentions in both terms of theory and experiment. The demon plays a key role to unify thermodynamics and information theory, which can extract the useful work from a heat bath by using the obtained information via feedback control. In this talk, I will talk about the recent development of thermodynamics of information. In particular, I will focus on the generalizations of the second law of thermodynamics and the Jarzynski equality in the presence of feedback control, where information contents and thermodynamic quantities are treated on an equal footing. I will also discuss recent experimental results that realized Maxwell’s demon by colloidal particles and single electrons.

1:39PM Z3.00005 Information and thermodynamics: Experimental verification of Landauer’s erasure principle. SERGIO CILIBERTO, ENSL-CNRS — Rolf Landauer argued that the erasure of information is a dissipative process. A minimal quantity of heat, proportional to the thermal energy, is necessarily produced when a classical bit of information is deleted. A direct consequence of this logically irreversible transformation is that the entropy of the environment increases unavoidably by a finite amount. We experimentally show the existence of the Landauer bound in a generic model of a one-bit memory. Using a system of a single colloidal particle trapped in a modulated double-well potential, we establish that the mean dissipated heat saturates at the Landauer bound in the limit of long erasure cycles. This result demonstrates the intimate link between information theory and thermodynamics. For a memory erasure procedure, which is a logically irreversible operation, a detailed Jarzynski Equality is verified, retrieving the
Friday, March 6, 2015 11:15AM - 2:03PM
Session Z4 GERA: Physics of Batteries, Supercapacitors and Fuel Cells  Mayor Cockrell Room 004 -

11:15AM Z4.00001 In-situ Studies of Structures and Processes at Model Battery Electrode/Electrolyte Interfaces1. PAUL FENTER, Argonne National Laboratory — The ability to understand and control materials properties within electrochemical energy storage systems is a significant scientific and technical challenge. This is due, at least in part, to the extreme conditions present within these systems, and the significant structural and chemical changes that take place as lithium ions are incorporated in the active electrode material. In particular, the behavior of interfaces in such systems is poorly understood, notably the solid-liquid interface that separates the electrode and the liquid electrolyte. I will review our recent work in which we seek to isolate and understand the role of interfacial reactivity in these systems through in-situ, real-time, observations of electrochemically driven lithiation/delithiation reactions. This is achieved by observing well-defined model electrode-electrolyte interfaces using X-ray reflectivity. These results reveal novel understandings of interfacial reactivity in conversion reactions (e.g., Si, Si, Ge, NiO) that can be used to control the complex reaction lithiation pathway through the use of thin-film and multilayer electrode structures.

1This work was supported by the Center for Electrochemical Energy Science, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, in collaboration with T. Fister, A. Gewirth, M.J. Bedzyk and others.

11:51AM Z4.00002 Hybrid Functional Calculations of Acceptor Doping in Protonic Conductor SrZrO3. LEIGH WESTON, University of Sydney; ANDERSON JANOTTI, University of California, Santa Barbara; XIANGYUAN CUI, CATHERINE STAMPFL, University of Sydney, CHRIS VAN DE WALLE, University of California, Santa Barbara — Perovskite oxides such as SrZrO3 (SZO), which exhibit high temperature proton conductivity, are promising electrolyte materials for use in solid oxide fuel cells (SOFCs). Proton conductivity in SZO is typically achieved via acceptor doping with trivalent cations substituting at the Zr site, where the formation of charge compensating oxygen vacancies facilitates proton solvation. We present a detailed study of Sc and Y dopants in SZO based on first-principles, hybrid density functional calculations. When substituting at the Zr site, both dopants form deep acceptors, where the neutral charge state forms a localized hole polaron state. Under certain growth conditions Sc and Y will form auto-compensating donor species by substituting at the Sr site, which would inhibit proton solubility. Moreover, the proton - dopant association was found to be strong, with proton binding energies of -0.41 eV and -0.31 eV for ScZr and YZr respectively, indicating that proton transport is limited by trapping. These new results will be useful in the development of zirconate based proton conducting electrolyte materials for solid oxide fuel cells.

12:03PM Z4.00003 Effect of Fe doping on O vacancy/interstitial formation and migration in PrBaCo2O5+δ. OMOTAYO SALAWU, LIYONG GAN, UDO SCHWINGENSCHLOGL, King Abdullah Univ — Oxygen vacancy formation and migration are key factors considered for the operation of cathodes in solid oxide fuel cell. First-principles calculations are used to investigate Fe doped PrBaCo2O5+δ as cathode material for intermediate temperature solid oxide fuel cells. We discuss the electronic properties of the pristine system and the effect of Fe doping on the structural and electronic properties. Different concentrations of the dopants are calculated. We find that the volume of the unit cell and O vacancy formation energy increase linearly with the Fe content concentration. We also investigate the formation of oxygen interstitial as a function of Fe substitution and the possibility of anisotropic diffusion of the O ion was also studied.

12:15PM Z4.00004 Short-lived K2S Molecules in Superionic Potassium Sulfide. YUSUKE OKEYA, KAZUO TSUMURAYA, Meiji University — The first principles molecular dynamics method allows us to elucidate the formation of short-lived K2S molecular states in superionic potassium sulfide. The covalent and the Coulomb bonds exist between the ionized mobile potassiums and the ionized immobile sulfurs. Both the bonds induces indirect covalent and indirect Coulomb attractions between the di-interstitial potasiums on the mid-sulfurs, which forms the short-lived K2S molecular states. The covalent electron density also exists between short-lived potassium dimers. The three attractions reduce Haven’s ratios of the potassiums in the conductor. The molecule formation indicates the electronic state of the conductor is intermediate between the ionic and covalent crystals. The absence of the long-lived potassium dimers implies a failure of the caterpillar diffusion model or the Frenkel-Kontorova chain model for the superionic diffusion of the potassiums in the sulfide. The incompletely ionized cations and anions reduce the Coulomb attractions between them which induces the sublattice melting of smaller size of the potassiums than the sulfurs.

12:27PM Z4.00005 First principles calculations of stability and lithium intercalation potentials of ZnCo2O4. L.C. YU, J. WU, H. LIU, Chengdu Green Energy and Green Manufacturing Technology R&D Center, Sichuan, 620107, China, Y.N. ZHANG, Chengdu Green Energy and Green Manufacturing Technology R&D Center, Sichuan; Beijing Computational Science Research Center, Beijing, China — Among the metal oxides, which are the most widely investigated alternative anodes for use in lithium ion batteries (LIBs), binary and ternary tin oxides have received smaller size of the potassiums than the sulfurs. The incompletely ionized cations and anions reduce the Coulomb attractions between them which induces the sublattice melting of smaller size of the potassiums than the sulfurs. The covalent and the Coulomb bonds exist between the ionized mobile potassiums and the ionized immobile sulfurs. Both the bonds induces indirect covalent and indirect Coulomb attractions between the di-interstitial potasiums on the mid-sulfurs, which forms the short-lived K2S molecular states. The covalent electron density also exists between short-lived potassium dimers. The three attractions reduce Haven’s ratios of the potassiums in the conductor. The molecule formation indicates the electronic state of the conductor is intermediate between the ionic and covalent crystals. The absence of the long-lived potassium dimers implies a failure of the caterpillar diffusion model or the Frenkel-Kontorova chain model for the superionic diffusion of the potassiums in the sulfide. The incompletely ionized cations and anions reduce the Coulomb attractions between them which induces the sublattice melting of smaller size of the potassiums than the sulfurs.

12:39PM Z4.00006 Density Functional Theory Study of the Conductivity of Manganese Dioxide Nanowires during Li+ Insertion. RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA 92697, USA, HUI WANG, Department of Physics, Fudan University, Shanghai 200433, China, MAY LE THAI, REGINALD M. PENNER, Department of Chemistry, University of California, Irvine, CA 92697, USA — Manganese oxide (δ-MnO2) as a battery material has various advantages such as low cost, high earth abundance and environmentally safe, and it has large interlayer space for lithium ion insertion and migration. In this work, the system of 200 MnO2 nanowire array is used to study the electrochemical changes through in situ conductivity measurements during the lithium ion insertion process. The result indicates that the conductivity of each MnO2 nanowire array increases as the lithium ion concentrations increases corresponding to more negative insertion potential. We perform ab initio molecular dynamic (AIMD) simulations and density functional theory (DFT) calculations with the van der Waals (vdW) correction to understand the fundamental electrochemical and structural properties of δ-MnO2 nanowires. We find that water molecules are important for the expansion of the interlayer distance of δ-MnO2, and reveal that the variation of conductivity of δ-MnO2 nanowires with different Li+ concentrations stems from the Li+-produced gap states.

1HW and RW were supported 1000 talent fund in Fudan U and by DOE-BES (Grant No. DE-FG02-05ER46237). MT and RP were supported by the U.S. DOE-EFRC (Award Number DESC0001160).
12:51PM Z4.00007 In Situ Correlation of Volumetric Expansion with Charge Storage in Nanostructured MnO2, Tetyana Ignatova, Brad Corso, Deng Pan, O. Tolga Gul, Phillip G. Collins, Department of Physics and Astronomy, University of California at Irvine — Pseudocapacitors aim to meet developing energy storage needs by combining the high energy density of batteries with the power performance of capacitors. However, degradation remains a critical issue for pseudocapacitor electrodes. After many cycles, nanostructured metal oxides lose their capacity through mechanisms that remain poorly understood. In this work, we studied the volumetric changes that accompany charge storage in nanoscale MnO2 electrodes by combining in-liquid atomic force microscopy (AFM) with 3-terminal electrochemical cycling. Typical samples consisted of thin films (100 to 400 nm) of porous, amorphous MnO2 deposited onto 2 µm Pt electrodes and then cycled in aqueous LiClO4 electrolyte. In situ measurements of film expansion during charge insertion observed 5-6% volumetric expansion for partial charging of 0.1 electron per Mn atom over a wide range of scan rates and voltage windows, even though these parameters change the balance between fast, double-layer capacitance and bulk, redox pseudocapacitance mechanisms. In fact, volume expansion is universally attributed to bulk charging, so the invariance highlights an unexpected role for surface processes in nanostructured electrode materials.

1:03PM Z4.00008 Topological defect dynamics in operando battery nanoparticles, Andrew Uleveland, Shirley Meng, Oleg Shpyrko, University of California: San Diego — Topological defects are ubiquitous in physics and manifest themselves as magnetic monopoles in quantum field theories and crystallographic imperfections in condensed matter systems. In the latter, the defect properties determine many of the material’s properties and such represent substantial novel opportunities for design and optimization of desired functionalities through deliberate defect engineering and manipulation. However, this approach of “defect choreography” currently suffers from the lack of suitable nanoscale probes to track buried single defects in situ and in operando. Here we report 3D imaging of single edge dislocations and their motion in an individual nanoparticle under operando conditions in a Lithium ion battery. We further observe the dislocation act as a nucleation point during the structural phase transformation. We find that the region near the dislocation enters a negative Poisson’s ratio, or auxetic, regime at high voltage. Dislocation imaging is thus a powerful nanotechnology approach to measure performance indicators such as exact Li vacancy concentration and hopping energy barriers. We hope that the “map” between structure and property provided here will speed optimization of the ionic conductivity via targeted doping strategies.

1:15PM Z4.00009 Structure and Stoichiometry in doped LLZO (Li2La3Zr2O12), Michelle Johnnies, Naval Research Laboratory, NOAM BERNSTEIN, NRL, ASHIA HUQ, Oak Ridge National Laboratory, SAIKAT MIKHOPADAY, ONRL, JEFF WOLFENTINE, Army Research Laboratory, JAN ALLEN, ARL, TRAVIS THOMPSEN, University of Michigan, JEFF SAKAMOTO, UMich, DEREK STEWART, HGST — LLZO has a tetragonal, Li-ordered phase with very low ionic conductivity and a cubic, Li-disordered phase with two orders of magnitude higher conductivity, relevant for solid electrolyte usage. The jump in conductivity can be correlated to dopant-induced Li vacancies that disorder the Li sublattice and cause the structural phase transitions this work presents a high-throughput, first-principles technique to show how both overall structure and selected local structural elements change as a function of dopant concentration. In particular, we examine how the local structure that defines the Li ion pathways changes with the lattice constant and how important microscopic quantities such as different Li site energies and hopping barriers change accordingly. Our work provides a link between the easily measurable lattice constant and extremely important but difficult to measure performance indicators such as exact Li vacancy concentration and hopping energy barriers. We hope that the “map” between structure and property provided here will speed optimization of the ionic conductivity via targeted doping strategies.

1:27PM Z4.00010 Compressive Sensing Cluster Expansion Studies of Lithium Intercalation and Phase Transformation in MoS2 for Energy Storage, Chi-Ping Liu, University of California, Los Angeles, FEI ZHOU, Lawrence Livermore National Laboratory, MIEDVUDZ OZOLINS, University of California, Los Angeles, UNIVERSITY OF CALIFORNIA, LOS ANGELES COLLABORATION, LAWRENCE LIVERMORE NATIONAL LABORATORY COLLABORATION — Bulk molybdenum disulfide (MoS2) is a good electrode material candidate for energy storage applications, such as lithium ion batteries and supercapacitors due to its high theoretical energy and power density. First-principles density-functional theory (DFT) calculations combined with cluster expansion are an effective method to study thermodynamic and kinetic properties of electrode materials. In order to construct accurate models for cluster expansion, it is important to effectively choose clusters with significant contributions. In this work, we employ a compressive sensing based technique to select relevant clusters in order to build an accurate Hamiltonian for cluster expansion, enabling the study of Li intercalation in MoS2. We find that the 2H MoS2 structure is only stable at low Li content while 1T MoS2 is the preferred phase at high Li content. The results show that the 2H MoS2 phase transforms into the disordered 1T phase and the disordered 1T structure remains after the first Li insertion/deinsertion cycle suggesting that disordered 1T MoS2 is stable even at dilute Li content. This work also highlights that cluster expansion treated with compressive sensing is an effective and powerful tool for model construction and can be applied to advanced battery and supercapacitor electrode materials.

1:39PM Z4.00011 Binder-free Carbon Nanotube Flexible Solid State Supercapacitor1, Kofi ADU, The Pennsylvania State University Altoona College, DANHAO MA, The Pennsylvania State University, RAMAKRISHNAN RAJAGOPALAN, The Pennsylvania State University-DuBois, CHENG-YU WANG, ANGELA LUEKING, CLIVE RANDELL, The Pennsylvania State University — We present a post synthesis self-assemble protocol that transforms the trillions of CNTs in powder form into densely packed flexible, robust and binder-free macroscopic membranes with hierarchical pore structure. The binder-free CNT membranes could be as thin as <10µm with mass density greater than that of water (1.0g/cc). As the thickness of the CNT membrane is increased, we observed a gradual transition from high flexibility to buckling and brittleness in the flexural properties of the CNT membranes. We have demonstrated the use of the CNT membranes as electrode in two-electrode 1M H2SO4 aqueous double layer supercapacitor that shows very high power density ~ 1040 kW/kg based on the mass of both electrodes and time constant of ~ 15 ms with no degradation in performance even after 10,000 cycles. Furthermore, we will show the designing of flexible 3-stack bipolar solid-state ultracapacitor and present results on energy/power densities, voltage, cyclability, temperature stability in relation to flexibility and weight. Preliminary results indicate high temperature stability >85°C and CV voltage ~ 3V with very low leakage current ~ 10nA.

This Work is Supported by Penn State Altoona Undergraduate Research Sponsored Program and Penn State Materials Research Institute, University Park.

1:51PM Z4.00012 X-ray absorption spectroscopy as a probe of dissolved polysulfides in lithium sulfur batteries, TOD PASCAL, DAVID PRENDERGAST, Lawrence Berkeley National Lab — There has been enormous interest lately in lithium sulfur batteries, since they have 5 times the theoretical capacity of lithium ion batteries. Large-scale adoption of this technology has been hampered by numerous shortcomings, chiefly the slow rate of utilization of the active material and rapid capacity fading during cycling. Overcoming these limitations requires methods capable of identifying and quantifying the products of the poorly understood electrochemical reactions. One recent advance has been the use of X-ray absorption spectroscopy (XAS), an element-specific probe of the unoccupied energy levels around an excited atom upon absorption of an X-ray photon, to identify the reaction products and intermediates. In this talk, we’ll present first principles molecular dynamics and spectral simulations of dissolved lithium polysulfide species, showing how finite temperature dynamics, molecular geometry, molecular charge state and solvent environment conspire to determine the peak positions and intensity of the XAS. We’ll present a spectral analysis of the radical (-1e charge) species, and reveal a unique low energy feature that can be used to identify these species from their more common dianion (-2e charge) counterparts.

Friday, March 6, 2015 11:15AM - 2:03PM
Session Z5 DMP DCOMP: Focus Session: Competing Order and ARPES in Fe-Based Superconductors
Jude Gorman Room 005 - Andrei Chubukov, University of Minnesota
Competing phases in iron-based superconductors — DONGHUI LU, SSRL SLAC — Stanford
A common aspect of high temperature superconductivity in both cuprates and iron-based superconductors is that it always appears in the vicinity of other competing phases, whose suppression brings the full emergence of superconductivity. In iron-based superconductors, the competing phases take the form of collinear spin-density-wave phase and nematic phase. Characterization of these competing phases and associated phase transitions is essential to establishing a comprehensive understanding of the phase diagram of high temperature superconductors and ultimately the mechanism of unconventional superconductivity. In this talk, I will present our angle-resolved photoemission study of different family of iron-based superconductors. Our early data on detwinned BaFe$_1-x$Co$_x$As$_2$ and NaFeAs not only revealed a symmetry breaking orbital anisotropy in the nematic phase, but also identified the spectroscopic signatures associated with each phase transition in our ARPES spectra [1,2]. More recent results from underdoped Ba$_1$Fe$_2$As$_2$, on the other hand, provided the direct spectroscopic evidence for the coexistence and competition between SDW phase, nematic phase, and superconducting phase [3]. Finally, our latest data on multilayer FeSe film demonstrate the presence of a nematic state without long range magnetic order, suggesting the importance of orbital degree of freedom in driving the nematicity [1,3]. M. Yi, D. H. Lu, J.-H. Chu, J. C. Analytis, A. P. Sorini, A. F. Kemper, B. Moritz, S.-K. Mo, R. G. Moore, M. Hashimoto, W.-S. Lee, Z. Hussain, T. P. Devereaux, I. R. Fisher, and Z.-X. Shen, Proc. Natl. Acad. Sci. 108, 6878 (2011). [2] M. Yi, H. Wen, Z.-X. Shen, and D. H. Lu; Nature Communications 5, 3711 (2014).

Electron correlation tuned superconductivity in iron chalcogenide superconductors — MING YI, MENG WANG, Univ of California - Berkeley, DONGHUI LU, Stanford Synchrotron Radiation Laboratory, ALEXANDER KEMPER, Lawrence National Laboratory, SUNG-KWAN MO, Advanced Light Source, Lawrence National Laboratory, ZHI-XUN SHEN, Stanford University, ROBERT BIRGENAU, Univ of California - Berkeley — The iron chalcogenide superconductors, A$_x$Fe$_2$-Se$_2$ (A=K, Rb, Cs), is an interesting system where superconductivity occurs without the existence of hole Fermi pockets, hence lacking the nesting conditions needed under a spin fluctuation mediated pairing scenario. It is then important to understand the ingredients needed for superconductivity in these materials. It has been shown that sulfur substitution for selenium in this system can continually reduce the $T_c$ from 30K to zero, providing an opportunity for understanding the occurrence of superconductivity in these materials. In this talk, I will present angle-resolved photoemission spectroscopy data on the Rb$_x$Fe$_2$(Se$_{1-y}$S$_y$)$_2$ series, where we show that electron correlation strength is the crucial parameter that tunes superconductivity in this family.

ARPES of K-doped iron selenide superconductor — TAKAYOSHI YOKOYA, MASANORI SUNAGAWA, KENSEI TERASHIMA, TAKAHIRO HAMADA, HIROKAZU FUJIIWARA, Okayama University, MASASHI TANAKA, HIROYUKI TAYEKA, YOSHIHIKO TAKANO, NIMS, MASASHI ARITA, KENYA SHIMADA, HIROFUMI NAMATAME, MASAKI TANIGUCHI, HISOR, Hiroshima University, KAT-SUHIRO SUZUKI, HIDETOMO USUI, KAZUHIKO KUROKI, Osaka University, TAKANORI WAKITA, YUJI MURAOKA, Okayama University — In iron pnictide superconductors, the characteristic Fermi surface (FS) peak, namely a nesting of hole-like FS at the zone center and electron-like FS at the zone corner, is considered to induce spin/orbital fluctuation leading to high-Tc superconductivity [1,2]. In K-doped iron selenide superconductors, however, ARPES studies reported absence of hole-like FS at the zone center, which is different from that observed in iron pnictides [3]. So far, proposed models for the superconductivity based on the FS topology appear to fail to explain available experimental results. In this talk, we present our recent ARPES studies on a K-doped iron selenide superconductor performed with careful tuning of experimental conditions, which show a hole-like FS around the zone center. [1] I. I. Mazin et al., Phys. Rev. Lett. 101, 057003 (2008); [2] K. Kuroki et al., Phys. Rev. Lett. 101, 087004 (2008); [3] Y. Zhang et al., Nat. Mater. 10, 273 (2011); T. Qian et al., Phys. Rev. Lett. 106, 187001 (2011).

What do we actually see in ARPES? Generalized unfolding method and application to Fe-based superconductors — MILAN TOMIC, HARALD O. JESCHKE, ROSER VALENTI, Goethe University — Interpretation of angle resolved photoemission (ARPES) measurements relies heavily on comparison with ab-initio (DFT) band structures. However, ARPES-observed band structures and DFT band structures often disagree on the unit cell periodicities as well as position of band structure features relative to the Brillouin zone. We present a novel, symmetry-based approach to band structure unfolding which utilizes irreducible representations of space groups. Within the unified framework we can treat both the translational and point group symmetries and explain how ARPES measurements sometimes reflect crystal structure features with a reduced unit cell. We will present some examples in the context of Fe-based superconductors.

ARPES investigations of parent compounds of 122 Fe-based superconductors and their 3d transition metal cousins — PIERRE RICHARD, W.-L. ZHANG, S.-F. WU, A. VAN ROEKEGHEM, P. ZHANG, H. MAO, T. QIAN, A. Kiryukhin, F. Milot, Institute of Physics, Chinese Academy of Sciences, T. KIM, M. HOESCH, Laboratoire de Photonique et d’Optique, Lyon, France (France), H. MIYAGAWA, H. MIAO, TIAN QIAN, XUN SHI, PIERRE RICHARD, Institute of Physics, Chinese Academy of Sciences, T. KIM, M. HOESCH, Diamond Light Source, LINGYI XING, XUAN GENG, HONG DING, Institute of Physics, Chinese Academy of Sciences — In conventional BCS superconductors, the quantum condensation of superconducting electron pairs is understood as a Fermi surface instability, in which the low-energy electrons are paired by attractive interactions. Whether this explanation is still valid in high-Tc superconductors such as cuprates and iron-based superconductors remains an open question. In particular, a fundamentally different picture of the electron pairs, which are believed to be formed locally by repulsive interactions, may prevail. Here we report a high-resolution angle-resolved photoemission spectroscopy study on LiFe$_1-x$Co$_x$As. We reveal a large and robust superconducting gap on a band sinking below the Fermi energy upon Co substitution. The observed Fermi surface free superconducting order is also the largest over the momentum space, which rules out a proximity effect origin and indicates that the superconducting order parameter is not tied to the Fermi surface as a result of a Fermi surface instability.

Observation of strong electron pairing on band without Fermi surfaces in LiFe$_1-x$Co$_x$As — HU MIAO, TIAN QIAN, XUN SHI, PIERRE RICHARD, Institute of Physics, Chinese Academy of Sciences, T. KIM, M. HOESCH, Diamond Light Source, LINGYI XING, XUAN GENG, HONG DING, Institute of Physics, Chinese Academy of Sciences — In conventional BCS superconductors, the quantum condensation of superconducting electron pairs is understood as a Fermi surface instability, in which the low-energy electrons are paired by attractive interactions. Whether this explanation is still valid in high-Tc superconductors such as cuprates and iron-based superconductors remains an open question. In particular, a fundamentally different picture of the electron pairs, which are believed to be formed locally by repulsive interactions, may prevail. Here we report a high-resolution angle-resolved photoemission spectroscopy study on LiFe$_1-x$Co$_x$As. We reveal a large and robust superconducting gap on a band sinking below the Fermi energy upon Co substitution. The observed Fermi surface free superconducting order is also the largest over the momentum space, which rules out a proximity effect origin and indicates that the superconducting order parameter is not tied to the Fermi surface as a result of a Fermi surface instability.

Dynamic coexistence of competing orders in multi-component superconductors — MAXIM DZERO, Kent State University, ALEX LEVCHENKO, Michigan State University — We study the nonequilibrium dynamics of an electronic model with competing spin-density wave and unconventional superconductivity in the context of iron-pnictides. Focusing on the collisionless regime we find that magnetic and superconducting order parameter varies may coexist dynamically after the quench even though the equilibrium state has only one order parameter. We consider different initial conditions concomitant with the phase diagram and in a certain regime identify new oscillatory amplitude modes with incommensurate frequencies for magnetic and superconducting responses. At the technical level we solve equations of motion for the electronic Green’s functions and self-consistency conditions by reducing the problem to a closed set of Bloch equations in the pseudospin representation.
1:03PM Z5.00008 Correlation-induced self-doping in iron-pnictide superconductor Ba$_2$Ti$_2$Fe$_{2}$As$_{1}$O$_{4}$, TIAN QIAN, JUNZHANG MA, Institute of Physics, Chinese Academy of Sciences, A. VAN ROEKEGHEM, Ecole Polytechnique, PIERRE RICHARD, Institute of Physics, Chinese Academy of Sciences, GUANGHAN CAO, Zhejiang University, SILKE BIERMANN, Ecole Polytechnique, HONG DING, Institute of Physics, Chinese Academy of Sciences — The electronic structure of the iron-based superconductor Ba$_2$Ti$_2$Fe$_{2}$As$_{1}$O$_{4}$ ($T_{ onset}^{c} = 23.5$ K) has been investigated by using angle-resolved photoemission spectroscopy and combined local density approximation and dynamical mean field theory calculations. The electronic states near the Fermi level are dominated by both the Fe 3d and Ti 3d orbitals, indicating that the spacer layers separating different FeAs layers are also metallic. By counting the enclosed volumes of the Fermi surface sheets, we observe a large self-doping effect, i.e. 0.25 electrons per unit cell are transferred from the FeAs layer to the Ti$_2$As$_2$O layer, leaving the FeAs layer in a hole-doped state. This exotic behavior is successfully reproduced by our dynamical mean field calculations, in which the self-doping effect is attributed to the electronic correlations in the 3d shells. Our work provides an alternative route of effective doping without element substitution for iron-based superconductors.

1:15PM Z5.00009 Extraordinary Doping Effects on Quasiparticle Scattering and Bandwidth in Iron-Based Superconductors, DONGLAI FENG, Dept. of Physics, Fudan University — Iron-based superconductors exhibit very rich phenomena with doping. We systematically investigate the behavior of dopants in a variety of iron-based superconductors with angle-resolved photoemission spectroscopy (ARPES), we find that dopants modify the carrier density, introduce quasiparticle scattering, and vary the bandwidth in extraordinary ways [1]. Particularly, we find that instead of Fermi surface topology or carrier density, the bandwidth, which is closely related to electronic correlations, is likely the most important parameter that determines the change in the electronic properties. By investigating the change in the coupling strength between electron and a bosonic mode, in addition, the size of the band splitting between the middle and inner hole bands at the Gamma point which was suggested to represent the size of Fermio-orbital fluctuation does not change, in a sharp contrast to the case of Co doped LiFeAs. This result suggests that the band splitting is not related to the $T_c$ suppression in LiFe$_1$-xMnxAs system.

1:39PM Z5.00011 Nematic order and Fermi surface reconstruction of chalcogen Fe-based superconductors, JUJUN-YUAN LIN, Institute of Physics, National Chiao Tung University, Hsinchu 30010, Taiwan — We utilized the transport property measurements and polarized Fe L-edge XAS to explore nematic order and Fermi surface reconstruction in FeSe. Temperature-dependent magnetoresistance— the Hall coefficient, and angle-resolved photoemission spectroscopy (ARPES) measurements on the charge density wave system’s (CDW) CeTe$_2$O$_4$. We found that the slopes of the middle and inner hole bands near the Fermi energy decrease upon Mn doping, resulting in downward shift of the band tops. Meanwhile, band positions away from the Fermi energy remain more or less the same. We attribute such change to the suppression in LiFe$_1$-xMnxAs system.

2:27PM Z5.00010 Electronic structure of LiFe1-xMnxAs (x=0, 0.04), JONGJIN SEO, Yonsei Univ, BUMSUNG LEE, KEE HOON KIM, Seoul National Univ, CHANGYOUNG KIM, Yonsei Univ — We studied the Mn substitution effect in LiFeAs with Angle Resolved Photoemission Spectroscopy. We found that the slopes of the middle and inner hole bands near the Fermi energy decrease upon Mn doping, resulting in downward shift of the band tops. Meanwhile, band positions away from the Fermi energy remain more or less the same. We attribute such change to the suppression in LiFe$_1$-xMnxAs system. This work is to elucidate the existence of Fermi surface reconstruction in FeSe in which no SDW was observed. Moreover, whether this electronic structure change has a nematic or magnetic origin will be answered.

This work was supported by MOST of Taiwan.

2:51PM Z5.00012 On the Phase Diagram of FeSe$_{1-y}$As$_y$, KHALIL ZIQ, T. OWOLABI, King Fahd University of Petroleum and Minerals, Physics Department — Structural, magnetic and transport measurements have been performed on FeSe$_{1-y}$As$_y$ samples in the normal and superconducting state in an effort to obtain the phase diagram. It is found that As-substitution drastically suppress the superconducting state while it has little effect of structural transformation as the temperature decreases. Moreover, low As-concentration (x ∼ 1%As) has been found very effective in stabilizing the β-FeSe phase.

This work has been supported by NSTIP under 11-ADV1631.


11:15AM Z7.00001 Electronic structure origins of the extremely large magnetoresistance in tungsten ditelluride, IVO PLETIKOSIC, MAZHAR ALI, ROBERT CAVA, Princeton Univ, TONICA VALLA, Brookhaven Natl Lab — WTe$_2$ is a layered transition metal dichalcogenide showing a structural reduction to one-dimensional tellurium-surrounded tungsten chains. The material exhibits an extremely large positive anisotropic magnetoresistance of a few million percent that increases as the square of the field and shows no saturation up to 60 T. We explored the possible electronic structure origins of the magnetoresistance by means of angle-resolved photoelectron spectroscopy (ARPES) and found electron and hole pockets of equal size along the direction of tungsten chains, forming a highly anisotropic quasi-two-dimensional Fermi surface. The perfect carrier compensation at low temperatures has been identified as the primary source of the magnetoresistive effect, and the change of the Fermi surface shape as well as the high-density-of-states band slightly below the Fermi level recognized as the cause of its diminishing at rising temperatures. [1] M.N. Ali et al. Nature 514, 205 (2014) [2] I. Pletikos? et al. arXiv:1407.3576 (2014)

11:27AM Z7.00002 Near Gap Excitation of Collective Modes in a Charge Density Wave, DOMINIK LEUENBERGER, JONATHAN SOBOTA, SHUOLONG YANG, Stanford University, ALEXANDER KEMPER, Lawrence Berkeley National Laboratory, PAULA GIRALDO, ROB MOORE, IAN FISHER, PATRICK KIRCHMANN, THOMAS DEVEREAUX, ZHI-XUN SHEN, Stanford University — We present time-and-angle-resolved photoemission spectroscopy (trARPES) measurements on the charge density wave system’s (CDW) CeTe$_2$. Optical excitation transiently populates the unoccupied band structure and reveals a CDW gap size of $\Delta = 0.59$ eV. In addition, the occupied Te-5p band dispersion is coherently modified by three collective modes. First, the spatial polarization of the modes is analyzed by fits of a transient model dispersion and DFT frozen phonon calculations. We thereby demonstrate how the rich information from trARPES allows identification of collective modes and their spatial polarization, which explains the mode-dependent coupling to charge order. Second, the exciting photon energy $h\nu$ was gradually lowered towards $2\Delta$, at constant optical excitation density. The coherent response of the amplitude mode deviates from the optical conductivity, which is dominated by direct interband transitions between the lower and upper CDW bands. The measured $h\nu$ dependence on the CDW gap size for transition between bands with different orbital character. This finding suggests, that the coherent response of the CDW amplitude mode is dominated by photo-doping of the charge ordering located in the Te-planes.
CaC$_6$ and BaC$_6$, we rule out C$_{xy}$ phonon mode as the origin of the superconductivity in CaC$_6$, which strongly suggests interlayer state driven superconductivity. For BaC$_6$, the graphene band Dirac point energy is smaller than that of CaC$_6$. Based on data from cell is supposed to contain three graphene layers. This suggests that c-axis ordering of Ca has little effect on the electronic structure of CaC$_6$. In addition to band possesses a weak $k_z$ dispersion. The overall electronic structure shows a peculiar single graphene layer periodicity in the $k_z$ direction although CaC$_6$ unit structures to investigate the interlayer states. The results reveal a spherical interlayer Fermi surface centered at the $\Gamma$ point.

BERG, JONATHAN DENLINGER, Advanced light source, CHANGYOUNG KIM, Yonsei Univ, YONSEI UNIVERSITY TEAM, POSTECH COLLABORATION, LEEM, CHUL KIM, YOONYUNG KOH, BEOMYOUNG KIM, Yonsei Univ, YEONGWOOK KIM, JUNSUNG KIM, KEUNSU KIM, Postech, ELI ROTEN.

Driven Superconductivity

Institute of Physics, Chinese Academy of Sciences, KEHUI WU, State Key Laboratory for Surface Physics, Institute of Physics, Chinese Academy of Science, DENLINGER, Advanced Light Source, Lawrence Berkeley National laboratory, Berkeley, California 94720, USA, MATS LEANDERSSON, Beamline I3, MAX LAB, SE-221 00, Lund, Sweden, CHANGYOUNG KIM, Institute of Physics and Applied Physics, Yonsei University, Seoul, 120-749, Korea. — Theoretical understanding of spin orbit coupling (SOC) effects in SrTiO$_3$ under 50-layers. This systematic study will provide insight in understanding the evolution of electronic structure and superconductivity from the single-layer up to 50-layers. This systematic study will provide insight in understanding the evolution of electronic structure and superconductivity from the single-layer to multiple-layer FeSe/SrTiO$_3$ films and eventually to the bulk FeSe superconductor.

CHEN, ZUYAN XU, Chinese Academy of Sci (CAS), XI CHEN, Tsinghua university, XUCUN MA, Chinese Academy of Sci (CAS), QIKUN XUE, Tsinghua university, XINGJIAN ZHOU, Chinese Academy of Sci (CAS) — the recent discovery of high-Tc superconductivity in a single-layer FeSe/SrTiO$_3$ film has attracted much attention... Our previous ARPES studies on the FeSe/SrTiO$_3$ films have observed distinct electronic structure of the single-layer FeSe/SrTiO$_3$ film, established a phase diagram and observed a signature of high Tc over 65K in the annealed single-layer FeSe/SrTiO$_3$ films, revealed the dichotomy of electronic structure and superconductivity between the single-layer and double-layer FeSe/SrTiO$_3$ films, and observed an insulator-superconductor transition in the single-layer FeSe/SrTiO$_3$ films. In this talk, we will present our new ARPES results on the FeSe/SrTiO$_3$ films with many different layers, from single-layer up to 50-layers. This systematic study will provide insight in understanding the evolution of electronic structure and superconductivity from the single-layer to multiple-layer FeSe film, to multiple-layer FeSe film and eventually to the bulk FeSe superconductor.
possible on the surface of a 3D SPT phase. The obstruction to defining a consistent topological theory involving both the original anyons and the gauge fluxes. We point out that a class of obstructions are necessary for identifying an anomalous SET which has a discrete unitary symmetry group $G$. SETs are anomalous in that they can only occur on the surface of a 3D symmetry protected topological (SPT) phase. In this paper we describe a procedure for identifying an anomalous SET. While the symmetry fractionalization is relevant for observing quantized transport. The phonons then smoothen this out leading to a non-trivial isotropic nonequilibrium distribution which has no memory of the initial state and initial switch-on protocol, and yet is distinct from a thermal state. An analytical expression for the distribution at the Dirac point is obtained. The general relations among fractional quantum numbers carried by different fractionalizations, including those relevant to space group symmetry and time reversal symmetry. Examples are given to apply this framework to exactly solvable local bosonic models with abelian or non-abelian topological order. In addition, the general relations among fractional quantum numbers carried by different anyon species are derived. This framework is applicable in particular to gapped quantum spin liquids, fractional Chern insulators, and fractional topological insulators. This research is supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award # DE-FG02-10ER46686. This work was supported by US Department of Energy (DOE-BES) under Award No. DE-SC0010821. We show that Se doping does not alter the behavior of topological insulators within staggered flux. Interestingly, gapless edge states consisting of counter-propagating states with opposite spins survive, and in some regions, a phase with two such pairs of edge states emerges. We examine the robustness of these phases in the presence of disorder and study the topological phase transitions by varying the disorder strength. These systems demonstrate topological properties similar to but different from the ones predicted by the well-known $Z_2$ topological theory.
12:03PM Z10.00005 Modular Anomalies in the Topological Classification of 2+1D and 3+1D Edge Theories1, MOON JIP PARK, Univ of Illinois - Urbana, CHEN FANG, B. ANDREI BERNEVIG, Princeton Univ, MATTHEW GILBERT, Univ of Illinois - Urbana — Classification of topological phases of matter in the presence of interactions is an area of intense interest. While much progress has been made on classification of interacting bosonic systems, the classification of fermionic systems is less established. One possible means of classification is via studying the partition function under modular transforms, as the presence of an anomalous phase arising in the edge theory of a D-dimensional system under modular transforms, or modular anomaly, signals the presence of a (D-1)-dimensional nontrivial bulk. In this work, we discuss the modular transforms of conformal field theories along a (2+1)-D and (3+1)-D edge. By both analytical and numerical methods, free chiral complex fermions in (2+1)-D and (3+1)-D are shown to be modular invariant, however, we show in (3+1)-D that a background U(1) gauge field results in the presence of a modular anomaly that is the manifestation of a quantum Hall effect in a (4+1)-D bulk.

1 Work supported by National Science Foundation (NSF) and Office of Naval Research (ONR).

12:15PM Z10.00006 Z2 topological invariants and gauge transformation of time reversal polarization, KLAUS KOEPERNIK, JEROEN VAN DEN BRINK, IFW Dresden, Germany — The $Z_2$ topological indices for 2D and 3D (strong and weak) topological materials can be calculated from the time reversal polarization as shown by Fu and Kane. These polarizations are defined up to a sign, which represents a gauge choice, since these signs do not influence the topological indices. We discuss the origin of this gauge invariance and its physical interpretation for materials with inversion center.

12:27PM Z10.00007 An exactly solvable model for twisted symmetry-enriched phases, NICOLAS TARANTINO, LUKASZ FIDKOWSKI, Stony Brook University — Topological phases in 2D have a long history of exotic behaviour, producing anyons and protected edge states. This trend continues when we impose an extra symmetry $G$, producing a symmetry-enriched topological (SET) phase. While the ground state will remain invariant under $G$, the set of anyons $\mathcal{A}$ may transform non-trivially. The different ways of implementing the symmetry are classified by the elements of the group cohomology $H^2(G, \mathcal{A})$, where $\mathcal{A}$ describes the action of $G$ on the set of anyons. Previously constructed models fix $\rho$ to be the identity, meaning that $G$ can only modify anyons by a phase, whereas we could easily envision a case where $G$ permutes anyon types, which we call twisted SETs. In this talk, we will propose a modified string-net model which allows $G$ to act on the anyons in exactly that manner, for any choice of $\rho$. We will also introduce a constructive method of gauging the global symmetry, which allows us to verify that the obtained twisted SETs are distinct by showing that discrete gauge theories produced by gauging $G$ are distinct.

12:39PM Z10.00008 “Gauging” Non-on-site Symmetries and Symmetry Protected Topological Phases1, CHANG-TSE HSIEH, GIL YOUNG CHO, SHINSEI RYU, Univ of Illinois - Urbana — We gauge non-on-site symmetries, such as parity symmetries, for a general (1+1)D conformal field theory (CFT) which is the boundary of (2+1)D symmetry protected topological (SPT) phases. This provides an efficient method to diagnose stability of SPT phases with the discrete non-on-site symmetries. To gauge the non-on-site symmetries, we are naturally led to consider field theories defined on a non-oriented manifold, such as Klein bottle. The partner states of the “vortices” (or twist operators) of the gauged non-on-site symmetries, the so-called crosscap states, provide information about the classification of the corresponding SPT phases. Our method also provide a way to gauging time-reversal symmetry, which is “topologically” related to parity symmetry by CPT theorem.

1 NSF grant DMR-1064319

12:51PM Z10.00009 Twist liquids and gauging anyonic symmetries, JEFFREY TEO, University of Virginia, TAYLOR HUGHES, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — Topological phases of matter in (2+1)D are frequently equipped with global symmetries that label anyons without changing the fusion and braiding structures. Twist defects are static symmetry fluxes that permute the labels of orbiting anyons. Gauging or melting these symmetries by quantizing defects into dynamical excitations leads to a wide class of more exotic topological phases known as twist liquids. We formulate a general gauging framework, characterize the anyon structure of twist liquids and provide soluble lattice models that capture the gauging phase transitions. Generalizing a discrete gauge theory, we represent the anyons by a phase, whereas we could easily envision a case where $G$ permutes anyon types, which we call twisted SETs. In this talk, we will propose a modified string-net model which allows $G$ to act on the anyons in exactly that manner, for any choice of $\rho$. We will also introduce a constructive method of gauging the global symmetry, which allows us to verify that the obtained twisted SETs are distinct by showing that discrete gauge theories produced by gauging $G$ are distinct.

12:03PM Z10.00010 Fluctuating Domain Wall Wavefunctions for Symmetry Protected Topological Phases1, SHENG-JIE HUANG, MICHAEL HERMELE, Department of Physics, University of Colorado at Boulder — Symmetry protected topological (SPT) phases have been argued to be classified by the group cohomology of the symmetry group. In general, it has been challenging to connect this classification directly and intuitively to physical properties. In this talk, we provide a simple picture of SPT ground state wave functions in terms of fluctuating domain walls, for SPT phases in one and two dimensions with a finite internal symmetry group. The structure of group cohomology has a simple physical manifestation in the wave functions we construct. We also employ the fluctuating domain wall picture to analyze physical properties of SPT phases, and relate these directly to the group cohomology structure of the wave function.

1 This research is supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award # DE-FG02-10ER46686.

12:15PM Z10.00011 Holographic entanglement renormalization of topological insulators, XUEDA WEN, Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green St, Urbana IL 61801, USA, YINGFEI GU, Department of Physics, Stanford University, Stanford, California 94305, USA, PEDRO LOPES, Instituto de Fisica Gleb Wataghin, Universidade Estadual de Campinas, Campinas, SP 13083-970, Brazil, GIL YOUNG CHO, Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green St, Urbana IL 61801, USA, XIAO-LIANG QI, Department of Physics, Stanford University, Stanford, California 94305, USA, SHINSEI RYU, Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green St, Urbana IL 61801, USA — In this work we study the real-space entanglement renormalization group (RG) flows and associated emergent holographic geometry of topological band insulators in (2+1) dimensions with continuum multi-scale entanglement renormalization ansatz (cMERA). Given a ground state of a topological insulator at the UV layer, we study how the Berry curvature as well as the quantum metric evolve in the bulk of cMERA. Besides the nontrivial topological properties in the bulk of cMERA, it is found that the UV state flows to a nontrivial IR state which carries a nonzero Berry flux. Our result is in parallel with the picture in lattice MERA that a nontrivial UV state corresponds to a nontrivial IR state. On the other hand, if we try to construct the UV state with a trivial IR state, we find there is a “phase transition” feature in the bulk of cMERA.
1:27PM Z10.00012 Classification of topological phases with reflection symmetry. TSUNEYA YOSHIDA, TAKAHIRO MORIMOTO, AKIRA FURUSAKI, RIKEN — In $Z_2$ topological band insulators, the time-reversal symmetry protects their topological structure. In these years such a notion is extended to correlated systems including bosonic systems, and these nontrivial phases are referred to as symmetry protected topological (SPT) phases. Parallel to this progress, a topological crystalline insulator, protected by spatial symmetry, is found for SnTe. Thus, SPT phases protected by this type of symmetry are naturally expected, and classifications of such phases are desired. In this article, we address this issue by focusing on a reflection symmetry. Our analysis based on the Chern-Simons approach proposes periodic tables for bosonic and fermionic SPT phases in two dimensions. Besides that, we show an SPT phase with the reflection symmetry is stabilized in a spin model of honeycomb lattice.

1:39PM Z10.00013 Gauging and Orbifolding Topological Phases[1], XIANG CHEN, UIUC, ABHISHEK ROY, Institute for Theoretical Physics, University of Cologne, JEFFREY TEO, Department of Physics, University of Virginia, Charlottesville, VA 22904 USA — Topological phases of matter in $2+1$D are commonly equipped with global symmetries, such as electric-magnetic duality in gauge theories and bilayer symmetry in fractional quantum Hall states. Gauging these symmetries into local dynamical ones is one way of obtaining exotic phases from conventional systems. We study this using the bulk-boundary correspondence and orbifolding the $(1+1)$D edge described by a conformal field theory (CFT). Our procedure puts twisted boundary conditions into the partition function, and predicts the fusion, spin and braiding behavior of anyonic excitations after gauging. We demonstrate this for the twofold-symmetric $Z_N$ gauge theory and the $S_3$-symmetric so(8)$_1$ state.

1:51PM Z10.00014 Sensing Coulomb impurities with 1/f noise in 3D Topological Insulator. SEMONTI BHATTACHARYYA, MITALI BANERJEE, HARIHARAN NHALIL, SUJA ELIZABETH, ARINDAM GHOSH, Indian Institute of Science, Bangalore — Electrical transport in the non-trivial surface states of bulk Topological Insulator (TI) reveal several intriguing properties ranging from bipolar field effect transistor action, weak antilocalization in quantum transport, to the recently discovered quantum anomalous Hall effect. Many of these phenomena depend crucially on the nature of disorder and its screening by the Dirac Fermions at the TI surface. We have carried out a systematic study of low-frequency 1/f noise in Bi$_2$Se$_3$ single crystals, to explore the dominant source of scattering of surface electrons and monitor relative contributions of the surface and bulk channels. Our results reveal that while trapped coulomb impurities at the substrate-TI interface are dominating source of scattering for thin (10 nm) TI, charged crystal disorder contribute strongly in thick TI (110 nm) channels. An unexpected maximum at 25K in noise from thick TI devices indicate scattering of the surface states by a cooperative charge dynamics in the bulk of the TI, possibly associated with the Selenium vacancies. Our experiment demonstrates, for the first time, impact of the bulk charge distribution on the surface state transport in TIs that could be crucial to the implementation of these materials in electronic applications.

Friday, March 6, 2015 11:15AM - 2:15PM –
Session Z16 DMP: Focus Session: Graphene - Growth

11:15AM Z16.00001 First-Principles Simulations for the Initial Stage of Graphene Growth Induced by Si Sublimation from Stepped SiC Surface[1], YOKY ONO, RIST, MARCEED, TAKAHIRO YAMASAKI, NIMS, MARCEED, TAKAHISA OHNO, NIMS, IIS Univ. of Tokyo, MARCEED — An epitaxial graphene sheet can be obtained by heat sublimation of Si atoms from the stepped SiC surface. Although this method is expected as one of the most encouraging procedure to make clean sheets, its atomic scale growth mechanism is yet not understood in detail. In this study, the initial stage of the graphene growth processes on a stepped SiC(0001) surface are analyzed by first-principles molecular dynamics (FPMD) simulations. A first-principles calculation code “PHASE”[1] which is appropriate for efficient large scale parallel calculations is used. Our FPMD simulations proceed as follows. Before the start, some of the Si atoms on the top layer are intentionally removed from the initial SiC substrate to emulate the Si heat sublimation. MD is executed for 1 ps, under the condition of high temperature and then relaxed. Next, additional Si atoms are removed from the 2nd top layer, and then the same MD is repeated again. We tracked the behavior of the redundant C atoms during the series of these procedures. Where, when and how do those C atoms start to re-create the new C-C networks will be discussed in detail by comparing the results from several different patterns of the SiC substrates.


A portion of this research was supported by the grant from MEXT’s project and carried out in partnership with the University of Tokyo.

11:27AM Z16.00002 Energy Efficient Growth of Epitaxial Graphene on Hexagonal SiC Surface with Molybdenum Plate Capping during UHV Annealing[1], KIBOG PARK, HAN BYUL JIN, YOUNGEUN JEON, SUNCHUL JUNG, VIJAYAKUMAR MODEPALLI, HYUNG-JOON SHIN, JUNG-WOO YOO, SUNG YOUB KIM, SOON-YONG KWON, UNIST, HYUN SUK KANG, BYUNG CHEOL LEE, KAERI, JAE-HYEON KO, Hallym University, DAEJIN EOM, KRISS — The quality of epitaxial graphene (EG) grown on a hexagonal SiC substrate is found to be improved greatly by capping the surface with a molybdenum plate (Mo-plate) during UHV annealing. The significant reduction of D-peak and increase of 2D-peak in the measured Raman spectra, compared with the spectra for no capping, confirm the crystallinity enhancement of EG film grown with Mo-plate capping. Mo-plate capping is considered to induce heat annealing on SiC surface by thermal radiation mirroring and raise Si partial pressure near surface by confining the sublimated Si atoms between SiC substrate and Mo-plate. These two phenomena can cooperatively facilitate an environment favorable for growing high-quality EG films. A top-gated field effect transistor is fabricated on EG film grown on Si-face 6H-SiC surface at ~ 950 degree C, showing the field effect mobility of ~ 1800 cm^2/Vs. With no need to heat the entire SiC substrate to high temperature over 1300 degree C as in the conventional annealing under UHV or Ar atmosphere, the Mo-plate capping can be an efficient method to reduce energy consumption significantly in growing high quality EG films.

V. I. Artyukhov, Y. Hao, R. S. Ruoff, and B. I. Yakobson, Proc. Natl. Acad. Sci. U.S.A. 11:51AM Z16.00004 CVD growth of single-crystal monolayer graphene on H-terminated germanium surface, DONGMOK WHANG, Sungkyunkwan University — Large-area graphene has been grown by catalytic chemical vapor deposition (CVD) on various metal substrates. However, the uniform growth of single-crystal graphene over wafer-scale areas remains a challenge toward the commercial realization of various electronic, photonic, mechanical, and other devices based upon the outstanding properties of graphene. In this talk, we present the growth of single-crystal monolayer graphene on hydrogen-terminatd germanium (Ge) surface. A single-crystal Ge substrate is a promising candidate for the growth of single-crystal graphene, because of (i) its catalytic activity for the catalytic decomposition of the formation of graphitic carbon on the surface; (ii) the extremely low solubility of carbon in Ge even at its melting temperature, enabling growth of complete monolayer graphene; (iii) the anisotropic atomic arrangement of single-crystal Ge surface, enabling aligned growth of multiple seeds; (iv) the availability of a large area single-crystal surface via epitaxial Ge growth on Si wafers. We observed that well-defined atomic arrangement on the single crystal Ge surface enabled aligned growth of multiple seeds which can merge to single crystal graphene. Furthermore very weak van der Waals interaction between graphene and underlying Ge surface enabled facile transfer of graphene and recycling of the Ge/Si wafer for continuing growth.

Supported by USNSF, USDOE, and NNSF of China.

11:39AM Z16.00003 Atomic Scale Studies of Graphene on Germanium, BRIAN KIRALY, Department of Materials Science and Engineering, Northwestern University, ROBERT JACOBBERGER, Materials Science and Engineering, University of Wisconsin - Madison, ANDREW MANNIX, MARK HERSAM, Department of Materials Science and Engineering, Northwestern University, MIKE ARNOLD, Materials Science and Engineering, University of Wisconsin - Madison, NATHAN GUISINGER, Center for Nanoscale Materials, Argonne National Laboratory — The successful growth of single crystal wafer-scale graphene directly on semiconducting Ge(110) substrates drastically shifted the graphene growth paradigm set in 2009. To further understand the interface between graphene and germanium, we performed ultra-high vacuum scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) experiments of graphene grown on Ge(001), Ge(110) and Ge(111) wafers. The STM studies confirm that graphene grown on the Ge(111) contains rotational disorder resulting in strongly scattering grain boundaries; conversely graphene on the Ge(110) surface demonstrates strong epitaxy. STS shows that the graphene on Ge(111) retains a nearly free-standing character. Upon in-situ annealing, reconstructed surface domains appear underneath the graphene covering up to 90% of the Ge(110) and Ge(111) surfaces. Raman spectroscopy reveals band shifts in graphene G/2D band of up to 12 cm$^{-1}$/50 cm$^{-1}$, attributed to substantial increase in doping from the underlying substrate. This work shows the electronic interaction between graphene and germanium is both tunable and closely related to the atomic reconfiguration of the underlying germanium surfaces.

11:51AM Z16.00004 CVD growth of single-crystal monolayer graphene on H-terminated germanium surface, DONGMOK WHANG, Sungkyunkwan University — Large-area graphene has been grown by catalytic chemical vapor deposition (CVD) on various metal substrates. However, the uniform growth of single-crystal graphene over wafer-scale areas remains a challenge toward the commercial realization of various electronic, photonic, mechanical, and other devices based upon the outstanding properties of graphene. In this talk, we present the growth of single-crystal monolayer graphene on hydrogen-terminatd germanium (Ge) surface. A single-crystal Ge substrate is a promising candidate for the growth of single-crystal graphene, because of (i) its catalytic activity for the catalytic decomposition of the formation of graphitic carbon on the surface; (ii) the extremely low solubility of carbon in Ge even at its melting temperature, enabling growth of complete monolayer graphene; (iii) the anisotropic atomic arrangement of single-crystal Ge surface, enabling aligned growth of multiple seeds; (iv) the availability of a large area single-crystal surface via epitaxial Ge growth on Si wafers. We observed that well-defined atomic arrangement on the single crystal Ge surface enabled aligned growth of multiple seeds which can merge to single crystal graphene. Furthermore very weak van der Waals interaction between graphene and underlying Ge surface enabled facile transfer of graphene and recycling of the Ge/Si wafer for continuing growth.

Supported by USNSF, USDOE, and NNSF of China.
1:15PM Z16.00009 Role of Surface Termination on the Growth of Graphene on Cu

1:27PM Z16.00010 Growth of Graphene by Catalytic Dissociation of Ethylene on CuNi(111)

1:30PM Z16.00011 ABSTRACT WITHDRAWN

2:03PM Z16.00013 Controlled growth of large area multilayer graphene on copper by chemical vapour deposition

Friday, March 6, 2015 11:15AM - 2:15PM

11:15AM Z18.00001 Structuring intuition with theory: The high-throughput way

11:51AM Z18.00002 The magnetic genome project
12:27PM Z18.00003 Distributed databases for materials study of thermo-kinetic properties
CORMAC TOHER, Duke Univ — High-throughput computational materials science provides researchers with the opportunity to rapidly generate large databases of materials properties. To rapidly add thermal properties to the AFLLOWLIB consortium [1, 2, 3, 4] and Materials Project repositories [5], we have implemented an automated quasi-harmonic Debye model, the Automatic GIBBS Library (AGL) [6, 7]. This enables us to screen thousands of materials for thermal conductivity, bulk modulus, thermal expansion and related properties. The search and sort functions of the online database can then be used to identify suitable materials for more in-depth study using more precise computational or experimental techniques. AFLLOW-AGL source code is public domain and will soon be released within the GNU-GPL license.

1:03PM Z18.00004 High-throughput evaluation of descriptors for thermoelectric materials
GEORG MADSEN, Ruhr Univ Bochum — Achieving optimal carrier and minimal thermal conductivity is necessary for a given material to be suitable for thermoelectric energy conversion. Both properties are computationally too demanding for brute force approaches which demands that simplified descriptors are developed. Based on the recent computational discovery of favorable thermoelectric performance in the commercially viable and environmentally friendly Ag:SnS [1], we discuss how doping limits can be computationally screened. We will discuss the effects of two ubiquitous effects that can result in decreasing the hole concentration and show how the surprising results of Li doping can be rationalized based on data made available through on-line repositories. Furthermore, we show how the lattice thermal conductivity can be rapidly and reliably screened based on the quasi harmonic approximation [2]. We contrast this to the information covered by the available phase space for three-phonon scattering processes.

1:39PM Z18.00005 Predicting lattice thermal conductivity with help from ab initio methods
DAVID BROIDO, Boston College — The lattice thermal conductivity is a fundamental transport parameter that determines the utility a material for specific thermal management applications. Materials with low thermal conductivity find applicability in thermoelectric cooling and energy harvesting. High thermal conductivity materials are urgently needed to help address the ever-growing heat dissipation problem in microelectronic devices. Predictive computational approaches can provide critical guidance in the search and development of new materials for such applications. Ab initio methods for calculating lattice thermal conductivity [1] have demonstrated predictive capability, but while they are becoming increasingly efficient [2], they are still computationally expensive particularly for complex crystals with large unit cells. In this talk, I will review our work on first principles phonon transport for which the intrinsic lattice thermal conductivity is limited only by phonon-phonon scattering arising from anharmonicity. I will examine use of the phase space for anharmonic phonon scattering and the Gruneisen parameters as measures of the thermal conductivities for a range of materials and compare these to the widely used guidelines stemming from the theory of Lieb fried and Schöllmann [3]. [1] D. A. Broido, M. Malorny, G. Birner, N. Mingo, and D. A. Stewart, Appl. Phys. Lett. 91, 231922 (2007); [2] Wu Li, J. Carrete, N. A. Katcho, and N. Mingo, Comp. Phys. Comm. 185, 1747 (2014); [3] G. Leibfried and E. Schöllmann, Nach. Akad. Wiss. Gottingen, Math. Phys. Klasse 4, 71 (1954).

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Friday, March 6, 2015 11:15AM - 2:15PM —
Session Z19 DFD GSOFT: Invited Session: Shear Thickening of Dense Suspensions Mission Room 103B - Heinrich Jaeger, University of Chicago

11:15AM Z19.00001 Dynamics of Discontinuous Shear Thickening suspensions
ERIC BROWN, Yale University — Concentrated suspensions of hard particles such as cornstarch in water exhibit Discontinuous Shear Thickening, in which an increasing shear rate drives a transition from liquid- to solid-like mechanical behavior. In steady-state shear this phenomena is a result of a dynamic version of jamming in which forces are transmitted along particle contact networks that span to system boundaries and repeatedly form and break up. Several dynamic phenomena observed in such suspensions have long been assumed to be a consequence of this shear thickening, but cannot be explained as a direct result of shear thickening, for example a uniquely strong impact response which allows a person to run on the fluid surface. We perform experiments in which a concentrated suspension is subjected to transient impact. In which we find that the strong impact response is due a short-lived jammed contact network spanning to the boundaries and a delay time required for this dynamically jammed region to propagate to the boundary. The resulting ability of this system-spanning solid-like region to support loads can explain the ability of a person to run on the surface of these fluids. This delay before a solid-like response may also explain several other dynamic phenomena observed in these fluids.

11:51AM Z19.00002 Disentangling the role of hydrodynamic and frictional forces in a shear-thickening suspension
ITAI COHEN, Cornell University — Who among us has not spent countless hours squeezing, rubbing, and smushing gooey substances like, tooth paste, silly putty, corn starch, and even bodily fluids between our fingers? If we could magnify our view and look deep within the substances we are handling what structures would we find? How, do these structures lead to the fascinating mechanical properties that we experience on the scale of our fingers. In this talk I will address the phenomenon of shear thickening in which the viscosity of a suspension increases with increasing shear rate. I will describe recent measurements we have made using a newly developed confocal rheoscope that, for the first time, experimentally visualize the hydrodynamically induced particle clusters. Such clusters have been implicated in continuous shear thickening. It remains controversial as to whether thickening in such suspensions also arises from frictional interactions between particles. The distinct contributions of frictional and hydrodynamic forces are typically difficult to measure independently using conventional techniques. Here, I will describe our approach for using both bulk rheometry techniques and our confocal rheoscope to disentangle their contributions to the total stress response.
12:27PM Z19.00003 Discontinuous Shear Thickening and Dilatancy: Frictional Effects in Viscous Suspensions, JEFFREY MORRIS, Levich Institute, City College of New York — Shear thickening in concentrated suspensions has been well-known for quite a long time, yet a firm consensus on the basis for very abrupt or “discontinuous” shear thickening (DST) seen in suspensions of large solid fraction, $\phi$, has not been reached. This work addresses the DST phenomenon, and proposes a simulation method based in the Stokesian Dynamics algorithm to explore the role of various forces between the particles, including hydrodynamic, conservative potential, and frictional interactions. This work shows that allowance for friction between spherical particles suspended in a viscous liquid causes a significant reduction in the jamming solid fraction of the mixture, $\phi_{\text{max}}$, taken as the maximum fraction at which the suspension will flow. A consequence of this is a shifting of the singularity in the effective viscosity, $\eta$, to smaller $\phi_{\text{max}}$, and the frictional suspension has a larger viscosity than does the frictionless suspension of the same solid fraction, as is clear from the standard empirical modeling of $\eta(\phi) = (1 - \phi)/\phi_{\text{max}}^{1-\alpha}$, $\alpha \approx 2$. When a counterbalancing repulsive force between the particles, representative for example of charge-induced repulsion, is incorporated in the dynamics, the mixture undergoes a transition from frictionless to frictional interactions, and from low to high effective viscosity, at a critical shear rate. Comparison with experimental data shows remarkable agreement in the features of DST captured by the method. The basic algorithm and results of both rate-controlled and stress-controlled simulations will be presented. Like the shear stress, the magnitude of the normal stress exerted by the suspended particles also increases abruptly at the critical shear rate, consistent with the long-standing notion that dilatancy and shear-thickening are synonymous. We will show that all shear thickening materials as dilatant is a misconception, but demonstrate the validity of the connection of dilatancy with DST in concentrated suspensions.

1:03PM Z19.00004 Role of frictional particle interactions for the jamming of dense suspensions, CLAUS HEUSSINGER, Institute for theoretical Physics, University of Goettingen — The jamming paradigm aims at providing a unified view for the elastic and rheological properties of materials as different as foams, emulsions, suspensions or granular media. The usefulness of such a unifying concept hinges on the presence or absence of phenomena that are in some sense universal. One such question is the form of the jamming phase itself. It has long been known that certain suspensions can undergo arrest when driving is strong enough. By way of contrast, standard yield-stress fluids, like dense emulsions, yield when the driving exceeds a threshold. This inversion of the jamming phase diagram can now be linked to the action of frictional forces between the suspended particles. Without frictional forces the material yields and flows at high forces, with friction the material only flows for low forces. As a corollary of this inversion one finds a discontinuous and hysteretic jamming transition as well as continuous and discontinuous shear-thickening regimes.

1:39PM Z19.00005 Setting of an object in a dense suspension, DEVARAJ VAN DER MEER, University of Twente — Constarsh suspensions exhibit remarkable behavior. Here, we present two surprising observations for an object settling in such a suspension. First, in the bulk of the liquid the velocity of the object oscillates around a terminal value, without damping. And secondly, near the bottom of the container the object comes to an expected full stop, but then accelerates again towards a second stop. This stop-go cycle is repeated up to seven times before the object comes to a final standstill close to the bottom. For the bulk oscillations we show that common shear thickening models cannot account for the observed phenomena and that the history of the suspension needs to be taken into account. A hysteretic model that goes beyond the traditional viscoelastic ones describes the experiments adequately, but due to its phenomenological origin lacks a solid physical interpretation. Subsequently, we propose a minimal jamming model to describe the behavior at the bottom. Finally, we will compare our experiments to other transient and steady state phenomena observed in dense suspensions and discuss them in the context of compressional and shear jamming.

Friday, March 6, 2015 11:15AM - 2:15PM — Session Z20 DPOLY: Invited Session: Physics of Entanglements
Ballroom B - Scott Milner, Pennsylvania State University

11:15AM Z20.00001 Shear banding in time dependent flows of polymers and wormlike micelles, SUZANNE FIELDING, Durham University — We study theoretically the formation of shear bands in time-dependent flows of polymeric fluids and wormlike micellar surfactant solutions, focussing in particular on the commonly studied experimental protocols of step shear stress and shear startup. For each protocol, we perform a linear stability analysis to provide a fluid-universal criterion (with some caveats in the case of shear startup) for the onset of shear banding (following Moorcroft and Fielding Phys. Rev. Lett. 2013). In each case this criterion depends only on the shape of the experimentally measured rheological response function for that protocol, independent of the constitutive properties of the material in question. In this way our criteria in fact concern all complex fluids and not just the polymeric ones of interest here. (See Fielding Rep. Prog. Phys. 2014 for a study of these effects in a broad class of soft glassy materials including dense emulsions, microgels and dense colloids.) An important prediction is that pronounced shear banding can arise transiently in each of these time-dependent protocols, even in fluids for which the underlying constitutive curve of the material (stress as a function of strain-rate) is monotonic and a steadily flowing state is accordingly unbanded. Further details can be found in Moorcroft and Fielding J. Rheol. 2014.

11:51AM Z20.00002 How polymer entanglement responds to fast large deformation: are we there yet?, SHI-QING WANG, University of Akron — Nearly all polymeric materials are of high molecular weight and therefore entangled in their liquid state. Significant melt elasticity arises from the transient networking due to chain entanglement. All rheological behavior stems from how the entanglement responds to external deformation of various forms. Unfortunately, the concept of entanglement still remains theoretically elusive to describe. On other hand, modeling the evolution of chain entanglement is the core questions in polymer rheology: a) where chain deformation comes from? b) when affine-like elastic molecular deformation ceases? In other words, yielding at both macroscopic (which is obviously taking place, e.g., signified by the stress overshoot response to startup shear) and molecular levels (through chain disentanglement) is an essential ingredient of any theoretical description of nonlinear polymer rheology. Macroscopic observations are valuable to afford useful insights, but it is the molecular dynamics simulations that are expected to address the foundational issues. This presentation will attempt to make a coherent discussion of what is known and where we are going from here.

1 National Science Foundation (DMR-1105135)

12:27PM Z20.00003 From molecules to non-linear rheology of highly branched, entangled polymers: getting your priorities right, DANIEL READ, The University of Leeds — The tube model for polymer dynamics offers the promise of predicting the flow properties of entangled polymeric liquids. Given a knowledge of the sizes and shapes of the polymers, the tube model suggests dynamical rules for the relaxation of stress carried by the molecules. Over the last couple of decades these rules have been, for the most part, established through experiments and simulations on liquids containing molecules of well-defined size and shape. For prediction of small amplitude flows, these rules are now codified in computer algorithms such as Larson’s hierarchical model (http://www.ingin.umich.edu/dept/che/research/larson/) and our own “BoB” model (http://sourceforge.net/projects/bob-rheology). As a result, it is now possible to make meaningful predictions for flow properties of industrial polymeric resins with distributions of randomly branched structures. Since real polymers are subjected to large deformations in realistic processing, we have recently extended the above work to prediction of the large-deformation response of branched polymers. This talk will describe the extra physics that applies in the non-linear flow regime, and how this has been implemented in our model: the central message is that one needs to know three quantities for every strand in the resin: 1) an orientation relaxation time, (2) a stretch relaxation time, and (3) a limiting value for the chain stretch. The latter is often discussed in terms of a topological quantity known as “priority.” Motivated by recent experiments on well defined “comb” molecules, we discuss some shortcomings in our current prediction of the “priority” and how this may be improved upon.
1:03PM Z20.00004 Entangled linear, branched and hyperbranched polymers in shear flow. DIMITRIS VLASTOSPOULOS, FORTH-IESL and University of Crete — Despite substantial progress in understanding the dynamics of long flexible polymers, several outstanding challenges remain. We address some of them. We discuss the response of well-characterized linear and branched (stars, combs, H) polymers to simple shear flow. The start-up stress behavior at high shear rates exceeding the inverse Rouse time, where according to tube-model theories polymer chains are oriented (and eventually stretched), is considered. We identify conditions under which combs are considered as effective diluted linear chains. We address the failure of stress-optical and Cox-Merz rules and the role of branching. Relaxation upon flow cessation is analyzed and a connection to convected constraint release is suggested. We apply the “probe rheology” approach to branched polymers diluted in polymeric matrix. Careful choice of matrix molar mass allows controlling constraint release effects. The shear response of asymmetric linear chain mixtures is also discussed in the context of recent studies in uniaxial extension suggesting enhancement of extensional viscosity. Entanglement-like effects are observed in dendronized polymers with branches below the entanglement limit, which interpenetrate to reduce inherent density heterogeneity.

Collaboration with S. Costanzo, F. Snijkers, H. Lentzakis, L. G. Leal (Santa Barbara), R. H. Colby (Penn State), N. Hadjichristidis (KAUST), A. D. Schelter (Zurich) and support from EU (Suplean, ESMI) and GGSRT (Aristea-Rings) are acknowledged.

1:39PM Z20.00005 Polymer twist: entanglement and packing ansatz. JIAN QIN, University of Chicago — Polymers in dense liquids (molten plastics) are severely constrained by surrounding chains, due to the fact that chains cannot cut through each other. Effectively, polymers may be considered as being confined inside a tube-like region. The tube diameter is the key parameter needed by the modern molecular theory for polymer rheology. But a molecular understanding of the tube diameter is missing. We summarize our recent attempts at estimating the tube diameter from simulated topologically equilibrated ring polymers, which have well-defined topological states and are free from the complication caused by chain end relaxation dynamics. We consider two non-invasive methods for estimating the tube diameter, one based on the extent of bead position spreading over an ensemble of short dynamic trajectories, and another based on statistics of topologically distinct states collected with the help of a generalized knot invariant.

Relaxation dynamics. We consider two non–invasive methods for estimating the tube diameter, one based on the extent of bead position spreading over an ensemble of short dynamic trajectories, and another based on statistics of topologically distinct states collected with the help of a generalized knot invariant. For simulated polymer melts, we get a tube diameter value that agrees with values obtained by more heuristic methods. We then present results on the effects of chain stretching and neutral solvent dilution on the tube diameter, and examine the three possible variants of the Lin-Noolandi packing arguments for the tube diameter, which all yield the same prediction for unperturbed polymer melts, but each gives different prediction when applied to stretched and diluted systems. The analyses are in favor of a binary view of polymer entanglement.

Friday, March 6, 2015 11:15AM - 1:15PM – Session Z21 Vanadium Oxides II

201 - Mengkun Liu, Stony Brook University

11:15AM Z21.00001 Study of microstructure effects on the photo-induced Metal-insulator transition in VO₂ thin films grown on Al₂O₃ and TiO₂¹. ELIZABETH RADUE, LEI WANG, College of William and Mary, SALINPORN KITTIWATANAKUL, JIWEI LU, STUART WOLF, University of Virginia, ENRICO ROSSI, R.A. LUKASZEW, IRINA NOVIKOVA, College of William and Mary — We studied the optical response of the VO₂ thin films undergoing photo-induced metal-insulator transition (MIT) of VO₂ and found the change in reflectivity over time to be highly dependent on the substrate on which the film was grown [1]. Specifically, we have looked at two different VO₂ thin film samples, one grown on TiO₂ and one grown on Al₂O₃, in a pump-probe configuration, and found that the strain and differences in microstructure resulted in substantial difference in the fluence threshold needed to induce MIT, as well as in the relaxation times back to the insulating state. By mounting the films in a cryostat, we also found that the fluence needed to achieve full MIT for the film on TiO₂ substrate did not depend on the sample temperature, implying that different mechanisms may be playing a stronger role in one film rather than the other for an optically induced transition.

¹This project was sponsored by the NSF, DMR-1006013. Plasmon Resonances and Metal Insulator Transitions in Highly Correlated Thin Film Systems, and Jeffress Trust Awards program in Interdisciplinary Research

11:27AM Z21.00002 Surface Plasmon Resonance and Insulator-Metal Transition in Gold and Vanadium Dioxide Bilayer Films. MELISSA BEEBE, LEI WANG, SCOTT E. MADARAS, J. MICHAEL KLOPF, ZHAOZHU LI, DAVID BRANTLEY, MATTHEW HEIMBURGER, COLLEGE OF WILLIAM & MARY, RUSSELL A. WINCHESKI, JIWEI LU, STUART A. WOLF, University of Virginia, R.A. LUKASZEW, College of William & Mary — Under certain conditions, thin films of noble metals such as gold and silver exhibit intense surface plasmon polaritons (SPP), in what is called surface plasmon resonance (SPR). These are charge oscillations along the air/film interface resulting from the interactions between an illuminating wave and the free electrons at the conductor’s surface. There are many possible applications of the SPR, including new plasmonic optoelectronic devices, biological sensors, and new imaging methods [1,2]. We now present correlated experimental studies and simulations on the modulation of the SPP in Au/VO₂ bilayers by the metal insulator transition (MIT) of VO₂, opening up new possible applications. The modification of the SPP wave vector by the thermally-induced MIT in VO₂ was investigated by measuring the optical reflectivity of the sample when SPP’s were excited via gratings patterned on the Au surface and also in Kretschmann configuration in Au/VO₂ bilayers.


11:39AM Z21.00003 Low-frequency noise spectroscopy of vanadium dioxide along the metal to insulator transition. SAHAR KESHAVARZ, PATRICK LECLAIR, Center for Materials for Information Technology (MINT), Department of Physics and Astronomy, University of Alabama Tuscaloosa, Al 35487, USA; ARUNAVA GUPTA, Center for Materials for Information Technology (MINT), Department of Chemistry, University of Alabama Tuscaloosa, Al 35487, USA; SANJOY SARKEY, Department of Physics and Astronomy, University of Alabama Tuscaloosa, Al 35487, USA — VO₂ exhibits ultrafast, reversible metal-insulator transition (MIT) around T ~ 340K. Origin and mechanism of VO₂ MIT has been controversial, since it simultaneously undergoes a structural transition. One key feature of the MIT is coexistence of metallic and insulating regions over a broad temperature range. We propose low-frequency noise spectroscopy to clarify the nature of this phase coexistence. Noise spectroscopy is more sensitive to details of current distribution, and thus the distribution of metallic and insulating regions, than traditional transport. Epitaxial films of VO₂ have been deposited on (100), (110) and (001) TiO₂ substrates by CVD and were tested by XRD, resistivity versus temperature, and AFM to ascertain quality. As the result, low-frequency 1/f noise amplitude diverges around onset of transition along c-axis, with noise depending non-monotonically on resistivity. On the other hand, it depends monotonically on resistivity along a-axis. This indicates the critical role of structural dynamics during the transition, and in particular strongly suggests that fluctuations of the V-V dimers along c-axis play a prominent role in MIT. Our findings contradict expectations for noise behavior based on simple percolation models.
11:51AM Z21.00004 Low temperature electric transport properties of hydrogen-doped VO2.

12:03PM Z21.00005 Hole doping in VO2 thin films.

12:15PM Z21.00006 Visualization of quasiparticle interference on the surface of SrVO3 film.


12:51PM Z21.00009 Direct Hall effect measurement on a single vanadium dioxide nanowire.
1:03PM Z21.00010 Crossbar structures of vanadium dioxide nanobeams1, ZHENG YANG, KETAKI SARKAR, University of Illinois at Chicago, YANG RESEARCH GROUP TEAM — A crossbar structure composed of two individual one-dimensional nanostructure such as nanowire, nanotube, graphene nanoribbon crossed with each other has been of great interest for nanoelectronic, photonic, and memory device applications as well as novel phenomena in fundamental science. Here we report crossbar nanostructures based on crossed vanadium dioxide nanobeams. Vanadium dioxide show a metal-insulator transition at \( \approx 340K \) with a sharp (3-5 orders of magnitude) resistance change accompanying with a structural change from monoclinic to tetragonal structures. Besides the thermal-triggering, other excitations in form of electrical, photo, strain can also trigger the phase transition. In recent years lots of efforts have been focused on how to utilize the metal-insulator phase transition in vanadium dioxide for device applications (ref: Zheng Yang et al, Oxide electronics utilizing ultrafast metal-insulator transitions, Annual Review of Materials Research, 2011, 41, 337). In this presentation, the growth, fabrication, structural and electrical properties of the vanadium dioxide nanobeam crossbars will be reported. The potential device applications of vanadium dioxide nanobeam crossbars will be discussed.

1Acknowledgement to the funding support from Discovery Award.

Friday, March 6, 2015 11:15AM - 2:03PM –
Session Z22 DMP: Focus Session: Carbon Nanotubes, Graphene, & Related Materials 202A -
Stephen Cronin, University of Southern California

11:15AM Z22.00001 Atomtronics: The Application of Organometallic Bis-Hexahapto Bonding to the Electrical Interconnection and Electronic Conjugation of the Graphitic Surfaces of Carbon Nanotubes and Graphene, ROBERT HADDON, University of California at Riverside — We have demonstrated the functionalization of epitaxial graphene with nitrophenyl groups and by the application of the Kobe reaction. The chemical formation of covalent carbon-carbon bonds involving the basal plane carbon atoms offers an alternative approach to the control of the electronic properties of graphene; the transformation of the carbon centers from sp\(^2\) to sp\(^3\) introduces a barrier to electron flow by saturating the carbon atoms and opening a band gap which potentially allows the generation of insulating, semiconducting and magnetic regions in graphene wafers.1 This raises the question of the role of covalent bonding in the interconnection of graphitic surfaces and the prospects for the use of such bonds in electronically conjugating neighboring carbon nanotube and graphene surfaces without saturating and destructively rehybridizing the carbon atoms at the point of attachment while simultaneously maintaining the band structures of the intact benzoid nanostructures. In this talk I will discuss our recent results on the covalent modification of the electronic structure and properties of graphene, and the application of organometallic chemistry to facilitate the interconnection of single-walled carbon nanotubes and to increase the dimensionality of graphitic surfaces. 1. Bekyarova, E.; Sarkar, S.; Wang, F.; Itkis, M. E.; Kalinina, I.; Tian, X.; Haddon, R. C., Effect of Covalent Chemistry on the Electronic Structure and Properties of Carbon Nanotubes and Graphene. Acc. Chem. Res. 2013, 46.

1Japan Society for the Promotion of Science

12:03PM Z22.00003 Theory of Chiral Transport in Chiral Carbon Nanotubes1, MASAKI NORO, Tokyo Institute of Technology, JYUNYA TANAKA, None, SHUICHI MURAKAMI, TAKEHITO YOKOYAMA, Tokyo Institute of Technology — In a chiral carbon nanotube, lower crystallographic symmetry allows chiral transport. Namely, when carriers exist by doping, an electric current along the tube axis induces a current around the tube. We calculate the chiral conductivity in carbon nanotubes induced by an electric field along the nanotube axis. We use a tight-binding model for various carbon nanotubes with different chiralities, and apply a constant relaxation time in Boltzmann transport equation. Because the band structure is different for each chiral carbon nanotube, we set electron concentration to be constant to compare quantitatively the chiral conductivity for each nanotube. We find that the chiral conductivity in chiral nanotube is in general non zero, and have either signs depending on their chiralities. We discuss the dependence on the chirality in comparison with the band structure in single-layer graphene, and attribute the chiral transport to the warping of the Fermi surface around the K and K’ point in graphene.

12:15PM Z22.00004 Electron and Optical Spectroscopies of Graphene Nanoribbons on Au(111): Insights from Ab-Initio Calculations, ANDREA FERRETTI, SHUDONG WANG, DEBORAH PREZZI, 53 Center, Istituto Nanoscienze, I-41125, Modena, Italy, ALICE RUINI, ELISA MOLINARI, University of Modena and Reggio Emilia, FIM dept & S3 Center, Istituto Nanoscienze, I-41125, Modena, Italy — Narrow graphene nanoribbons (GNRs) exhibit substantial electronic band gaps and optical properties expected to be fundamentally different from the ones of their parent material graphene. Unlike graphene the optical response of GNRs may be tuned by the ribbon width and the directly related electronic band gap. In this work we perform ab initio calculations and compute quasiparticle energies and optical properties of GNRs within the so-called GW-BSE scheme. We focus on a specific armchair nanoribbon (7-AGNR). The presence of the substrate is accounted for by means of a classical image charge model for the screened Coulomb interaction. Our findings show that the metallic substrate induces a significant reduction of the energy gap as compared to the isolated 7-AGNR, bringing the GW gap from 3.7±0.1 eV to 2.3-2.7 eV on Au(111). On the contrary, the position of the optical peaks remains unaltered. Our results are in very good agreement with the experimental values obtained by STS, ARPES, and differential reflectance data, indicating that this scheme can provide quantitative predictions for electron and optical spectroscopies of nanoribbons on weakly coupled substrates such as Au.

12:27PM Z22.00005 First-principles calculations of the phonon transport in carbon atomic chain systems based on atomistic Green’s function formalism1, HU SUNG KIM, YONG-HOON KIM, Graduate School of EEEWS, Korea Advanced Institute for Science and Technology — We report on the phonon transport in carbon chain systems, and cumulene. We utilized first-principles calculation with localized atomic basis sets to calculate interatomic forces. Calculated phonon dispersion of polyyne and cumulene were well-matched with theoretical expectations. In addition, we considered the strain effect on the phonon properties of the carbon chain systems. The applied strain affected bond-length alternation (BLA) and force interaction range. Finally, even and odd carbon atomic chains bridging two zigzag graphene nanoribbons were investigated. Increase in the phonon contribution on thermal conductivity was found in case of even carbon chains with proper amount of strain.

1Global Frontier Program (2013M3A6B1078881), Basic Science Research Grant (2012R1A1A2044793), and EDISON Program (No. 2012M3C1A6035684), KISTI Supercomputing Center (KSC-2014-C3-021)
12:39PM Z22.00006 Anomalous transport in nanotubes with resonant adsorbates

L. Colombier et al., PRL 109, 197402.
B. Yuma et al., PRB 87, 205412;
I. V. Bondarev, PRB 83, 153409;

Support by DOE-DE-SC0007117.

12:51PM Z22.00007 Exploring SAMO states of fullerenes with angle-resolved fs photoelectron spectroscopy

Eleanor Campbell, Elvira Bohl, Olof Johansson, University of Edinburgh, Benjamin Mignolet, Stanford University, Francois Remacle, University of Liege — Femtosecond photoelectron spectroscopy of fullerenes provides a powerful means to study excited Rydberg-like states that cannot be probed via conventional spectroscopy. The photoelectron spectra (PES) show a thermal electron background with a superimposed peak structure for photoelectron kinetic energies that lie below the laser photon energy. The peak structure has been assigned to one-photon ionisation of diffuse low-angular momenta states, so-called superatom molecular orbitals (SAMOs) centred on the hollow fullerene core, based on photoelectron angular distributions (PADs) and TD-DFT calculations. The relative photoionisation probabilities of the s-SAMO to p-SAMO were analysed for photon energies from 2-3.5 eV and showed good agreement with theoretical calculations. Here we look at the photoionisation probabilities and photoelectron angular distributions as a function of laser wavelength and, in particular, directly probe the influence of an endohedrally-trapped atom on the photoelectron spectra by directly comparing C60 and Li@C60. We also provide preliminary measurements to probe the timescale for thermal emission prior to coupling to vibrational degrees of freedom.

12:59PM Z22.00008 Relative stability of excitonic complexes in quasi-one-dimensional semiconductors

Igor Bondarev, North Carolina Central University — A configuration space approach first implemented in Ref.[1] to evaluate biexciton binding energies in carbon nanotubes (CNTs), is developed to obtain the universal asymptotic relations for the lowest energy trion and biexciton binding energies in quasi-1D semiconductors. Triions are shown to be generally more stable (have greater binding energy) than biexcitons in strongly confined quasi-1D structures with small reduced electron-hole masses, while biexcitons are more stable than triions in less confined quasi-1D structures with large reduced electron-hole masses. As such, there is a crossover behavior whereby triions get less stable than biexcitons as the nanostructure transverse size increases — an interesting, quite a general effect which could likely be observed through comparative measurements on semiconducting CNTs of increasing diameter. For a specific case of CNTs with diameters ≤ 1 nm, the model predicts the triion binding energy greater than that of the biexciton by a factor ≈ 1.4, decreasing with the CNT diameter, thus revealing the general physical principles that underlie recent experimental observations [2,3].

12:59PM Z22.00009 Optical detection of highly delocalized superorbitals in fullerenes

Guoping Zhang, Yihua Bai, Indiana State University; Thomas F. George, University of Missouri-St. Louis — Superatom molecular orbitals (SAMOs) in C60 are a group of highly delocalized orbitals, extending several nanometers outside the carbon cage, but unfortunately they are hard to detect optically. Here we employ three independent first-principles methods to show that the optical detection of SAMOs is possible for the multiphoton excitation, where successive absorptions of photons boost the optical cross section. In the case of the 1f orbital, we find that our theoretical photoelectron angular distribution matches the unpublished experimental one quantitatively. Experimental confirmation of our prediction will help explain why the mysterious 4-nm separation between C60 and organic compounds is essential to the efficiency of all the fullerene-based organic solar cells.

12:59PM Z22.00010 Understanding Faceting in Boron-Nitride and Carbon Nanotubes

Robert Guerra, International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy; Itai Leven, Department of Chemistry School of Chemistry, The Raymond and Beverly Sackler Faculty of Exact Sciences, Tel-Aviv University, Tel-Aviv 69978 (Israel); Andrea Vanossi, CNR-IOM Democritos National Simulation Center, Via Bonomea 265, 34136 Trieste, Italy; Erio Tosatti, International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy; Oded Hod, Department of Chemistry School of Chemistry, The Raymond and Beverly Sackler Faculty of Exact Sciences, Tel-Aviv University, Tel-Aviv 69978 (Israel); NanoFriction Group Trieste TEAM, Oded Hod Group @ Tau TEAM — Graphite and hexagonal boron nitride (h-BN) are known to share many structural characteristics such as interlayer spacing and bond length, in spite of their completely different atomic bond types, nonpolar homonuclear and strongly polar, respectively. Only recently, a connection of static polarizability and bond polarity with the interlayer spacing and stacking energetics in the two materials has been elucidated [1]. Yet, in the case of curved sheets forming a nanotube (NT), the presence of angular strain and non-uniform stacking between the layers give rise to complex force patterns that subtly differ in the two cases. By means of classical MD simulations of h-BN and carbon NTs we reveal how the interplay between angular strain and lateral interlayer forces enable the formation of facets in the two materials. The role of the curvature (NT size) and of chirality is discussed along with the important consequences of faceting in the static and frictional properties of multiwall NTs.

1:55PM Z22.00011 Exploring SAMO states of fullerenes with angle-resolved fs photoelectron spectroscopy

Eleanor Campbell, Elvira Bohl, Olof Johansson, University of Edinburgh, Benjamin Mignolet, Stanford University, Francois Remacle, University of Liege — Femtosecond photoelectron spectroscopy of fullerenes provides a powerful means to study excited Rydberg-like states that cannot be probed via conventional spectroscopy. The photoelectron spectra (PES) show a thermal electron background with a superimposed peak structure for photoelectron kinetic energies that lie below the laser photon energy. The peak structure has been assigned to one-photon ionisation of diffuse low-angular momenta states, so-called superatom molecular orbitals (SAMOs) centred on the hollow fullerene core, based on photoelectron angular distributions (PADs) and TD-DFT calculations. The relative photoionisation probabilities of the s-SAMO to p-SAMO were analysed for photon energies from 2-3.5 eV and showed good agreement with theoretical calculations. Here we look at the photoionisation probabilities and photoelectron angular distributions as a function of laser wavelength and, in particular, directly probe the influence of an endohedrally-trapped atom on the photoelectron spectra by directly comparing C60 and Li@C60. We also provide preliminary measurements to probe the timescale for thermal emission prior to coupling to vibrational degrees of freedom.

1:55PM Z22.00012 Optical detection of highly delocalized superorbitals in fullerenes

Guoping Zhang, Yihua Bai, Indiana State University; Thomas F. George, University of Missouri-St. Louis — Superatom molecular orbitals (SAMOs) in C60 are a group of highly delocalized orbitals, extending several nanometers outside the carbon cage, but unfortunately they are hard to detect optically. Here we employ three independent first-principles methods to show that the optical detection of SAMOs is possible for the multiphoton excitation, where successive absorptions of photons boost the optical cross section. In the case of the 1f orbital, we find that our theoretical photoelectron angular distribution matches the unpublished experimental one quantitatively. Experimental confirmation of our prediction will help explain why the mysterious 4-nm separation between C60 and organic compounds is essential to the efficiency of all the fullerene-based organic solar cells.

Supported by U.S. Department of Energy under Contract No. DE-FG02-06ER46304
The Origin of Negative Thermal Expansion in sp-sp² Hybridized Carbon Systems: Rigid Unit Modes

1:39PM Z22.00011

Cheol-Woon Kim, Seoung-Hun Kang, Young-Kyun Kwon, Kyung Hee University — Based on first-principles density functional theory, we investigate the thermal expansion behaviors of three kinds (α, β, and γ) of graphene, which is two-dimensional carbon allotrope composed of sp² and sp³ hybridized bonds. Using quasi-harmonic approximation, their Gibbs free energies are calculated as a function of 2D area and temperature to evaluate their temperature-dependent area variations. We find that all three kinds of graphene exhibit negative thermal expansion behaviors up to quite high temperature as similarly seen in graphene. Their thermal contraction can be explained partially by the ripple effect as observed in graphene, which seems, however, somewhat insufficient for their much larger thermal contraction than that of graphene. Their anomalously huge thermal contraction behaviors are attributed mainly to unusual phonon modes with a frequency of a few hundreds of cm⁻¹, which do not exist in graphene. These modes are identified to "rigid unit modes (RUMs)". The librational modes of "rigid units" composed only of sp³-bonds. RUMs are unusual in 2D materials, but known to be resolvable for the negative thermal expansion in various metal oxides composed of rigid polyhedra, such as MoO₃, where M is a metal cation.

1:51PM Z22.00012

Spectroscopy and microscopy of coronene-carbon nanotube hybrid structures

Katalin Kamaras, Beata Nagy, Hajnalka Tohati, Wigner Research Centre for Physics, Budapest, Hungary, Bea Botka, Rudi Hackl, Walther Meissner Institute, Garching, Germany, Thomas Chamberlain, Andrei Khlobystov, University of Nottingham, United Kingdom — The flat, disc-shaped polyaromatic hydrocarbon coronene and its derivatives can form various hybrid structures with carbon nanotubes: its size makes encapsulation possible for the most abundant carbon nanotubes, and its conjugated π-electron structure enables π–π bonding on the surface of the nanotubes. Depending on synthesis conditions, adsorption, encapsulation and polymerization reactions are all possible, resulting in coronene-based polymers, graphene nanoribbons or double-walled carbon nanotubes. Synthesis and characterization of such hybrid structures will be reported. Synthesis variations included sublimation temperature and exchanging the hydrogen atoms on the perimeter of the molecule for other atoms. Characterization was performed by transmission electron microscopy, as well as infrared, Raman and photoluminescence spectroscopy. We will present how synthesis conditions affect the reaction of the molecular species to form polymers or nanoribbons. We find that the nanotube surface catalyses the polymerization of coronene, and that non-carbon atoms other than hydrogen on the perimeter facilitate nanoribbon formation.

Supported by OTKA Grant No. 107580

Friday, March 6, 2015 11:15 AM - 2:03 PM – Session Z23 APS: General Physics 2028

11:15AM Z22.00001

Classifying symmetry-protected topological phases through the anomalous action of the symmetry on the edge

Dominic Else, Chetan Nayak, Department of Physics, University of California, Santa Barbara, CA — It is well known that (1 + 1)-D bosonic symmetry-protected topological (SPT) phases with symmetry group G can be identified by the projective representation of the symmetry at the edge. Here, we generalize this result to higher dimensions. We assume that the representation of the symmetry on the spatial edge of a (d + 1)-D SPT is local but not necessarily on-site, such that there is an obstruction to its implementation on a region with boundary. We show that such obstructions are classified by the cohomology group H^{d+1}(G, U(1)), in agreement with the classification of bosonic SPT phases proposed by Chen et al [Science 338, 1604 (2012)]. Our analysis allows for a straightforward calculation of the element of H^{d+1}(G, U(1)) corresponding to physically meaningful models such as non-linear sigma models with a theta term in the action. SPT phases outside the classification of Chen et al are those in which the symmetry cannot be represented locally on the edge. With some modifications, our framework can also be applied to fermionic systems in (2+1)-D.

11:27AM Z22.00002

Topological phase transition in a bilayer toric code model

Hong-Chen Jiang, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Yuan-Ming Lu, Department of Physics, The Ohio State University, Ashvin Vishwanath, Department of Physics, University of California, Berkeley — We study a bilayer toric-code model in two spatial dimensions by density matrix renormalization group approach. We show that as the interlayer coupling is increased, the system goes through a continuous phase transition from two decoupled copies of Z₂ topological orders (bilayer limit) to a single Z₂ topological order (monolayer limit). This phase transition is revealed by a jump of topological entanglement entropy. Moreover, the two phases are featured by distinct topological properties: in the bilayer limit the system supports symmetry protected gapless edge states, while the edge states are fully gapped in the monolayer limit. The nature of this continuous topological phase transition is also investigated.

11:39AM Z22.00003

Predicting Heat Transport across Multiple Tokamaks with Neural Networks

Christopher Luna, Arizona State University, Robert Budny, Princeton Plasma Physics Laboratory, Orso Meneghini, Sterling Smith, General Atomics, James Penna, MIT — Three multi-layer, feed-forward, back-propagation neural networks have been built and trained on heat transport data from DIII-D, TFTR, and JET respectively. A comparative analysis shows that previous success of neural networks in predicting heat transport in DIII-D [1] is reproduced for TFTR and JET. The effect of using different neural network topologies has been investigated across all of the devices. It is found that the neural networks can consistently predict the total species' heat fluxes for all of the devices, however they have difficulty in predicting the individual transport modes identified to "rigid unit modes (RUMs)", the librational modes of "rigid units" composed only of sp³-bonds. RUMs are unusual in 2D materials, but known to be resolvable for the negative thermal expansion in various metal oxides composed of rigid polyhedra, such as MoO₃, where M is a metal cation.

1:51AM Z22.00004

ABSTRACT WITHDRAWN

12:03PM Z22.00005

Incompleteness of General Relativity, Einstein’s Errors, and Related Experiments

C.Y. Lo, Applied and Pure Research Institute — General relativity is incomplete since it does not include the gravitational radiation reaction force and the interaction of gravitation with charged particles. Einstein’s covariance principle is invalid. There is no bounded dynamic solution for the Einstein equation. Thus, Gullstrand is right and the 1993 Nobel Prize for Physics press release is incorrect. Awards to Christodoulou reflect the blind faith toward Einstein and accumulated errors. The Einstein equation with an electromagnetic source has no valid solution unless a photonic energy-stress tensor with an anti-gravitational coupling is added. Thus, the photonic energy includes gravitational energy and Einstein’s theory needs improvement. The existence of anti-gravity coupling implies that the energy conditions in space-time singularity theorems of Hawking and Penrose cannot be satisfied in physics. The positive mass theorem of Yau and Schoen is misleading in physics, though considered an achievement by the Fields Medal. E = mc² is not valid for the electromagnetic energy alone. The discovery of the charge-mass interaction establishes the need for unification of electromagnetism and gravitation and would explain many puzzles. Experimental investigations for further results are important.

1 This publication is supported by the Chan Foundation, Hong Kong
various concentrations of Li. In the alloy, we investigated the range of the validity of the ANN potential. Our results show that ANN potentials are widely transferable to Li-Si alloys with accurately predict total energies and equilibrium structures of Li, Si and Li-Si alloys. Using several training databases that include different concentrations of Li, we developed an ANN potential for Li-Si alloys. Our calculations based on the geometry optimizations and molecular dynamic simulations show that the developed potential can be a promising approach to construct the potential energy surface is using artificial neural networks (ANN) that extends the time scales of simulations without interatomic potentials that can capture the dependence of structure on chemical composition. Compared with the fixed functional form of empirical potentials, and requires large numbers of atoms and long time scales which is generally inaccessible with first-principle approaches. These simulations can be carried out using massively parallel computers. We demonstrate that negative thermal expansion can result solely from the differential expansion of the bonds. Implications for materials design will be discussed.

12:27PM Z23.00007 ABSTRACT WITHDRAWN —

12:39PM Z23.00008 Derivative Structure Enumeration: Trimming a Combinatoric Tree1. WILEY S. MORGAN, Department of Physics and Astronomy Brigham Young University, RODNEY W. FORCADE, Department of Mathematics Brigham Young University, ANDREW RAPPE, University of Pennsylvania — In computational material science, one frequently needs to have a list of the “derivative superstructures” of a given lattice. For example many phases in metal alloys are merely “superstructures” of fcc, bcc, or hcp lattices (L12, B2, D019, etc.). When modeling potential alloys one needs to explore all possible arrangements of atoms on the lattice sites. The simple solution to this combinatorics problem is to generate the list of all possible configurations and then eliminate those that are symmetrically equivalent. This approach, however, suffers from the combinatoric explosion that happens when the supercell size is large or when there are more than two atom types. This problem persists even when there are only a relatively small number of unique configurations that survive the elimination process. Our new algorithm avoids this problem by generating “partial configurations,” then using group theory, it eliminates large classes of configurations in a single step. With this approach one can consider larger systems, such as multinary ground state searches, high entropy alloys, etc.

1WSM, RWD, CWR and GLWH acknowledge support from ONR (MURI N00014-13-1-0635).

12:51PM Z23.00009 Robust Computational Physics and Automated Sanity Checks1, CONRAD W. ROSENBROCK, GUS L.W. HART, Brigham Young University - Provo — A good computational physics course teaches students to say ‘well that’s completely wrong’ anytime the computer gives them a result. Once cast in doubt, it is the scientist’s responsibility to convince themselves that the result is in fact correct. As programs become more complicated, it usually becomes more difficult to guarantee that the final output is right. I will present a new framework that automates the production of robust, high quality Fortran code. The talk will include a brief overview of good coding principles and a demonstration of the most useful features of the framework that help automate implementation of these principles. By providing an XML-based documentation standard and automated unit testing, Fortpy1 helps researchers ensure that their code produces accurate physics and is easier to use by others.


1CWR and GLWH acknowledge support from ONR (MURI N00014-13-1-0635)

1:03PM Z23.00010 Equilibrium shape of colloidal crystals. DIMITRIOS MAROUDAS, RAY SEHGAN, Univ of Mass - Amherst — Clusters of colloidal crystals exhibit a wide range of size dependent properties. Leveraging such properties requires a strong fundamental understanding of the thermodynamics of colloidal clusters. A first step in developing this understanding is to accurately describe the equilibrium structure and morphology of these assemblies. In this presentation, we report the results of a generalized Wulff construction that is able to accurately describe the equilibrium, i.e., of minimum free energy, shape of an assembly of colloidal particles. The colloidal system that we focus on is modeled with an interparticle interaction consisting of two terms, an electrostatic repulsion and an Asakura-Oosawa (AO) depletion attraction. The generalized Wulff construction can account for both surface facet and surface edge effects on the stable colloidal crystalline morphology. This construction results in a configuration of minimum free energy for given crystal volume. We carry out these equilibrium shape calculations over a range of crystal sizes to examine size dependent effects on the stability of colloidal clusters. These calculations enable the determination of cluster sizes which exhibit improved stability (lower free energy) compared to that of similar-size clusters.

1:15PM Z23.00011 Coarsening Simulation with an Energy-Stable, Semi-Implicit Time Step. BENJAMIN VOLLMAYR-LEE, Bucknell University — Coarsening dynamics is effectively described by phase field models, which provide nonlinear field equations of motion that can be integrated numerically. However, these simulations are hampered by a numerical instability that imposes time marching with a fixed-size time step decomposition in any model and use an artificial viscosity, which adds an additional restriction, and that has the additional feature of being linear in the implicit fields, allowing for efficient calculation with fast Fourier transforms. Using this method enables simulations to extend decades farther into the coarsening scaling regime. I will report measurements of a variety of coarsening exponents obtained with this method.

1:27PM Z23.00012 ABSTRACT WITHDRAWN —

1:39PM Z23.00013 Developing Accurate and Transferable Artificial Neural Network Potentials for Li-Si Alloys1. BERK ONAT, EKIN DOGUS CUBUK, BRAD MALONE, EFFTHIMIOS KAXIRAS, Department of Physics and School of Engineering and Applied Sciences, Harvard University — Investigation of the lithiation and delithiation of Si anode in Li-ion batteries using realistic simulations is important and requires large numbers of atoms and long time scales which is generally inaccessible with first-principle approaches. These simulations can be carried out using interatomic potentials that can capture the dependence of structure on chemical composition. Compared with the fixed functional form of empirical potentials, a promising approach to construct the potential energy surface is using artificial neural networks (ANN) that extends the time scales of simulations without sacrificing the accuracy and transferability. Using ab-initio density functional theory data for training, we developed an environment-dependent high-dimensional ANN potential for Li-Si alloys. Our calculations based on the geometry optimizations and molecular dynamic simulations show that the developed potential can accurately predict total energies and equilibrium structures of Li, Si and Li-Si alloys. Using several training databases that include different concentrations of Li in the alloy, we investigated the range of the validity of the ANN potential. Our results show that ANN potentials are widely transferable to Li-Si alloys with various concentrations of Li.

1This work was supported in part by TUBITAK under post-doctoral research grant no 2219.
1:51PM Z23.00014 Mass, Energy, Space, and Time Systemic Unified Theory-MEST. DAYONG CAO, Avoid Earth Extinction Association — Massenergy and spacetime build up a balance system of flat universe; massenergy equals negative spacetime. Like mass attract, opposite mass repel; like energy repel, opposite energy attract; like space attract, opposite space repel; like time repel, opposite time attract. In the balance macrosystem: http://meetings.aps.org/link/BAPS.2014.MARY.33.9 In the balance microsystem: $E + E'\psi = m^2 + m'\psi'^2 = 0$. http://meetings.aps.org/link/BAPS.2011.MAR.1.06 There is a unified balance between macro-micro system. In cold area of CMB, the dark massenergy, the spacetime particle which has spacetime center, causes an expanding of period-wavelength of light and redshift which equals negative gravitational redshift of massenergy particle; in hot area, the dark massenergy causes more redshift of light. The sun and dark hole are a balance system-SDS which triggered periodic mass extinctions and created new life on our earth. The quantum orbits both of planets and dark comets of dark hole decided the period. Consciousness remotely change output voltages of solar cell and a balance between Electrons and electron holes which is a negative balance of SDS. By the nuclear energy of spacetime, consciousness should change the orbit of the balance of SDS for avoiding impact.

Friday, March 6, 2015 11:15AM - 2:15PM — Session Z24 DCOMP: Quantum Many-Body Systems and Methods II 203AB - Gopal Priya

11:15AM Z24.00001 Tenfold speed up of DFT: Improving k-point integration. GUS HART, Brigham Young University, DEREK C. THOMAS, University of Texas at Austin, JEREMY J. JORGENSEN, MATTHEW M. BURBIDGE, BRENT C. HESS, CONRAD W. ROSENBROCK, Brigham Young University, IAN H. SLOAN, University of New South Wales, RODNEY W. FORCADE, Brigham Young University, STEFANO CURTAROLO, Duke University — The amount of recent cpu time (> 100 mega cpu hours) spent in our group on high-throughput materials prediction led us to re-examine convergence issues in standard DFT calculations. For total energy calculations, k-point convergence can be increased two-fold and ten-fold for semiconductor and metals, respectively. For semiconductors, the popular “rectangle approximation method” using Monkhorst-Pack grids converges much faster than expected (for reasons that will be explained), which explains why it gained popularity in the early development of DFT codes. (Its simplicity is also a likely factor.) However, it is not possible to adapt the method to the case of partially-occupied bands in metals while preserving the rapid convergence of semiconductors. Using a rectangle rule for metals, irrespective of any smearing method, leads to the well-known problem that convergence rates are 100s times worse than for semiconductors. Revisiting the k-point integration issue in light of modern DFT practice, we demonstrate that this “metal deficit” can be reduced to only a factor of 5–10 worse than semiconductors. The further complication of integrating inside the Fermi surface for metals is solved with our approach without the need for smearing and its associated ad hoc parameters.

11:27AM Z24.00002 Strongly Interacting Molecular Subsystems Using DFT-in-DFT Embedding Theory with External Orbital Orthogonality. PATRICK TAMUKONG, MARK HOFFMANN, Univ of North Dakota, YURIY KHAIT, None — Since most ab initio methods for molecular electronic structure are limited in applicability by polynomially increasing computational costs with system size, localization and embedding techniques are among the leading research efforts in the development of methods that can well describe large systems. Since embedding schemes naturally use a “divide and conquer” approach, they are particularly attractive. We recently introduced a new variant of DFT-in-DFT embedding theory that enforces orbital orthogonality between subsystems, thereby completely obviating the use of error-prone kinetic energy functionals; moreover, no calculation of the total system is required at any stage. Here, we present density difference maps and potential energy curves for selected strongly interacting subsystems, including complete dissociation of covalent bonds, obtained with our new embedding protocol. The electron density difference maps presented here compare densities obtained with the new embedding method, and with conventional DFT-in-DFT, to Kohn-Sham (KS)-DFT selected strongly interacting subsystems, including complete dissociation of covalent bonds, obtained with our new embedding protocol. The electron density difference maps presented here compare densities obtained with the new embedding method, and with conventional DFT-in-DFT, to Kohn-Sham (KS)-DFT densities. It is shown that whereas conventional DFT-in-DFT leads to large density deviations, particularly at the interfaces between subsystems, the new method accurately represents the density at all points in space and leads to only negligible density deviations ($\approx 10^{-5} e/\text{a}_0^3$). To our knowledge, this new embedding method is the first variant of DFT-in-DFT to accurately dissociate actual covalent bonds.

11:39AM Z24.00003 Effect of uniaxial and biaxial strain on the electronic and dynamical properties of CdO: ACBN0 functional study. JACOB GALLAWAY, University of North Texas, PRIYA GOPAL, MARCO FORNARI, Central Michigan University, STEFANO CURTAROLO, Duke University, MARCO BUONGIORNO NARDELLI, University of North Texas — We have investigated the influence of uniaxial and biaxial strain on the electronic and vibrational properties of CdO in the rocksalt structure using Density functional theory calculations with our newly developed ACBN0 pseudo–hybrid Hubbard density functional. ACBN0 is a fast, accurate and parameter-free extension of traditional DFT+U proved to correct both the band gap and the relative position of the different bands in transition metal compounds. CdO is a technologically important materials with a direct band-gap of 2.2 eV, which makes it a potential candidate for applications as transparent conductor (TCO) in optoelectronic devices. In such devices, CdO is often grown as a thin film on a substrate and this substrate induces strain that alters the electronic properties. It is clearly very important to understand this phenomenon to properly predict the performance of these devices. All earlier first principles making the system semi-metallic. In this talk, we show that the newly developed ACBN0 functional opens up the gap in closer agreement with the experiments, thus making possible to study band-gap modulation. We will discuss in detail the variation of the electronic and vibrational properties under epitaxial strain.

1Agapito, L. et.al., arXiv:1406.3259

11:51AM Z24.00004 Bulk and surface properties of rutile TiO$_2$: an ACBN0 case study. LAALITHA LIYANAGE, University of North Texas, PRIYA GOPAL, Central Michigan University, LUIS AGAPITO, University of North Texas, MARCO FORNARI, Central Michigan University, STEFANO CURTAROLO, Duke University, MARCO BUONGIORNO NARDELLI, University of North Texas — Using the newly developed Agapito–Curtarolo–Buongiorno–Nardelli (ACBN0) functional, we investigate bulk and surface properties of rutile TiO$_2$. ACBN0 is a pseudo-hybrid Hubbard density functional that is a fast, accurate and parameter-free extension of traditional DFT+U that has been proved to correct both the band gap and the relative position of the different bands in transition metal compounds. Within ACBN0, the values of U and J are functionals of the electron density and depend directly on the chemical environment and crystalline field, thus providing a direct way of computing the Hubbard corrections for any individual atom in any local environment. With rutile TiO$_2$ as a stringent test-bed, we have applied ACBN0 to the evaluation of a broad range of physical and electronic properties of the bulk and surfaces (((100), (110), and (001)), including electronic structure, vacancy formation energy, surface formation energy and water adsorption energy. Our results compare favorably with existing GGA, traditional GGA+U$^+$ and hybrid functional calculations, demonstrating the versatility and accuracy of the ACBN0 approach.

1Agapito, S. Curtarolo, M. Buongiorno Nardelli, arXiv:1406.3259
12:03PM Z24.00005 Improved predictions of the electronic and structural properties of Zn- and Cd-based compounds. An ACBN0 study , PRIYA GOPAL, MARCO FORNARI, Central Michigan University, STEFANO CURTAROLO, Duke University, LUIS AGAPITO, LAALITHA LIYANGAN, MARCO BUONGIORNO NARDELLI, University of North Texas — In this talk, we will present our results of the performance of the recently developed ACBN0 pseudo-hybrid Hubbard density functional in predicting the electronic and structural properties of the Zn- and Cd-based semiconductors. ACBN0 is a fast, accurate and parameter-free extension of traditional DFT+U proved to correct the band gap in transition metal compounds. Within ACBN0, the values of U and J are functions of the electron density and depend directly on the chemical environment and crystalline field. We will compare the structural and electronic properties of ZnX and CdX (X=0,S,Se,Te) semiconductors calculated in rs,kz and zb phases using ACBN0 with the results obtained by semi-local PBE, hybrid HSE06 functionals and experiments whenever available. Our results demonstrate that the lattice constants, bulk modulii and band-gaps are more accurately described by ACBN0 compared to the PBE functionals. Overall, we show that ACBN0 is a powerful tool which preserves the accuracy of the HSE calculations with higher computational efficiency.

1L. Agapito, S. Curtarolo and M. Buongiorno Nardelli, arXiv:1406.3259

12:15PM Z24.00006 First-principles Evidence for Intermediate Hole Polaron in ZnO , HONGHUI SHANG, CHRISTIAN CARBONOGO, Fritz-Haber-Institut der MPG, Berlin, DE, PATRICK RINKE, Fritz-Haber-Institut der MPG, Berlin, DE and Aalto University, Helsinki, FI, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, DE, HIKMET SEZEN, FABIAN BEBENSEE, CHENGWU YANG, MARIA BUCHHOLZ, ALEXEI NEFEDOV, STEFAN HEISSLER, CHRISTOF WÖLL, Karlsruhe Institute of Technology, Karlsruhe, DE — We performed density functional theory calculations at the hybrid-functional level (HSE06) to investigate the nature of the polaronic states in ZnO. Our calculations confirm that neither small (i.e., strong coupling) electron nor hole polarons are stable in ZnO, in agreement with previous studies [1]. The binding energy of large polarons (i.e., weak coupling) was determined by evaluating the renormalization of the band edges due to the zero-point motion of the atoms [2]. However, for intermediate polarons at intermediate coupling strength, the harmonic approximation breaks down, and there is currently no first-principle theory. We use the HSE06 effective mass matrices to calculate the Fröhlich coupling constants \( \alpha \). Feynman’s path integral technique then yields an intermediate hole polaron, whose binding energy of 245 meV and associated peaks in the optical absorption spectrum are consistent with infrared reflection absorption spectroscopy.


12:27PM Z24.00007 Numerical detection of symmetry enriched topological phases with space group symmetry 1, LING WANG, ANDREW ESSIN, California Institute of Technology, MICHAEL HERMELE, University of Colorado at Boulder, OLEXEI MOTRUNICH, California Institute of Technology — Topologically ordered phases of matter, in particular so-called symmetry enriched topological (SET) phases, can exhibit quantum number fractionalization in the presence of global symmetry. In \( Z_2 \) topologically ordered states in two dimensions, fundamental translations \( T_x \) and \( T_y \) acting on anyons can either commute or anticommute. This property, crystal momentum fractionalization, can be seen in a periodicity of the excited-state spectrum in the Brillouin zone. We present a numerical method to detect the presence of this form of symmetry enrichment given a projected entangled pair state (PEPS); we study the minima of spectrum of correlation lengths of the transfer matrix for a cylinder. As a benchmark, we demonstrate our method using a modified toric code model with perturbation. An enhanced periodicity in momentum clearly reveals the nontrivial anti-commutation relation \( \{ T_x, T_y \} = 0 \) for the corresponding quasiparticles in the system.

1This work was supported by the Institute for Quantum Information and Matter through Grant GBMF1250, by the U.S. Department of Energy (DOE), under Award # DE-FG02-10ER46686 (M.H.), and by the National Science Foundation through grant DMR-1206096 (O.M.).

12:39PM Z24.00008 Chiral d-Wave Superconductivity in coupled ladders 1, JEAN PAUL LATYR FAYE, Université de Sherbrooke, Québec, Canada, SYED R. HASSAN, P.V SRLUCKSHMY, The Institute of Mathematical Sciences, Chennai, India, GANAPATHY BASKARAN, The Institute of Mathematical Sciences, Chennai, India and Perimeter Institute of Theoretical Physics, Waterloo, Ontario, Canada, DAVID SÉNÉCHAL, Université de Sherbrooke, Québec, Canada — We study the Hubbard model on the trellis lattice, a two-dimensional frustrated lattice of coupled two-leg ladders, with hopping amplitude \( t \) within ladders and \( t' \) between ladders. For large \( U/t \) this is a model for the cuprate \( Sr_{1−x}Ca_xCu_2O_4 \). We use the variational cluster approximation (VCA), with clusters of sizes 8 to 12. We investigate the phase diagram as a function of doping, \( U/t \) and \( t'/t \) and find a superconducting dome ending at roughly 20% doping. Repulsion-induced spin singlet correlations within ladders block inter-ladder single electron tunneling, but allow pair tunneling and help establish 2D superconductivity. However, the nature of the order parameter depends on doping. At small doping \( (t < 3\% \) for \( t' = 0.15t \) and \( U = 10t \)), the order parameter is real and its interladder component grows steeply with \( t' \). Beyond that value, the order parameter becomes complex for a finite range of doping and gives the bulk chiral, PT violating, two-dimensional superconductivity. In all cases, the ladder component of the order parameter has d-wave character.

1Computational resources were provided by Compute Canada and Calcul Quebec

12:51PM Z24.00009 Density matrix of disjoint regions as a way of determining dominant correlations in interacting systems , HITESH CHANGLANI, OLABODE SULE, SHINSEI RYU, University of Illinois at Urbana-Champaign — In the context of strongly correlated systems, studying the ground state reduced density matrix (or derived quantities, such as the entanglement entropy and spectrum) of a local region has turned out to be useful for characterizing a wide variety of phases. However, to make definitive quantitative mappings of lattice simulations to field theories one needs to go beyond the density matrix of a single region. We use critical spin chains to demonstrate how information from the density matrix of disjoint regions (obtained from the density matrix renormalization group) [1,2] can be used to calculate the low-lying scaling dimensions (and operators) of the corresponding conformal field theory. In a related context, we will also discuss the use of density matrices that involve more than just the ground state, as a way of detecting order in the system [3]. [1] W. Muender, A. Weichselbaum, A. Holzer, J. von Delft, C. L. Henley, New. J. Phys., 12, 075027 (2010) [2] H.J. Changlani, O. Sule, S. Ryu (in preparation) [3] C. L. Henley and H.J. Changlani, J. Stat. Mech. 2014(11), 11002 (2014)
1:03PM Z24.00010 Real-time decay of a highly excited charge carrier in the one-dimensional Holstein model\footnote{Supported by the DFG through FOR 1807, and Alexander von Humboldt foundation.}. LEV VIDMAR, FLORIAN DORFNER, FABIAN HEIDRICH-MEISNER, University of Munich, CHRISTOPH BROCKT, ERIC JECKELMANN, University of Hanover — We study the real-time dynamics of a highly excited charge carrier coupled to quantum phonons via a Holstein-type electron-phonon coupling \cite{1}. This is a prototypical example for the non-equilibrium dynamics in an interacting many-body system where excess energy is transferred from electronic to phononic degrees of freedom. We use an efficient numerical method \cite{2,3}, i.e., diagonalization in a limited functional space, to study the non-equilibrium dynamics on a finite one-dimensional chain. We perform a comprehensive analysis of the time evolution in different parameter regimes by calculating the electron, phonon and electron-phonon coupling energies, and the electronic momentum distribution function. For example, we demonstrate that in the weak coupling regime, the relaxation dynamics obtained from the Boltzmann equation agrees very well with the numerical data. We also study the time dependence of the eigenstates of the single-site reduced density matrix, the so-called optimal phonon modes, unveiling that their structure in non-equilibrium contains very useful information for the interpretation of the numerical data. \cite{1} Dorfner et al, submitted (2014) \cite{2} Vidmar et al, PRB 83, 134301 (2011) \cite{3} Golez et al, PRL 109, 236402 (2012)

1:15PM Z24.00011 ABSTRACT WITHDRAWN –

1:27PM Z24.00012 ABSTRACT WITHDRAWN –

1:39PM Z24.00013 Basic Variables of Quantum Mechanics for Electrons in Electrostatic and Magnetostatic Fields, XIAO-YIN PAN, Ningbo University, VIRAIHT SAHNI, The Graduate Center, CUNY — We consider a system of \(N\) electrons in an external electrostatic \(E = -\nabla v(r)\) and magnetostatic \(B(r) = \nabla \times A(r)\) fields, and the Hamiltonian to include the interaction of the latter with both the orbital and spin angular momentum. We prove the one-to-one relationship \{\(v(r)\), \(A(r)\)\} \(\rightarrow\) \{\(\rho(r)\), \(j(r)\)\}, where \(\rho(r)\) and \(j(r)\) are the nondegenerate ground state density and current operator, respectively. The proof accounts for the many-to-one relationship between the \{\(v(r)\), \(A(r)\)\} and the ground state \(\Psi\). In parallel with the Hohenberg-Kohn theorem proof in which the wave function \(\Psi\) of the different physical systems considered is constrained to a fixed electron number \(N\), the corresponding \(\Psi\) in our proof is constrained to having the same total orbital \(L\) and spin \(S\) angular momentum. Thus, \{\(\rho(F)\), \(j(F)\)\} constitute the basic variables in the rigorous HK sense.

1:51PM Z24.00014 Corner Contributions to the Entanglement Entropy of Strongly Interacting Systems in 2+1 Dimensions, EDWIN MILES STOUDENMIRE, Perimeter Institute for Theoretical Physics, PETER GUSTAINIS, RAVI JOHAL, University of Waterloo, STEFAN WESSEL, RWTH Aachen University, ROGER MELKO, University of Waterloo, Perimeter Institute for Theoretical Physics — In \(D=2+1\) quantum critical systems, the entanglement entropy of a region with a sharp corner in its boundary contains a subleading logarithmic scaling term with a universal coefficient. In certain cases it is known that this coefficient captures the number of low-energy degrees of freedom in the associated field theory. Using a combination of density matrix renormalization group and numerical linked cluster calculations to isolate the corner coefficient for critical systems in the \(O(N)\) Wilson-Fisher universality class, we observe a striking confirmation of the universality of this quantity and find that, to leading order, the corner coefficient is proportional to the number of field components \(N\).

2:03PM Z24.00015 Spin-coherent states and instanton calculus on a Riemann surface, TOBIAS GULDEN, MICHAEL JANAS, Department of Physics, University of Minnesota, ALEX KAMENEV, Fine Theoretical Physics Institute, University of Minnesota — Semiclassical instanton calculations require solutions to the classical equations of motion, however in complexified phase space of spin-coherent states these are rarely attainable. But identification of the constant energy submanifold of the phase space with a Riemann surface allows to evaluate the semiclassical actions without explicitly knowing the actual classical paths. Furthermore we show that such actions may be solely derived from monodromy properties of the corresponding Riemann surface. Among other results, we prove that the period of quenched tunneling in an external magnetic field is semiclassically exact.

Friday, March 6, 2015 11:15AM - 2:03PM –
Session Z25 DCMP: Hubbard and Other Models: Theory 203B -

11:15AM Z25.00001 The 2D Hubbard Model: Diagrammatic Extensions from Two-Particle Vertex Functions, JAMES LEBLANC, EMANUEL GULL, Univ of Michigan - Ann Arbor — There are now a number of approaches to computing self energies at finite temperatures in the 2D Hubbard model. The dynamical mean field theory, and finite cluster extensions such as the dynamical cluster approximation (DCA), has typically provided an excellent image of local properties of correlated systems. However, towards low temperatures finite size effects occur due to the neglect of non-local correlations beyond the length scale of the impurity cluster. We explore one proposal to mitigate this effect by simulating on the two-particle level. By computing the full and two-particle irreducible vertex functions from DCA we present a first quantitative description on the reliability of this approach and compare against existing large cluster DCA results.

11:27AM Z25.00002 Antiferromagnetism, Superconductivity and Pseudogap of the 2D Hubbard Model\footnote{University of Michigan, Simons foundation}. XI CHEN, EMANUEL GULL, JAMES LEBLANC, Univ of Michigan - Ann Arbor — The phase diagram of the two-dimensional Hubbard model in the strongly correlated regime captures some important features that have been observed in high \(T_c\) cuprate superconductors such as superconductivity and pseudogap states. We study the model on a square lattice using dynamical mean field theory and dynamical cluster approximation at various doping, temperature and next nearest neighbor hopping. By measuring the two-particle correlation functions we are able to extend beyond previous work to determine the antiferromagnetic and d-wave superconducting phase transition temperatures. Further, the pseudo gap crossover is estimated by the density of states obtained via analytic continuation, and also from the imaginary time Green’s function. We will discuss the relation between pseudo gap and superconductivity based on the simulation results.
11:51 AM Z25.00044 Cluster dynamical mean-field theory study of Mott transition in the triangular lattice Hubbard model. **HUNG DANG,** Institute for Theoretical Solid State Physics, JARA-FIT and JARA-HPC, RWTH Aachen University, 52056 Aachen, Germany, XIAO YAN XU, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, KUANG-SHING CHENG, Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany, ZI YANG MENG, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, STEFAN WESSEL, Institute for Theoretical Solid State Physics, JARA-FIT and JARA-HPC, RWTH Aachen University, 52056 Aachen, Germany — In strongly correlated electron systems, geometric frustration can significantly affect the Mott metal-insulator transition. Using the dynamical cluster approximation, a cluster extension of the dynamical mean-field theory, we examine the evolution of the metal-insulator transition phase boundary as a function of temperature and interaction strength for the anisotropic triangular lattice Hubbard model as the degree of geometric frustration varies. We show that (i) the slope of this phase boundary changes systematically along with the frustration, and (ii) there exists a critical frustration at which this phase boundary is vertical. We discuss in details the connection between this critical degree of frustration and the suppression of the antiferromagnetic order due to frustration, which may be related to the emergence of exotic insulator phases as observed in several organic charge transfer salts.

12:03 PM Z25.00005 ABSTRACT WITHDRAWN —

12:15 PM Z25.00006 ABSTRACT WITHDRAWN —

12:27 PM Z25.00007 Mott metal-insulator transition in a metallic liquid — Gutzwiller molecular dynamics simulations. **KIPTON BARROS,** GIA-WEI CHERN, CRISTIAN D. BATISTA, JOEL D. KRESS, Los Alamos National Laboratory, GABRIEL KOTLIAR, Rutgers University — Molecular dynamics (MD) simulations are crucial to modern computational physics, chemistry, and materials science, especially when combined with potentials derived from density-functional theory. However, even in state of the art MD codes, the on-site Coulomb repulsion is only treated at the self-consistent Hartree-Fock level. This standard approximation may miss important effects due to electron correlations. The Gutzwiller variational method captures essential correlated-electron physics yet is much faster than, e.g., the dynamical-mean field theory approach. We present our efficient Gutzwiller-MD implementation. With it, we investigate the Mott metal-insulator transition in a metallic fluid and uncover several surprising static and dynamic properties of this system.

12:39 PM Z25.00008 Quantum electrodynamical time-dependent density functional theory for many-electron systems on a lattice1. **MEHDI FARZANEHPOUR,** ILYA TOTAKLY, Nano-Bio Spectroscopy group and, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, NANO-BIO SPECTROSCOPY GROUP AND ETSF SCIENTIFIC DEVELOPMENT CENTRE TEAM — We present a rigorous formulation of the time-dependent density functional theory for interacting lattice electrons strongly coupled to cavity photons. We start with an example of one particle on a Hubbard dimer coupled to a single photonic mode, which is equivalent to the single mode spin-boson model or the quantum Rabi model. For this system we prove that the electron-photon wave function is a unique functional of the electronic density and the expectation value of the photonic coordinate, provided the initial state and the density satisfy a set of well defined conditions. Then we generalize the formalism to many interacting electrons on a lattice coupled to multiple photonic modes and prove the general mapping theorem. We also show that for a system evolving from the ground state of a lattice Hamiltonian any density with a continuous second time derivative is locally v-representable.

1:03 PM Z25.00010 Spontaneous Breaking of $U(N)$ symmetry in invariant Matrix Models1. **FABIO FRANCHINI,** SISSA/M.I.T. — Matrix Models have a strong history of success in describing a variety of situations, from nuclei spectra to conduction in mesoscopic systems, from strongly interacting systems to various aspects of mathematical physics. Traditionally, the requirement of base invariance has lead to a factorization of the eigenvalue and eigenvector distribution and, in turn, to the conclusion that invariant models describe extended systems. I will show that deviations of the eigenvalue statistics from the Wigner-Dyson universality induce an effect on the eigenvectors and that the phase transition observed when the eigenvalue density become disconnected correspond to a breaking of the $U(N)$ symmetry to a smaller one. This spontaneous symmetry breaking is essentially a Higgs mechanism, due to the strongly correlated nature of matrix models and opens the possibility to a variety of applications.

1:15 PM Z25.00011 Free fermion description of a paramagnetic Mott insulator. **JOHAN NILSSON,** Uppsala University — A scheme is presented that enables a description of a paramagnetic Mott insulator in terms of free fermions. The main idea is to view the physical fermions as a part of a multi-band system and to allow for a correlation between the physical fermions and the auxiliary ones. Technically this is implemented through a non-linear canonical transformation, which is conveniently formulated in terms of Majorana fermions. The transformed Hamiltonian is in the next stage approximated with a free fermion theory. The approximation step is variational and provides an upper bound on the ground state energy at zero or the Free energy at finite temperature. In this way we are able to extend the domain of applicability of mean field theory and free fermions.
misalignment is then shown by extensive sliding simulations to increase the dynamic friction by a considerable factor over the aligned case. More generally, this recent importance as a frictional model, also develops in full equilibrium a small rotation angle, easy to detect in the Moiré pattern. The colloidal monolayer epitaxial rotation from aligned to misaligned relative to a periodic substrate. We show first of all that a model 2D colloidal monolayer in an optical lattice, of ICTP, SISSA and CNR-IOM Democritos — It is well known in surface science that incommensurate adsorbed monolayers undergo a spontaneous, energy-lowering

... positions of rutile TiO2 (110) and WO3 (001) surfaces in water. We obtain non-negligible solvation effects of such surfaces. We develop minimally-empirical continuum solvation models suitable for treating such surfaces ing of new materials. However, traditional solvation models are extensively fit to describe organic solutes and hence extrapolate poorly to highly-polar inorganic photo-electrochemical cell. Direct theoretical calculations of solid-liquid interfaces are expensive and simplified models are desirable for rapid theoretical screen-

... of the superfluid state in repulsively interacting three-component (colors) fermionic atoms in optical lattices. When two of the three color-dependent repulsions are much larger than the other, pairing symmetry is an extended s wave although the superfluid state appears adjacent to the paired Mott insulator in the phase diagram [1]. As the difference between the three repulsions is decreased in square optical lattices, the extended s-wave pairing changes into a nodal d-wave pairing, and then into a d−x2+y2-wave pairing. This change in pairing symmetry is attributed to the competition among the density fluctuations of unpaired atoms, the quantum fluctuations of the color-density wave, and those of the color-selective antiferromagnet [2]. This phenomenon can be studied in Li atoms and Yb,Yb mixtures in optical lattices using existing experimental techniques.

...energies & limit, where only ring exchange occurs, the Hamiltonian is sign problem free. Using Green’s function Monte Carlo, we investigate the phase diagram of this ring exchange only fermionic model and report our results.

1:39PM Z25.00013 Môbius molecules and fragile Mott insulators, LUKAS MEUCHELR, Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA, JOSEPH MACIEJKO, University of California, Santa Barbara — There has been significant recent interest in understanding non-Fermi liquid phases and searching for candidate Hamiltonians which may support them. DMRG and variational Monte Carlo students on 2-leg ladders have suggested the presence of such a phase, the d-wave metal, in certain regime of the t = J − K model on the 2D square lattice. K is a nearest neighbor exchange term. Non-variational quantum Monte Carlo studies of this model are hampered by the presence of a fermionic sign problem over most of the parameter space. However, in the t = J = 0 limit, where only ring exchange occurs, the Hamiltonian is sign problem free. Using Green’s function Monte Carlo, we investigate the phase diagram of this ring exchange only fermionic model and report our results.

1:51PM Z25.00014 Controlled superfluid pairing symmetry of repulsively interacting three-component fermionic atoms in optical lattices, SEI-ICHIRO SUGA, University of Hyogo — We investigate the pairing symmetry of the superfluid state in repulsively interacting three-component (colors) fermionic atoms in optical lattices. When two of the three color-dependent repulsions are much larger than the other, pairing symmetry is an extended s wave although the superfluid state appears adjacent to the paired Mott insulator in the phase diagram [1]. As the difference between the three repulsions is decreased in square optical lattices, the extended s-wave pairing changes into a nodal d-wave pairing, and then into a d−x2+y2-wave pairing. This change in pairing symmetry is attributed to the competition among the density fluctuations of unpaired atoms, the quantum fluctuations of the color-density wave, and those of the color-selective antiferromagnet [2]. This phenomenon can be studied in Li atoms and Yb,Yb mixtures in optical lattices using existing experimental techniques.

...energies & limit, where only ring exchange occurs, the Hamiltonian is sign problem free. Using Green’s function Monte Carlo, we investigate the phase diagram of this ring exchange only fermionic model and report our results.

This work was supported by Grant-in-Aid for Scientific Research (B) (No. 25287104) from the JSPS.

Friday, March 6, 2015 11:15AM - 1:51PM — Session Z26 DCP: Surfaces, Interfaces, Colloids and Catalysis II 204A - David Chandler, Sandia National Laboratories

11:15AM Z26.00001 Band offsets across solid-liquid interfaces from continuum solvation methods, RAVISHANKAR SUNDARRAMAN, YUAN PING, GIULIA A. GALLI, WILLIAM A. GODDARD III, Joint center for artificial photosynthesis, CA — The band edge positions of photo-electrodes relative to water redox potentials play an important role in determining the efficiency of the photo-electrochemical cell. Direct theoretical calculations of solid-liquid interfaces are expensive and simplified models are desirable for rapid theoretical screen-

This material is based upon work performed by the Joint Center for Artificial Photosynthesis, a DOE Energy Innovation Hub, supported through the Office of Science of the U.S. Department of Energy under Award Number DE-SC0004993.


M. G. Walter et al., Chem. Rev. 110, 6446, (2010)


J. Yourey et al., J. Mat. Chem. 21, 7651, (2011)

11:27AM Z26.00002 Friction boosted by spontaneous epitaxial rotations, DAVIDE MANDELLI, SISSA, ANDREA VANONI, CNR-IOM Democritos and SISSA, NICOLA MAJNIINI, Università degli studi di Milano, SISSA and CNR-IOM Democritos, ERIOS TOSATTI, ICTP, SISSA and CNR-IOM Democritos — It is well known in surface science that incommensurate adsorbed monolayers undergo a spontaneous, energy-lowering epitaxial rotation from aligned to misaligned relative to a periodic substrate. We show first of all that a model 2D colloidal monolayer in an optical lattice, of recent importance as a frictional model, also develops in full equilibrium a small rotation angle, easy to detect in the Moiré pattern. The colloidal monolayer misalignment is then shown by extensive sliding simulations to increase the dynamic friction by a considerable factor over the aligned case. More generally, this example suggests that spontaneous rotations are rather ubiquitous and should not be ignored in all tribological phenomena between mismatched lattices.

This work was mainly supported by the ERC Advanced Grant No. 320796-MODPHYSFRICT, and partly by SINERGIA contract CRSI2 136287, by PRIN/COFIN Contract 2010/LKJXB 004, by COST Action MP1303.
11:39AM Z26.00003 Surface Electric Potential of Macroions between the Limits of Small Ions and Charged Nanocolloids, BENXIN JING, Y. ELAINE ZHU. Department of Chemical and Biomolecular Engineering, University of Notre Dame — The surface electric potential of macroions in the size of 1-10 nm in aqueous solutions is critical to understand the supramolecular assembly involving biomacromolecules, charged nanoparticles and nanoclusters and their resulting material properties. However, the electric potential of these macroions could not be accurately determined because their sizes fall in between the limits of small ions and plain charged nanocolloids, while solving the non-linear Poisson-Boltzmann equation remains a grand challenge to date. In this work, we investigate polyether oligomeric silsesquioxane (POSS) with 8 amine terminal groups as a model macroion. We employ a new computational technique, fluorescence correlation spectroscopy (FCS), to measure the excited electron and core hole (PCH) to quantitatively measure the local proton concentration, which is the local co-ion concentration in vicinity of POSS with 1.5 nm in diameter. By changing the ionic strength of aqueous solution and the distance between pH-sensitive fluorescence probe and POSS, we quantitatively determine the proton concentration gradient. The distance dependent local pH can be simply analyzed to obtain the surface electric potential of the POSS macroion without the necessity to solve the non-linear Poisson-Boltzmann equation.

11:51AM Z26.00004 X-ray absorption spectroscopy of lithium sulfur battery reaction intermediates, KEVIN VUJCIK, Dept. of Chemical and Biomolecular Engineering, University of California, Berkeley, TOD PASCAL, DAVID PRENDERGAST, Molecular Foundry, Lawrence Berkeley National Laboratory, NITASH BALSARA, Dept. of Chemical and Biomolecular Engineering, University of California, Berkeley — Lithium sulfur batteries have a theoretical energy density nearly five times greater than current lithium ion battery standards, but questions still remain regarding the reaction pathways through which soluble lithium polysulfide (Li2Sx, “x” ranging from 2 to 8) reaction intermediates are formed. Complicating spectroelectrochemical approaches to elucidate redox pathways is the challenge of obtaining spectral standards for individual Li2Sx species. Lithium polysulfides cannot be isolated as individual component and exist only in solution as a distribution of different Li2Sx molecules formed via disproportionation reactions (e.g. 2Li2S4 goes to Li2S3 + Li2S5). X-ray absorption spectroscopy (XAS) at the sulfur K-edge has recently been employed as a technique to study Li-S chemistry. We have recently obtained XAS standards for individual Li2Sx species via first principles DFT simulations and the excited electron and core hole approach. Here, experimental sulfur K-edge XAS of Li2Sx species dissolved in poly(ethylene oxide) are compared to spectra obtained from analogous theoretical calculations. The impact that polysulfide solution concentration and the presence of other lithium salts (e.g. LiNO3) have on X-ray spectra of Li2Sx species is explored via experiment and theory.

12:03PM Z26.00005 Depth profile of halide anions under highly charged biological membrane, WOONGMO SUNG, Department of Physics, Sogang University, WENJIE WANG, Ames National Lab., JONGGWAN LEE, Department of Physics, Sogang University, DAVID VAKNIN, Ames National Lab., DOSEOK KIM, Department of Physics, Sogang University — Halide ion (Cl− and I−) distribution in cationic Langmuir monolayer consists of 1.2-palmitoyl-3 dimethylammonium-propane (DPTAP) molecules was investigated by vibrational sum-frequency generation (VSFG) and X-ray spectroscopy. From VSFG spectra, it was observed that large halide anions (I−) screen surface charge more efficiently so that interfacial water alignment becomes more randomized. On the other hand, number density of ions directly measured by X-ray fluorescence spectroscopy at grazing incidence angle reveals that the ion densities within 6 ~ 8 nm are the same for both I− and Cl−. Since the observed ion densities in both cases are almost equal to the charge density of the DPTAP monolayer, we propose that larger halide anions are attracted closer to the surface making direct binding with the charged headgroups of the molecules in the monolayer, accomplishing charge neutrality in short distance. This direct adsorption of anions also disturbs the monolayer structure both in terms of the conformation of alkyl chains and the vertical configuration of the monolayer, with iodine having the stronger effect. Our study shows that the length scale that ions neutralize a charged interface varies significantly and specifically even between monovalent ions.

12:15PM Z26.00006 Electrochemical Growth of Ag Junctions and Diffusion Limited Aggregate (DLA) Fractal Simulation, ZAK OLSON, SAM TUPPAN, WOO-JOONG KIM, Seattle Univ, SEATTLE UNIVERSITY TEAM — We attempt construction of a single atom connection between two copper wires. By applying a DC voltage across the wires when immersed in a silver nitrate solution, we deposit silver until a junction is formed. The deposited silver forms a fractal structure that can be simulated with a diffusion limited aggregation model.

12:27PM Z26.00007 Single crystal growth and properties of two layered oxytellurides1, TIGLET BESARA, DANIEL RAMIREZ, THEO SIEGRIST, National High Magnetic Field Laboratory/Florida State University, JIFENG SUN, JEFFREY WHALEN, TAKAHISA TOKUMOTO, STEPHEN MCGILL, RYAN STILLWELL, STANLEY TOZER, National High Magnetic Field Laboratory, DAVID SINGH, Oak Ridge National Laboratory — We report on the synthesis, structure, and physical properties of two layered oxytellurides: Ba2Yb2O6Te and Ba2TeO. Both compound were grown in single crystalline form using a molten metal flux, and crystallize in a tetragonal space group: P43/mmm for Ba2Yb2O6Te and P43/mmm for Ba2TeO. Ba2Yb2O6Te consists of Ba2Yb2O6 perovskite double layers separated by a CsCl-type BaTe slab, while Ba2TeO consists of an inverse PbO-type BaO layer separated by an NaCl-type BaTe slab. Ba2Yb2O6Te displays short range 2D magnetic ordering below 4 K, and a sharp optical absorption feature at 1.27 eV consistent with a F7/2 → F5/2 transition of Yb3+. For Ba2TeO, optical measurements display a sharp increase in absorbance, a manifest of a band edge. DOS corroborates the band gap, at 2.93 eV, indicating semiconducting behavior.

1 DOE DE-SC0008832 (TB, DR, JS, TS), NSF DMR-1157490 (NHMFL)

12:39PM Z26.00008 ABSTRACT WITHDRAWN —

12:51PM Z26.00009 Superhydrophilic - Superhydrophobic Transition in Vertically Aligned Titania Nanotubes, OOMMAN VARGHESE, RAM NEUPANE, MAGGIE PAULOSE, University of Houston — Both hydrophilic (wetting) and hydrophobic (non-wetting) surfaces find applications in a variety of technological areas. For example, hydrophilic surfaces are used in microfluidic devices to provide antifoaming and antifouling functions whereas hydrophobic coatings are used in clothes to attribute stain resistance. While in superhydrophilic surfaces the contact angle that water droplets make with the surface is nearly zero, the surfaces that make contact angles greater than about 120° are considered superhydrophobic. Oxide ceramics generally exhibit hydrophilic behavior. Surface texturing or organic coatings are often used to make the surface hydrophobic or superhydrophobic. We prepared highly ordered titania nanotube arrays on titanium foils using anodic oxidation that showed superhydrophobic behavior upon fabrication. We noticed a strong correlation between fabrication conditions and the wettability. We have become successful in converting such a superhydrophobic nanostructure into superhydrophobic without modifying the surface with organic molecules or texturing. Contact angles in excess of 145° have been obtained. We will present these results and discuss the physiochemical processes that decide wetting properties of oxide nanostructures.
1:03PM Z26.00010 Size-dependent melting of single and stacked silver alkanethiolate layers: experiment and phenomenological model1, ZICHAO YE, Univ of Illinois - Urbana, LITO DE LA RAMA, SanDisk Corporation, LIANG HU, Intel Corporation, MIKHAIL EFREMOV, University of Wisconsin-Madison, LESLIE ALLEN, Univ of Illinois - Urbana — We report a systematic study of melting of silver alkanethiolate (AgSCn) lamellar crystals. A new synthesis method enables us to control their thickness by either modulating alkanethiol chain length (n = 7-18) or stacking them to a specific layer number (n = 1-10). Nanocalorimetry shows stepwise increase in the melting point, T\text{m}_n, of single layer AgSCn as an increment of chain number. Layer stacking also results in a size-dependent melting. An odd/even alternation is observed in the T\text{m}_n of 2, 3, and 4-layer lamellae, but absent in that of single and multilayer samples. We develop a phenomenological model for lamellae melting based on the cumulative excess free energy contributions of four spatially separate layers in Ag\text{SCn} crystal: free surface, Ag–S central plane, substrate interface, and interlayer interface. Surface excess free energy is revealed to be independent of chain length. The selective appearance of the odd/even effect is due to the significant stabilization of interlayer interfaces of odd-chain samples, possibly due to registration/packing. Such interface stabilization occurs most significantly for 2-layer samples. XRD results support the model as the measured van der Waals gap is smaller for crystals with odd chains.

1Supported by NSF-DMR-1409953 and NSF-DMR-1006385.

1:15PM Z26.00011 Control and expression of –NH\textsubscript{2}, –SH, –COOH and SiO\textsubscript{2} on the surface of silicon carbide quantum dots, MUNUVE MWANIA, SUSANA AGUINRE-MEDEL, PETER KROLL, None — We present simple protocols of interlayer interfaces of odd-chain samples, possibly due to registration/packing. Such interface stabilization occurs most significantly for 2-layer samples. 4-layer lamellae, but absent in that of single and multilayer samples. We develop a phenomenological model for lamellae melting based on the cumulative excess free energy contributions of four spatially separate layers in Ag\text{SCn} crystal: free surface, Ag–S central plane, substrate interface, and interlayer interface. Surface excess free energy is revealed to be independent of chain length. The selective appearance of the odd/even effect is due to the significant stabilization of interlayer interfaces of odd-chain samples, possibly due to registration/packing. Such interface stabilization occurs most significantly for 2-layer samples. XRD results support the model as the measured van der Waals gap is smaller for crystals with odd chains.

1:27PM Z26.00012 Effects of Surface Treatments on Nylon 6,6 via Non-thermal Atmospheric Plasma for Thermoplastic Adhesives, CHI-CHIN WU, ANDRES BUJANDA, JOHN DEMAREE, JASON ROBINETTE, AMANDA WEERASOORIYA, DAVID FLANAGAN, Army Research Laboratory, ARL PLASMA GROUP, CCEP, WMRD TEAM — This work aims to modify the properties of Nylon 6,6 surfaces for attaining improved interfacial adhesion to thermoplastic composites utilizing atmospheric non-thermal plasma treatments followed by silane treatments using 3-aminopropyltriethoxysilane (APS) in some cases. An L-shaped dielectric barrier discharge configuration was employed to expose nylon substrates to oxygen-containing gas plasmas such as He/O\textsubscript{2} and He/H\textsubscript{2}O, respectively, at room temperature. The chemically-modified surface of the substrate after plasma exposure was immediately examined by static water contact angle wettability measurements and X-ray photoelectron spectroscopy. It was found that the surface hydrophilicity was substantially enhanced and the amount of surface oxygen was significantly increased after a three-minute plasma exposure due to the increased surface energy and additional O-H bonds. The enhancements on interfacial adhesion were evaluated with lap shear tests using three types of adhesives: EPON 825/D230, EPON 825/D2000 and sikaflex252, respectively. The results of tensile tests on the adhesive joints showed an almost 300% increase in interfacial adhesive strength for EPON 825/D230 bonds after plasma treatments. Finite element modeling of adhesive joints for bond strength is underway to compare with experimental results and study the quantitative relations between the mechanical properties within the bond and at interfaces.

1:39PM Z26.00013 Theoretical evidence for unexpected O-rich phases at corners of MgO surfaces, DANIEL BERGER, Technische Universität München, Garching, DE, KARSTEN ROESCH, Technische Universität München, Garching, DE, LUCA M. GHIRARDELLI, Fritz-Haber-Institut der MPG, Berlin, DE, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, DE, Technische Universität München, Garching, DE — Introducing charge carriers into MgO via p doping greatly reduces formation energy of an O-vacancy in the bulk and at the (100) surface [1]. In this work, we use hybrid density functional theory to explore O-vacancy and O/O\textsubscript{ad}-species defects at corners of MgO surfaces. The defects are modelled using MgO clusters embedded into a field of norm-conserving pseudopotentials and point charges. The long-range response of the oxide to the charge carriers trapped at the defects is taken into account using a polarizable force field. The low-energy defect atomic structures are found using an \textit{ab initio} genetic algorithm [2]. Concentrations of O-vacancies and O-ad-species at realistic temperatures and pressures are obtained with \textit{ab initio} atomistic thermodynamics. Unexpectedly, we find that O-ad-species rather than O-vacancies are dominating defects at realistic conditions. The stability of the O-ad-species over O-vacancies and pristine corners is explained by an interplay between bond-breaking, bond-making, and charge-carrier trapping. — [1] N. Richter et al., Phys. Rev. Lett. 111, 045502 (2013); [2] S. Bhattacharya et al., New J. Phys., in press (2014)

Friday, March 6, 2015 11:15AM - 2:03PM – Session Z28 GMAG DMP: Focus Session: Kagome Antiferromagnets II

11:15AM Z28.00001 Simplex valence-bond crystal in the spin-1 kagome Heisenberg antiferromagnet1, WEI LI, Ludwig-Maximilians-Universität, TAO LIU, University of Chinese Academy of Sciences, ANDREAS WEICHSELBAUM, JAN VAN DELFT, Ludwig-Maximilians-Universität, GANG SU, University of Chinese Academy of Sciences — We investigate the ground state properties of a spin-1 kagome antiferromagnetic Heisenberg model using tensor-network (TN) methods. We find a ground state with trimerization (simplex) valence-bond order, and obtain the energy per site $\varepsilon_{0} = -1.4099 \left( D = 16 \right)$ by accurate calculations directly in the thermodynamic limit. The symmetry between the two kinds of triangles is spontaneously broken, with a relative energy difference of $\delta \approx 20\%$. The spin-spin, dimer-dimer, and chirality-chirality correlation functions are found to decay exponentially with a rather short correlation length, showing that the ground state is gapped. We thus identify the ground state be a simplex valence-bond crystal (SVBC). We also discuss the spin-1 bilinear-biquadratic Heisenberg model on a kagome lattice, and determine its ground state phase diagram, find a quantum phase transition between the SVBC and a ferro-quadrupolar nematic state. Moreover, we implement non-abelian symmetries, here spin SU(2), in the TN algorithm, which improves the efficiency greatly and provides insight into the tensor structures.

1This work was supported in part by the MOST of China (Grant No. 2012CB932900 and No. 2013CB933401), and the Strategic Priority Research Program of the Chinese Academy of Sciences (Grant No. XDB07010100). WL was also supported by the DFG through SFB-TR12
11:27 AM Z28.00002 Quantum Kagome Ice. JUAN CARRASQUILLA, Perimeter Inst for Theo Phys, ZHIHAO HAO, University of Waterloo, ROGER MELKOV, University of Waterloo and Perimeter Institute — Two-dimensional quantum spin liquids (QSLs) are exotic phases of matter where magnetic moments remain disordered even at extremely low temperatures. Despite ongoing searches, QSLs remain elusive, due to a lack of concrete knowledge of the microscopic mechanisms that inhibit magnetic order in real materials. Here, we study a theoretical model for a broad class of frustrated magnetic rare-earth pyrochlore materials called “quantum spin ices”. When subject to an external magnetic field along the [111] crystallographic direction, the resulting spin interactions create a mix of geometric frustration and quantum fluctuations in decoupled two-dimensional kagome planes. Using large-scale quantum Monte Carlo simulations, we identify a simple set of interactions sufficient to promote a groundstate with no magnetic long-range order, and a gap to excitations, conjectured to be a $Z_2$ spin liquid phase. This suggests a systematic experimental procedure to search for two-dimensional QSLs within the broader class of three-dimensional pyrochlore quantum spin ice materials.

11:39 AM Z28.00003 The $J_1$-$J_2$ Kagome Heisenberg Model with Dzyaloshinskii-Moriya Interaction. TZEZAR SEMAN, Northern Illinois University, CHENG-CHIEN CHEN, Argonne National Laboratory, RAJIV SINGH, University of California, Davis, MICHEL VAN VEENENDAAL, Northern Illinois University, Argonne National Laboratory — We study the static and dynamic properties of an $S = 1/2$ kagome antiferromagnetic (AFM) Heisenberg model using large-scale exact diagonalization. We map out the phase diagram as functions of the next-nearest-neighbor exchange $J_2$ and the $z$-axis Dzyaloshinskii-Moriya interaction $D_z$. In particular, the phase boundary between a magnetically disordered state and a $Q = 0$, $120^\circ$ AFM state appears. We also identify a long-range spin-spin correlation function. We also compute the dynamical structure factor for the resulting spin-liquid phase. The implications of our numerical results to AFM long-range order is identified through finite-size extrapolation of the transverse spin-spin correlation function. We also compute the dynamical structure factor of Na4Ir3O8. Starting from these states, we will discuss.

11:51 AM Z28.00004 Frustration and Dzyaloshinsky-Moriya anisotropy in the kagome francisites Cu$_3$Bi(SeO$_2$)$_2$O$_X$. ALEXANDER TSIRLIN, National Institute of Chemical Physics and Biophysics, Tallinn, Estonia, IOANNIS ROUSOCHATZAKIS, Max Planck Institute for Complex Systems, Dresden, Germany, RONALD ZINKE, JOHANNES RICHTER, Institute for Theoretical Physics, University of Magdeburg, Germany — Kagome spin lattice is an abundant source of magnetic frustration. We will present density-functional as well as analytical and numerical calculations that elucidate the microscopic magnetic model of spin-1/2 francisite materials Cu$_3$Bi(SeO$_2$)$_2$X ($X =$ Cl, Br). Their weakly distorted kagome lattice features ferromagnetic nearest-neighbor and antiferromagnetic next-nearest-neighbor couplings that result in an infinitely degenerate classical ground state for the isotropic spin model restricted to Heisenberg exchanges. This degeneracy is lifted by quantum fluctuations, although the canted magnetic order observed experimentally is only marginally lower in energy than other competing states. We argue that in francisites this canted state is primarily stabilized by the Dzyaloshinsky-Moriya (DM) anisotropic quantum magnet. We derive the hierarchy of the DM exchanges in francisites and explain qualitatively the anisotropic magnetic response of these frustrated quantum magnets.

12:03 PM Z28.00005 Using the Density-Matrix Renormalization Group to Explore a Proposed Hamiltonian for Volborthite. EDWARD PARKER, Univ of California - Santa Barbara — Volborthite (Cu$_3$V$_2$O$_7$(OH)$_2$: 2H$_2$O) is a strongly geometrically frustrated system of spin-1/2 ions on a Kagomé lattice whose magnetic ordering temperature is more than two orders of magnitude below its Curie temperature. Measurements of its magnetization curve show an extremely broad magnetization plateau extending over a range of at least 100 Tesla. Density functional theory calculations suggest a nontrivial anisotropic spin coupling structure with both ferromagnetic and antiferromagnetic bonds. Prior studies of similar (but simpler) systems suggest the possibility of a spin nematic phase containing gapless bound states of two or more magnons, which can condense and spontaneously break the $U(1)$ spin symmetry about the applied field down to a discrete cyclic symmetry. We will report Density-Matrix Renormalization Group studies of this model to investigate plateau formation and possible spin nematic and spin density wave phases. Techniques include approximating the full 2-D lattice using interchain mean-field theory and spin ladders.

12:15 PM Z28.00006 Thermal transport study of $S = 1/2$ kagome frustrated system Volborthite. DAIKI WATANABE, Kyoto University, MINORU YAMASHITA, MASAAKI SHIMOZAWA, YOSHITAKA SUZUKI, HAJIME ISHIKAWA, ZENJI HIROI, ISSP, University of Tokyo, YUJI MATSUDA, Kyoto University — The nature of spin liquid states of 2D frustrated magnetic systems has been discussed over decades. Recently, some candidate materials of 2D quantum spin liquid have been reported from the absence of long range order in low temperatures. However, the elementary excitations which characterize the ground state have yet to be observed. It is suggested that thermal Hall measurement is a powerful probe to identify the elementary excitations of 2D quantum spin liquid[1]. Here we report the results of thermal-transport measurements of Volborthite (Cu$_3$V$_2$O$_7$(OH)$_2$: 2H$_2$O) which possesses the 2D kagome planes. We observed double anomalies in the thermal conductivity around 1K. These anomalies correspond magnetic orderings reported by the NMR measurements and the specific heat measurements[2,3]. We will also talk about our thermal Hall measurements above the ordering temperature. [1] H. Katsura et al., Phys. Rev. Lett. 104, 066403 (2010). [2] H. Yoshida et al., Nat. Commun. 3, 860 (2012). [3] M. Yoshida et al., J. Phys. Soc. Jpn. 81, 024703 (2012).

12:27 PM Z28.00007 New Realisations of Frustrated Quantum Spin Systems from Vanadium Based Oxyfluorides. LUCY CLARK, FARIDA AIDOUDI, CAMERON BLACK, RUSSELL MORRIS, PHILIP LIGHTFOOT, University of St Andrews — We recently presented the first example of a material containing a kagome network of antiferromagnetically interacting V$^{4+}$ $S = 1/2$ cations, DQVOF (Diammonium Quinolinilidium Vanadium Oxyfluoride). The $S = 1/2$ kagome layers within DQVOF are separated by V$^{4+}$ $S = 1$ cations. Our low temperature magnetic study of DQVOF suggested that the kagome layers remain decoupled from these inter-layer spins and that the system adopts a gapless QSL ground state[1]. Here, we will discuss how variations in the chemical methods used to prepare DQVOF can be employed to extend this family of frustrated V$^{4+}$ based oxyfluorides. In particular, we will focus on a new phase InMVOF (Imidazolium Vanadium Oxyfluoride), which consists of V$^{4+}$ $S = 1/2$ kagome layers like DQVOF, but the connectivity between the kagome layers is remarkably different. Single crystal X-ray diffraction reveals that the inter-layer vanadium species in InMVOF also sit on a kagome network. Magnetic susceptibility data of InMVOF reveal an absence of long range magnetic magnetic order down to 2 K despite significant antiferromagnetic exchange exchange (6~ ~ 50 K), which suggests that interesting physics is at play. [1] L. Clark et al., Phys. Rev. Lett. 110, 207208 (2013)

12:39 AM Z28.00008 ABSTRACT WITHDRAWN —
1:03PM Z28.00010 Quantum Phase Transitions and De-Coupling of Magnetic Sublattices in the Quasi-Two-Dimensional Ising Magnet Co3V2O8 in a Transverse Magnetic Field, K. FRITSCH, Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), Berlin, Germany; Dept. of Physics and Astronomy, McMaster University, Hamilton, Canada, G. EHLERS, Neutron Scattering Science Division, ORNL, Oak Ridge, USA, K. C. RULE, HZB; ANSTO, Lucas Heights, Australia, K. HABICHT, HZB, M. RAMAZANOGLU, Dept. of Physics and Astronomy, McMaster University, H. A. DABKOWSKA, Brockhouse Institute for Materials Research (BIMR), Hamilton, Canada, B. D. GAULIN, Dept. of Physics and Astronomy, McMaster University; BIMR, Canadian Institute for Advanced Research, Toronto, Canada - The application of a magnetic field transverse to the easy axis, Ising direction in the quasi-two-dimensional Kagome staircase magnet, Co3V2O8, induces three quantum phase transitions at low temperatures, ultimately producing a novel high field polarized state, with two distinct sublattices. New time-of-flight neutron scattering techniques, accompanied by large angular access, high magnetic field infrastructure allows the mapping of a sequence of ferromagnetic and incommensurate phases and their accompanying spin excitations. At least one of the transitions to incommensurate phases at \( \mu_0 H_{c3} \approx 6.25 \text{T} \) and \( \mu_0 H_{c2} \approx 7 \text{T} \) are discontinuous, while the final quantum critical point at \( \mu_0 H_{c3} \sim 13 \text{T} \) is continuous.

1:15PM Z28.00011 \(^{17}\)O Single Crystal NMR Evidence for a Gapped Spin-liquid Ground State in the S=1/2 Kagome Lattice ZnCu3(OH)6Cl2, MINGXUAN FU, Department of Physics and Astronomy, McMaster University, TAKASHI IMAI, Department of Physics and Astronomy, McMaster University and Canadian Institute for Advanced Research, TIANHENG HAN, Department of Physics, University of Chicago, YOUNG S. LEE, Departments of Applied Physics and Photon Science, Stanford University and SLAC National Accelerator Lab — The two-dimensional S=1/2 Kagome lattice in Herbersmithite ZnCu3(OH)6Cl2 is the best candidate for experimental realization of a quantum spin liquid ground state known to date. The recent discovery of a continuum of spinon excitations using inelastic neutron scattering in this material has drawn strong attention to its exotic magnetic properties. Understanding the nature of the paramagnetic ground state of ZnCu3(OH)6Cl2, however, remains a challenge, due to excess magnetic Cu defects occupying the interlayer Zn sites. We conducted single crystal NMR measurements of the \(^{17}\)O Knight shift, and succeeded in measuring the intrinsic spin susceptibility of the Kagome layer down to \( T \approx 0.011 \text{(J} \sim 17 \text{meV}) \) for the first time. We demonstrate that the intrinsic spin susceptibility decays exponentially at low temperatures, revealing the presence of a spin gap \( \Delta \approx 0.13 \). Moreover, we show that application of a high magnetic field suppresses the gap. These results provide direct evidence for a gapped spin-liquid ground state realized in ZnCu3(OH)6Cl2.

1:27PM Z28.00012 Spin liquid state in the S=1 vanadium kagome YCa3(VO)3(BO)4, CHRISTOPHER WIEBE, University of Winnipeg, HARLYN SILVERSTEIN, University of Manitoba, JASON GARDNER, NIST NCNR, HAIDONG ZHOU, University of Tennessee-Knoxville — Over the last decade, the search for model kagome compounds has been fruitful for S=1/2 Cu\(^{2+}\) spins in the minerals Herbersmitheite and Volborthite [1-2]. There are fewer comparable materials for S=1 analogues, but recent progress has been made with the discovery of YCa3(VO)3(BO)4, which has a network of V\(^{3+}\) kagome spins [3]. Previous reports were made of no magnetic ordering down to 1.5 K in this compound, despite strong antiferromagnetic exchange [3]. Here we report a new synthesis method for this material which reduces impurity levels, resulting in high quality polycrystalline samples of YCa3(VO)3(BO)4. Neutron scattering experiments show no evidence for long-ranged magnetic ordering down to 50 mK, with gapped inelastic excitations developing similar to S=1/2 kagome compounds. Heat capacity and susceptibility measurements also show a lack of long-range magnetic order and a lack of spin glassiness, placing this compound as a new spin liquid candidate.

1:39PM Z28.00013 Infrared phonons as a probe of spin liquid in kagome antiferromagnet Herbertsmithite, ANDREI SUSHKOV, GREGORY JENKINS, DENNIS DREW, Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742, USA, TIAN-HENG HAN, University of Chicago, Chicago, IL 60637, USA, YOUNG LEE, Massachusetts Institute of Technology, Cambridge, MA 20139, USA — Phonons are sensitive to magnetic interactions between ions through the spin-phonon coupling mechanism where the phonon resonance frequency is proportional to \( S_i S_j \) spin-spin correlation function. In our earlier work [1], we observed strong magnetic phonon splitting at the magneto-structural transition in cubic spinel ZnCr2O4. In Herbertsmithite ZnCu3(BO)4Cl2, neither magnetic ordering nor structural transition was observed down to mK temperatures. Recent theoretical work predicts a resonating bond ground state in Herbertsmithite that breaks p6 chiral symmetry and lifts the degeneracy between two zone center optical phonon modes [2]. From fits to reflectivity spectra we have obtained the temperature dependence of all IR-active phonons polarized both in and perpendicular to the kagome plane. Observed signatures of magnetic interaction effects on the phonon parameters will be discussed.

1:51PM Z28.00014 Barlowite: a new mother compound of spin liquids, TIAN-HENG HAN, University of Chicago, JOHN SINGLETON, Los Alamos National Laboratory, JOHN SCHLUETER, Argonne National Laboratory — Experimental investigations of spin liquids start with finding suitable materials. Existing candidate compounds have limitations, even though the observation of spinons in herbertsmithite has marked a breakthrough. I will introduce a new mother compound of kagome spin liquids, barlowite, with its properties characterized using thermodynamic techniques. The advantages of barlowite will be discussed.
11:15AM Z29.00001 High precision measurements of quantum critical properties for 3D quantum antiferromagnets. ZI YANG MENG, YAN QI QING, Institute of Physics, Chinese Academy of Sciences, BRUCE NORMAND, Renmin University, ANDERS SANDVik, Boston University — Using large-scale quantum Monte Carlo (QMC) simulations, we study the quantum phase transitions in three-dimensional $S=1/2$ dimerized Heisenberg antiferromagnets. We obtain high precision results on the quantum critical properties of the transition from antiferromagnetically ordered phase to the magnetically disordered dimerized phase. With careful finite size scaling analysis and improved estimator of physical observables in the QMC simulations, we are able to extract the precise logarithmic corrections to quantum phase transition in our system governed by the $3+1$ O(3) universality class. Finite temperature quantum critical properties in excitation spectra are obtained as well.

11:27AM Z29.00002 Calculation of the Curie temperature of Ni using first principles based Wang-Landau Monte-Carlo. MARKUS EISENBACH, Oak Ridge National Lab, JUNQI YIN, University of Tennessee, YING WAI LI, Oak Ridge National Lab, DON NICHOLSON, University of North Carolina, Asheville — We combine constrained first principles density functional with a Wang-Landau Monte Carlo algorithm to calculate the Curie temperature of Ni. Mapping the magnetic interactions in Ni onto a Heisenberg like model to underestimate the Curie temperature. Using a model we show that the addition of the magnitude of the local magnetic moments can account for the difference in the calculated Curie temperature. For ab initio calculations, we have developed our Locally SelfConsistent Multiple Scattering (LSMS) code to constrain the magnitude of the local moments in addition to their direction and apply the Replica Exchange Wang-Landau method to sample the larger phase space efficiently to investigate Ni where the fluctuation in the magnitude of the local magnetic moments is of importance equal to their directional fluctuations. We will present our results for Ni where we compare calculations that consider only the moment directions and those including fluctuations of the magnetic moment magnitude on the Curie temperature. This research was sponsored by the Department of Energy, Offices of Basic Energy Science and Advanced Computing. We used Oak Ridge Leadership Computing Facility resources at Oak Ridge National Laboratory, supported by US DOE under contract DE-AC05-00OR22725.

11:39AM Z29.00003 Thermodynamic properties of a 2D itinerant ferromagnet - a sign-problem free quantum Monte Carlo study. SHENG-LONG XU, University of California, San Diego, YI LI, Princeton Center for Theoretical Sciences, Princeton University, CONGJUN WU, University of California, San Diego — We investigate thermodynamic properties of itinerant ferromagnetism by using the non-perturbative method of quantum Monte Carlo simulation, which is shown free of the sign problem in a multi-orbital Hubbard model in the square lattice in a large region of fermion density. The spin magnetic susceptibility is local-moment-like exhibiting the Curie-Weiss law in the off-critical temperature region, while the compressibility typically exhibits the itinerant nature, which is finite and weakly temperature-dependent. The spin magnetic susceptibility further grows exponentially as approaching zero temperature for the SU(2) invariant models. The long-range ferromagnetic ordering appears when the symmetry is reduced to the Ising class, and the Curie temperature can be accurately determined.

11:51AM Z29.00004 A benchmark study of the two-dimensional Hubbard model with auxiliary-field quantum Monte Carlo. MINGPU QIN, HAO SHI, SHIWEI ZHANG, College of William and Mary — The ground state properties of the two-dimensional Hubbard model are calculated with the auxiliary-field quantum Monte Carlo (AFQMC) method. With general twist boundary conditions, the shell effect is eliminated. We use large lattice sizes ($L \times L$ lattices with $L$ up to 24) and average over many twist angles to extrapolate to the thermodynamic limit and ensure convergence of the calculated physical quantities. At half filling, we obtain accurate results for the ground-state energy, sublattice magnetization and double occupancy, while the compressibility typically exhibits the itinerant nature, which is finite and weakly temperature-dependent. The spin magnetic susceptibility further grows exponentially as approaching zero temperature for the SU(2) invariant models. The long-range ferromagnetic ordering appears when the symmetry is reduced to the Ising class, and the Curie temperature can be accurately determined.

11:03PM Z29.00005 Entropic and magnetic properties of Ni-Mn-In magnetocaloric materials. JING-HAN CHEN, Department of Physics and Astronomy, Texas AM University, NICKOLAUS BRUNO, Department of Mechanical Engineering, Texas AM University, IBRAHIM KARAMAN, Department of Materials Science and Engineering, Texas AM University, YUJIN HUANG, JIANGOU LI, School of Materials Science and Engineering, Shanghai Jiaotong University, JOSEPH H. ROSS, JR., Department of Physics and Astronomy, Texas AM University — We report magnetization and field-dependent calorimetry studies of phase transitions in Ni-Mn-In. Off-stoichiometric alloys based on NiMnIn have drawn attention due to the coupled first order magnetic and structural transformation, and the large magnetocaloric entropy associated with this martensitic transformation. We have analyzed materials with compositions NiMnIn, NiMnInNd, NiMnInMn, which differ in that the former exhibits a paramagnetic to antiferromagnetic transition, while the others exhibit an additional ferromagnetic transition. Our results show that in the NiMnIn materials, the total entropy change at the phase transition can be modeled solely according to a magnetic contribution due to local moments on the Mn sites. On the other hand, NiMnInMn includes a larger contribution which can be described in terms of a magneto-elastic coupling. This we will discuss in terms of the Bean-Rodbell model and a renormalization of the Debye temperature coupled with magnetism. We will also discuss the low-temperature properties, which show divergent behavior including antiferromagnetic, ferrimagnetic and superparamagnetic behavior.

12:03PM Z29.00006 Abstract Withdrawn —

12:27PM Z29.00007 Magnetoelectric effect in non-centrosymmetric Kondo lattices. Ilya Vekhter, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA, USA, Leonid Isaev, JILA and Department of Physics, University of Colorado, Boulder, CO, USA — We study magnetoelastic (ME) response in Kondo lattices without the center of inversion. In such materials the conduction electrons move under the influence of an odd in momentum spin-orbit interaction (SOI). The interplay between this SOI and Kondo screening enables manipulation of the net magnetization of the system by an applied electric field. As a simple model for this phenomenon, we consider a Kondo bilayer (a pair of two-dimensional Kondo lattices) with Rashba-type SOI, and treat it within a generalized hybridization mean field theory. We demonstrate that the ME response, strongest inside the heavy-fermion phase, has a very pronounced dependence on the magnitude of the spin-orbit coupling. These results provide a new pathway to the ME effect in strongly correlated materials.
related to a Fermi surface effect. 

Our recent measurements using both time-of-flight and reactor based inelastic scattering reveal magnetic excitations that are again greater in magnitude than the exchange constant in the basal plane. Despite this unusual feature the observed excitations could be described using a classical description. 


derived both the Nambu-Goldstone mode, already known for ferromagnetic systems, as well as another massive, gapped mode. This mode was found to be associated with fluctuations in the order parameter by Zhang, Farinas, and Bedell and was identified as the Higgs amplitude mode, which had never been identified in a weak ferromagnetic system [2]. They applied their model to the weak ferromagnet MnSi using existing experimental results for the material, 

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A large number of these materials reported. (ND4)2[FeCl5-D2O] is a rare case where improper ferroelectricity has been observed in a molecular material. 

We have used single crystal and powder neutron diffraction to study its crystal and magnetic structures and hence determine the mechanism of multiferroicity in this compound. From the crystal structure determinations above and below 79 K, we have observed an order-disorder phase transition, which is related with the ordering of the ammonium counterion. Below TN, at zero magnetic field, we have determined the magnetic structure, which corresponds with a cycloidal spin arrangement where the magnetic moments are confined in the ac-plane and propagate along the c-direction. All the cycloids in (ND4)2[FeCl5-D2O] compound have the same chirality and therefore the ferroelectricity can be explained via the inverse Dzyaloshinskii-Moriya mechanism. 

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Laboratory — We study the electronic and magnetic properties of individual transition metal atoms (Ti, V, Cr, Mn, Fe, Co and Ni) deposited on a Cu surface topological transition at Joseph Betouras, Loughborough University, ANDREY CHUBUKOV, Department of Physics, University of Wisconsin-Madison, Madison, WI 53706, USA. — We analyze the temperature and doping dependence of the specific heat \(C(T)\) in \(\text{Na}_2\text{CoO}_2\). This material was conjectured to undergo a Lifshitz-type topological transition at \(x = x_c = 0.62\), in which a new electron Fermi pocket emerges at the \(\Gamma\) point, in addition to the existing hole pocket with large \(k_F\). The data show that near \(x = x_c\), the temperature dependence of \(C(T)/T\) at low \(T\) gets stronger as \(x\) approaches \(x_c\) from below and then reverses the trend and changes sign at \(x ≥ x_c\). We argue that this behavior can be quantitatively explained within the spin-fluctuation theory. We show that magnetic fluctuations are enhanced near \(x_c\) at momenta around \(k_F\), and their dynamics changes between \(x ≤ x_c\) and \(x ≥ x_c\), when the new pocket forms. We demonstrate that this explains the temperature dependence of \(C(T)/T\). We show that at larger \(x (x > 0.65)\) the system enters a magnetic quantum critical regime where \(C(T)/T\) roughly scales as \(\log T\). This behavior extends to progressively lower \(T\) as \(x\) increases towards a magnetic instability at \(x ≈ 0.75\).

1 EPSRC grants EP/H049797/1 and EP/I02609X/1, DOE grant DE-FG02-ER4000 and a Leverhulme Trust visiting professorship held at Loughborough University.

Friday, March 6, 2015 11:15AM - 1:51PM – Session Z30 GMAG DMP: Focus Session: Frontiers in Magnetism II

11:15AM Z30.0001 Electronic properties of transition metal atoms on Cu2 N/Cu(100): a DFT comparative study1, ALEJANDRO FERRON, JOSÉ LADO, JOAQUIN FERNÁNDEZ-ROSSIERS, International Iberian Nanotechnology Laboratory — We study the electronic and magnetic properties of individual transition metal atoms (Ti, V, Cr, Mn, Fe, Co and Ni) deposited on a \(\text{Cu}_2\text{N/Cu}(100)\) surface by means of spin-polarized density functional theory (DFT) calculations. We focus our work on a comparative study of the various quantities, such as magnetic moment, orbital occupation, structural properties, hybridization with the substrate and spin polarization of the substrate, paying attention to the trends as the transition metal is changed. In this work we try to go beyond existing theoretical works by providing a comprehensive and comparative study of the electronic, magnetic and structural properties of these seven atoms including also Ni, for which there are no published calculations to the best of our knowledge. In the case of Mn, Fe and Co, we connect our results with the existing scanning tunneling microscope experiments [1,2].


1 AF acknowledges funding from the European Union’s Seventh Framework Programme for research, technological development and demonstration, under the PEOPLE programme, Marie Curie COFUND Actions, grant agreement number 600375 and CONICET.

11:27AM Z30.0002 Ni adsorption on MgO(001): A Comparison of DFT and DFT+U, OLIVER ALBERTINI, AMY LIU, Georgetown University, BARBARA JONES, IBM Almaden Research Center — The study of magnetic atoms on surfaces has drawn recent attention due to possible applications in the realm of magnetic storage and quantum computing. Researchers are looking across the 3d transition metal series for candidates with high magnetic anisotropy. Here we examine the MgO/Ag surface with a Ni adatom using DFT and DFT+U computational approaches. We investigate the preferential binding site and the interesting physics involved in the resulting magnetic moment, drawing comparisons with a recent study of Co on MgO/Ag.

11:39AM Z30.0003 Magnetocrystalline anisotropy “space” distribution over atoms from different first principles approaches, ROMAN CHEPULSKYY, DMYTRO APALKOV, New Memory Technology, Samsung Semiconductor R&D Center, Samsung Electronics — Interplays between bulk vs interface and electron hybridization vs stress contributing into the magnetocrystalline anisotropy are studied from first principles. Fe/MgO system is considered as example with variable Fe thickness. The effect of stress is modeled by consideration of a number of fixed in-plane lattice parameters with full relaxation in z-direction. Different approaches to calculate separate atom contributions into the total magnetocrystalline anisotropy are compared and controversies are discussed.

11:51AM Z30.0004 Electric field control of Martensitic Phase Transitions in Thin Films of Ni-Mn-In, NABIL AL-AQTASH, University of Nebraska - Omaha, ANDREI SOKOLOV, University of Nebraska Lincoln, RENAT SABIRIANOV, University of Nebraska - Omaha — We propose the electric field control of martensite transformation of Ni-Mn-In thin films deposited on ferroelectric (FE) substrate. DFT- based calculations indicate that the off-stoichiometric Ni2Mn1.5In0.5 alloy shows that the ferromagnetic (FM) cubic phase undergoes transformation to tetragonal ferromagnetic (FIM) martensite phase at low temperature. The presence of FE substrate changes the relative stability of FM austenite and FIM martensite phases. \((\text{SrZrO}_3/\text{PbZrO}_3)\) superlattices were considered as FE substrates with polarization perpendicular to the interface. The relative stability of two phases of the thin films can be tuned by polarization reversal in FE due to the change in sign of induced charges at the interface. The energetically favorable structures of the FE/Ni2Mn1.5In0.5 systems depend on interface structure between FE and Ni2Mn1.5In0.5 layers, e.g. Ni-(Pb-O) interface. The energy difference \((\text{per NiMnIn } \text{f.u.})\) between FM austenite and FIM martensite states of the film on FE substrate is \(\Delta E = 0.22 \text{ eV}\) with polarization away from interface, upon polarization reversal \(\Delta E = 0.75 \text{ eV}\), compared to \((\Delta E = 0.24 \text{ eV})\) in the bulk. Additionally Pb atoms in PbO3 planes shifted in opposite direction with respect to oxygen planes and alter the chemical bonding of Pb with Ni atoms of the thin films. These changes possibly cause the shift of the martensite transition temperature. These results clearly indicate the possibility of control of martensitic transition in Ni-Mn-In thin films by FE substrate.

12:03PM Z30.0005 Ab initio calculation of magnetic interactions and time-dependent density functional theory simulation for ultrafast magnetic dynamics, ZHANGHUI CHEN, LIN-WANG WANG, Lawrence Berkeley Nat Lab — The competition between exchange interaction and spin-orbital coupling, especially in the presence of the symmetry-breaking of interfaces, provides a path to magnetic interactions which can cause novel magnetic structures like skyrmions. We will use a noncollinear spin ab initio calculation to predict the spin-spin interactions near such interfaces. A new algorithm is developed for such calculations. Similarly, a newly developed fast time-dependent density functional theory algorithm will be used to study femtosecond spin relaxation after an initial excitation by a fast laser pulse. Such simulation is mean to reveal the underlying mechanism which causes fast magnetic decays.
The use of supercritical fluids was found to lead to a homogeneous microstructure with an average grain size of 35 nm. The magnetic properties show an enhancement of magnetization and coercivity from $M(3T)$. They also observed that the magnetic phase by subjecting ball milled powders with micron size grains to the supercritical conditions of fluids at high pressure of 850 psi and temperature of 250 °C. The study concludes that the Mn-based alloys have attracted much interest lately for the development of rare earth-free permanent magnets.

**Enhancement of Magnetization and Coercivity from $M(3T)$**

AHMED A. ELGENDY, GEORGE HADJIPANAYIS, University of Delaware — Mn-based alloys have attracted much interest lately for the development of rare earth-free permanent magnets. The work was funded by NSF-G8. References: Cui, B. Z.; Marinescu, M.; Liu, J. F., Nature Comm., 5, 3333 (2014).

**Magnetization studies and spin Hamiltonian modelling of Li2(Li1-xFex)N**

JAMES H. ATKINSON, Department of Physics, University of Central Florida, Orlando, FL, USA, ANTON JESCHE, The Ames Laboratory, Iowa State University, Ames, Iowa, IA, and the Institute for Physics, University of Augsburg, Augsburg, Germany, ENRIQUE DEL BARCO, Department of Physics, University of Central Florida, Orlando, FL, USA, PAUL C. CAPFIELD, The Ames Laboratory, Iowa State University, Iowa, USA — The study of ferromagnetic materials that yield many examples of compounds which exhibit large energy barriers to a reversal of magnetization and correspondingly wide magnetization versus field hysteresis loops. Some materials, such as members of the class called “single-molecule magnets” (SMMs), even display vivid signatures of quantum tunneling effects, manifested as step-like features in hysteresis loop measurements of crystalline ensembles. The compound Li2(Li1-xFex)N has been previously shown to display an extremely high blocking temperature ($\sim 20$ K) and large coercive fields ($\sim 11$ T), as well as step-like features like those seen in SMMs. Here we report the results of low-temperature Hall sensor magnetization studies on a crystalline sample of Li2(Li1-0.006Fe0.006)N in which we detailed evidence of a preferential orientation for the observed features, as well as their dependence upon transverse component fields in their magnitude, behavior which we attempt to model with a giant spin Hamiltonian. [1] A. Jesche, R.W. McCallum, S. Thimmaiah, J.L. Jacobs, V. Taufour, A. Kreyszig, R.S. Houk, S.L. Bud'ko & P.C. Canfield. Nature Comm., 5, 3333 (2014).

1 This work is supported by the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358

**Nanostructured Mn2Ga Alloys with High Magnetization and Coercivity**

AHMED A. ELGENDY, GEORGE HADJIPANAYIS, University of Delaware — Mn-based alloys have attracted much interest lately for the development of rare earth-free magnets because of their high magnetocrystalline anisotropy. [1] In this study, we have prepared nanostructured Mn2Ga alloys with the pure D022 phase by subjecting ball milled powders with micron size grains to the supercritical conditions of fluids at high pressure of 850 psi and temperature of 250 °C. The use of supercritical fluids was found to lead to a homogeneous microstructure with an average grain size of 35 nm. The magnetic properties show an enhancement of magnetization and coercivity from $M(3T)= 30$ emu/g and $HC = 3$ kOe in the micron size powders to $M(3T)$ and $HC$ of 48 emu/g and 4.7 kOe, respectively in the nanosize powders. This new method of grain size reduction to nanoscale with the subsequent increase in coercivity via the high pressure cell opens new routes for rare earth-free permanent magnet development. The work was funded by NSF-G8. References. Cui, B. Z.; Marinescu, M.; Liu, J. F. Ferromagnetic Tetragonal L10-type Mn2Ga Isotropic Nanocrystalline Microparticles. IEEE Trans. Mag. 2013, 49(7), 3322-3325.

**Application of Barkhausen noise and ferromagnetic hysteresis for magnetic non-destructive evaluation of multiphase composites and structures**

NEELAM PRABHU GAUNKAR, ORFEAS KYPRIS, CAJETAN NILEBEDIM, DAVID JILES, Department of Electrical and Computer Engineering, Iowa State University — Composite ferromagnetic materials with multiple magnetic phases are increasingly used in applications such as magnetic data storage, magnetic sensors and actuators and exchange-spring magnets. These materials occur in single or multiphase conditions and can undergo phase changes over time or during processing. For these materials, we examine the interrelation between magnetic hysteresis, Barkhausen noise and the material microstructure. We observe that the presence of a second phase in these materials can be detected with the help of Barkhausen noise signals due to the occurrence of additional peaks in the magnetization envelope. This behavior in the magnetic response can serve as a tool for non-destructive evaluation of ferromagnetic materials for which phase constitution and phase changes affect the structural performance.

**Development of Gallium-Indium Alloys, Nonmagnetic Test Masses for Exotic Spin-Dependent Force Searches**

MARIAN KHOSRAVI, RAKSHYA KHATIWADA, WILLIAM M. SNOW, Indiana Univ - Bloomington, Center for the Exploration of Energy and Matter — Possible new spin-dependent short-range forces of nature in the mm to μm range which couple to nucleons are now sought in most experiments. Most experiments search for this possible interaction through NMR frequency shifts of polarized nuclei with the introduction of an unpolarized test mass nearby [1]. However, any nonzero magnetic susceptibility of this test mass can produce a systematic error in the measurement. We therefore seek materials with magnetic susceptibilities as close as possible to zero. We synthesized Gallium-Indium (Ga-In) alloys with various Indium percentages which are liquid at room temperature and measured their magnetic susceptibilities using a torsion balance-based commercial device. The measured magnetic susceptibilities range from $-0.06E-06$ to $-0.12E-06$ cgs volume susceptibility and are consistent with the weighted average of the component susceptibilities. The values are about an order of magnitude lower than water for a substance possessing 4.7 times larger nuclear density. [1] P. H. Chu, A. Dennis, C. B. Fu, H. Gao, R. Khatiwada, G. Laskaris, K. Li, E. Smith, W. M. Snow, H. Yan, and W. Zheng, Phys. Rev. D 87, 011105(R) (2013)

1 NSF PHY-1068712
11:15AM Z31.00001 Tuning Dirac states at grain boundaries in the topological insulator Bi2Se3. LIAN LI, University of Wisconsin, Milwaukee — Symmetry protected Dirac states have been experimentally observed in topological insulator (TI) bismuth chalcogenides. Recently, we have further demonstrated direct electrical generation and detection of spin accumulation induced by spin-momentum locking of Dirac surface states in Bi2Se3, a critical step forward towards future electronic and spintronic applications. In this talk, I will give an overview of the opportunities and challenges in the epitaxial growth of these layered TIs that exhibit a strong (covalent) intra-layer bonding and weak (van der Waals) inter-layer bonding. Using Bi2Se3 as an example, I will show that this characteristic anisotropic bonding facilitates a spiral growth mode on virtually any substrates by molecular beam epitaxy [2]. The coalescence of these spirals results in a high density of grain boundaries (GBs) [3,4]. Using scanning tunneling and transmission electron microscopies, and density functional theory calculations, I will further show that near the zero-angle GBs (i.e., anti-phase domain boundaries), caused by vertical shifts of a fraction of a Bi2Se3 quintuple layer, the Dirac states are robust against scattering by these extended structural defects. However, electrostatic fields on the order of 108 V/m are found, which locally charge the Dirac state, shifting the Dirac point by up to 120 meV [3]. On the other hand, low-angle (<15°) GBs are found to be of the tilt variant, consisting of alternating edge dislocation pairs [4], resulting in periodic in-plane stretching and compression. Scanning tunneling spectroscopy reveals that in-plane stretching reduces the van der Waals gap, enhancing the Dirac states; while in-plane compression expands the inter-quintuple separation, therefore destroying the Dirac states and opens a gap in the local density of states. These findings demonstrate the tunability of Dirac states by electric field and strain at the atomic scale, and also highlight the inherent formation of GBs during vapor phase epitaxy of layered TIs. Finally, I will discuss methods to possibly control the density and types of GBs to minimize their impact on carrier transport. [1] C. H. Li, O. M. J. van’t Erve, J. T. Robinson, Y. Liu, L. Li, and B. T. Jonker, Nat. Nanotechnol. 9, 218 (2014). [2] Y. Liu, M. Weinert, and L. Li, Phys. Rev. Lett. 108, 115501 (2012). [3] Y. Liu, Y. Y. Li, D. Gilks, V. K. Lazarov, M. Weinert, and L. Li, Phys. Rev. Lett. 110, 186804 (2013). [4] Y. Liu, Y. Y. Li, S. Rajput, D. Gilks, L. Lari, P. L. Galindo, M. Weinert, V. K. Lazarov, and L. Li, Nat. Phys. 10, 294 (2014).

1. NSF (DMR-1105839).

11:51AM Z31.00002 Magnetic Correlations in the Quasi-2D Semiconducting Ferromagnet CrSiTe2. TRAVIS WILLIAMS, ADAM ACZEL, MARK LUMSDEN, STEVE NAGLER, MATT STONE, JIANQIANG YAN, Oak Ridge National Laboratory, DAVID MANDRUS, University of Tennessee — The quasi-two-dimensional, semiconducting ferromagnet CrSiTe2 is a particularly attractive candidate for spintronics applications due to its relatively accessible magnetic phase transition and large magnetic moment. In this study, we use neutron scattering to measure the static and dynamic magnetic properties. Neutron diffraction shows 3D ordering below TC = 33K, but two dimensional static correlations persist up to at least 300K. The inelastic neutron scattering data shows two distinct spin wave bands, which are nearly dispersionless along the c-axis. The exchange constants extracted from the data suggest that the spins are very nearly Heisenberg, but only weakly coupled perpendicular to the 2D planes. Above the Curie temperature, the spin wave intensity decreases drastically but, like the static correlations, these dynamic magnetic correlations persist within the 2D planes up to room temperature.

12:03PM Z31.00003 Infrared spectroscopy of Cr and V doped Sb2Te3: dilute magnetic semiconductors. DAVID CRANDLES, JASON MANSON, ANTHONY MADUBUONU, Department of Physics, Brock University, Canada, CTIRAD UHER, Department of Physics, University of Michigan, USA, PETR LOSTAK, Department of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, Czech Republic — Temperature dependent optical reflectance measurements on well characterized samples of non-intentionally doped, Cr-doped and V-doped Sb2Te3 show that both the parent compound and the Cr-doped version are narrow-gap semiconductors (Eg ≈ 0.25 eV) with a conventional Drude free carrier absorption. The carrier density increases slightly with decreasing temperature while the scattering rate increases quadratically with temperature which is a sign of optical phonon scattering. Vanadium doping introduces a change in the temperature dependence of the scattering rate as well as higher electrical resistivity than Cr-doped Sb2Te3. Analysis of the literature values of the saturation magnetization for H || c suggests that V is in a mixed valence state V3+/V4+.

3. Work support by NSERC.
12:27PM Z31.00005 Electrical detection of spin-momentum locking in topological insulators\textsuperscript{1}, CONNIE LI, OLAF VAN ’T ERVE, JEREMY ROBINSON, Naval Research Lab, YAOYI LI, LIAN LI, University of Wisconsin, Milwaukee, BERRY JONKER, Naval Research Lab — One of the most striking properties of topological insulators (TIs) is that of spin-momentum locking – the spin of the TI surface state lies in-plane, and is locked at right angle to the particle momentum. While anticipated by theory, direct electrical access to this spin system in a simple transport structure had been challenging, due to that the bulk is typically unintentionally doped and contributes to transport. Using a ferromagnet/tunnel barrier detector contact that preferentially probes surface/ interface spins, we have demonstrated the first direct electrical detection of spin-momentum locking in the TI surface states in Bi\textsubscript{2}Se\textsubscript{3}.\textsuperscript{1} However, as the bulk carrier concentration for Bi\textsubscript{2}Se\textsubscript{3} is typically in the 10\textsuperscript{19} cm\textsuperscript{-3} range, the Fermi level is well within the conduction band, where a significant portion of the current is shunted through the bulk. Moving the Fermi level to within the gap is desirable to eliminate current shunting, as well as contribution from Rashba 2DEG states that may dilute the signal.\textsuperscript{[2]} These results, as well as how they affect the spin signal measured will be discussed at the meeting.\textsuperscript{[1]} C. H. Li, et. al., Nat. Nanotech. 9, 218 (2014).\textsuperscript{[2]} S. Hong et. al., PRB 86, 085131 (2012).

\textsuperscript{1}Supported by NRL core funds and Nanoscience Institute.

12:39PM Z31.00006 The effect of low-symmetry defects in semiconductors on spin Hall conductivity\textsuperscript{1}, MATTHEW D. MOWER, MICHAEL E. FLATTÉ, University of Iowa — We study the effect of low-symmetry defects in semiconductors on the spin Hall conductivity of carriers. It has previously been shown that these defects, e.g. DX centers in direct-gap III-V semiconductors, couple to carriers via a rather large, novel spin-orbit interaction. Compared to translational- or bulk-asymmetry based spin-orbit interactions, this spin-orbit interaction considerably enhances the carrier spin relaxation rate. However, we find that it does not make appreciable contributions to transverse spin currents. At the level of the 1st and 2nd Born approximations, there is neither side-jump nor skew scattering from these defects. Thus, we imagine a scenario where shifting impurities between substitutional and interstitial (low symmetry) positions quickly relaxes a spin system with negligible effects on existing transverse spin currents.

\textsuperscript{1}This work was supported in part by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA.

12:51PM Z31.00007 Intraband and interband spin-orbit torques in non-centrosymmetric ferromagnets, H. LI, KAUST, K. VYBORNY, T. JUNGWIRTH, Institute of Physics ASCR, H. GAO, J. SINOVA, Texas A&M University, A. MANCHON, KAUST — Experimental observations of the spin-orbit torque in non-centrosymmetric ferromagnets such as multilayered ferromagnetic metals and dilute magnetic semiconductors, have recently been reported\textsuperscript{[1]}. Two scenarios have been invoked to explain the origin of these current-driven torques. In the first one, the spin orbit coupling generates an in-plane non-equilibrium spin density and exerts a field-like torque on the magnetization. In the second one, the torque originates from the spin Hall effect occurring in the normal metal placed below the ferromagnet. Recently, a large (anti-)damping-like torque has been observed in a single magnetic GaMnAs layer\textsuperscript{[2]}. Obviously, the torque cannot be attributed to the spin Hall effect owing to the absence of the adjacent heavy metal. Such a torque might be attributed to the interband contribution to the non-equilibrium spin polarization in the linear-response Kubo formula. This intrinsic (scattering-independent) mechanism is related to (a specific type of) the Berry curvature and our calculations corroborate its link to actual experiments. Our numerical results show the paramagnetic dependence of the different torque components, they exhibit similarities to the analytical results for the Rashba two-dimensional electron gas in the weak disorder limit and open new perspectives in the development of current-driven spin-orbit torques by structural design.\textsuperscript{[1]} A. Chernyshev, et.al., Nat. Phys. 5, 656(2009).\textsuperscript{[2]} L. Liu et al. Science 336, 555 (2012)

1:03PM Z31.00008 Current induced spin orbit torques in antiferromagnets, HUAWEI GAO, Texas A&M University, JAKUB ZELEZNY, T. JUNGWIRTH, Institute of Physics ASCR, Czech Republic, JAIRO SINOVÁ, Institute fur Physik, Johannes Gutenberg Universität Mainz, Germany — In magnetic material with bulk inversion asymmetry or structure inversion asymmetry, unpolarized electric current can induce non-equilibrium spin polarization due to spin orbit coupling. This non-equilibrium spin polarization is exchange coupled with the magnetic order and act on them as torques. These torques are called spin orbit torques(SOT) which can be used to manipulate the magnetic orders. In ferromagnets, SOT effects have been observed experimentally. We extend the study of SOT to antiferromagnetic systems. Besides similar effects as in ferromagnets, we show staggered SOT in antiferromagnets following exactly the antiferromagnetic lattice which couple with the Neel order directly. We’ll report the study in both a 2D collinear antiferromagnetic model and a non-collinear antiferromagnet IrMn.

1:15PM Z31.00009 Spin Hall Effect and Irreversible Thermodynamics; Center-to-Edge Transverse Current-Induced Voltage, WAYNE SASLOW\textsuperscript{1}, Texas A&M University — For the first time the Dyakonov and Perel theory of the Spin Hall Effect (SHE) is examined from the viewpoint of irreversible thermodynamics, which is significantly more constraining than the symmetry arguments of pure phenomenology. As thermodynamic driving forces we include the thermal gradient, the gradient of the electrochemical potential (rather than the potential gradient and density gradient separately), and the “internal” magnetic field that is thermodynamically conjugate to the magnetization. In turn, we obtain the form of bulk transport coefficients relating the fluxes to the thermodynamic forces. Relative to Dyakonov and Perel, in addition to the new terms due to thermal gradients, the Onsager relations require three new (non-linear) terms in the current density, and minor revisions in the current density and spin current density. For a longitudinal current along a strip, the center-to-edge transverse voltage difference, due both to the $-β\vec{P} \times \vec{E}$ term of the number current density $\vec{q}$ and to one of the new current density terms, is determined. An ac capacitative probe likely would not significantly disturb this effect. We estimate a $\Delta V_{\perp}$ as large as $10^{-1}$ V for GaAs, but only $10^{-8}$ V for Pt.

\textsuperscript{1}This work was performed while a guest of the Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD, 20878

1:27PM Z31.00010 Disentangling the spin torques in a ferromagnet/semiconductor bilayer, TIMOTHY D. SKINNER, London Centre for Nanotechnology, University College London, KAMIL OLEJNIK, Institute of Physics, ASCR, LUCY K. CUNNINGHAM, University of Cambridge, HIDEKAZU KUREBAYASHI, London Centre for Nanotechnology, University College London, RICHARD P. CAMPION, BRYAN L. GALLAGHER, University of Nottingham, TOMAS JUNGWIRTH, Institute of Physics, ASCR, ANDREW J. FERGUSON, University of Cambridge — Current-induced spin torques measured in ferromagnet/paramagnetic metal bilayers can originate from the spin-Hall effect (SHE) and inverse spin galvanic effect (ISGE). Distinguishing the two effects has proved difficult as they can both possess the same symmetries, but it is essential for our basic physical understanding of the spin torques at the ferromagnet/paramagnetic interface to experimentally disentangle the SHE and ISGE contributions. In our approach, we look to zinc-blende crystals (such as III-V semiconductors), where the ISGE has a symmetry which depends on the crystal orientation. The field-like [1] and antidamping [2] torques, arising from the ISGE in the magnetic III-V semiconductor (Ga,Mn)As, are well understood because of low-temperature spin-torque ferromagnetic resonance (ST-FMR) measurements. Through new ST-FMR measurements, we show that in a room-temperature ferromagnetic metal/paramagnetic semiconductor bilayer, the SHE and ISGE co-exist and can be unambiguously separated and quantified by their symmetries.


1:39PM Z31.00011 ABSTRACT WITHDRAWN
11:15AM Z32.00001 Turning a strongly correlated Mott insulator into a weakly correlated metal\textsuperscript{1}, Y. F. KUNG, SIMES, SLAC National Accelerator Laboratory and Stanford University, E. A. NOWADNICK, Cornell University, C. J. JIA, SIMES, SLAC National Accelerator Laboratory and Stanford University, S. JOHNSTON, University of Tennessee, Knoxville, B. MORITZ, SIMES, SLAC National Accelerator Laboratory, T. P. DEVEREAUX, SIMES, SLAC National Accelerator Laboratory and Stanford University — As Mott insulators, such as cuprate superconductors, are doped with charge carriers, strong electron-electron interactions give rise to fascinating novel phenomena. Much of the interesting physics arises in the intermediate doping regime where the system displays metallic behavior strongly renormalized by correlations, in contrast with the naive expectation that the correlations would weaken rapidly away from half filling. To shed light on this issue, we examine the doping evolution of spin and charge excitations in the strongly correlated single-band Hubbard model using determinant quantum Monte Carlo (DQMC). Compared to the behavior predicted by the random phase approximation (RPA), the evolution of the excitations from DQMC shows that significant correlations remain up to relatively high doping levels (40\% hole doping and 15\% electron doping), near the maximum of what can be achieved in cuprates. The comparison improves with additional doping (up to 75\% hole doping) as the system approaches a metallic state in which the spin and charge excitation spectra are essentially the same.

\textsuperscript{1}This work was supported by the NSF Graduate Research Fellowship Program and the NDSEG Fellowship

Friday, March 6, 2015 11:15AM - 1:39PM –

Session Z32 GMAG DMP: Focus Session: Strongly Correlated Oxide Systems

11:15AM Z32.00002 The electromagnetic field induced excitation of magnons in spin-orbit coupled Mott insulators\textsuperscript{2}, ROHIT HEGDE, ALLAN MACDONALD, University of Texas, Austin — The spin-only description of the Hubbard model’s low-energy states belies an active charge degree of freedom that can in principle couple to external electromagnetic fields. The precise way in which the charge and current densities manifest in the spin sector is constrained when the electronic system possesses SU(2) spin-rotational symmetry, thus limiting the response to electric and magnetic fields. This constraint lifts in the presence of spin-orbit coupling, leading to the emergence of novel responses like that of an electron’s spin to an external magnetic field resulting from induced orbital currents in addition to the usual direct Zeeman coupling. Magnons mediate the linear response of electrons to time varying fields of low-frequency ($\hbar \omega \ll U$). We study the electric and magnetic susceptibilities of single band Hubbard models with spin-dependent hopping on various lattices, and comment on the applicability to magnetically ordered materials like the iridates.

\textsuperscript{2}This work was supported by SCOPE, CREST, NICT, and KAKENHI.

11:27AM Z32.00003 Sub-gap optical conductivity in the Mott insulator in one-dimensional Hubbard model with randomness, CHENG-JU LIN, OLEXEI MOTRUNICH, California Institute of Technology — We demonstrate a non-zero optical conductivity within the Mott gap in the one-dimensional Hubbard model with randomly distributed onsite potential. The effective Hamiltonian in the spin sector is described by the random exchange coupling spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model, which is in the random-singlet phase. An electric field couples to the electric polarization operator, and we first find its expression in terms of the spin variables in the Mott insulator regime. We then apply the decimation renormalization-group analysis pioneered by Dasgupta, Ma and Fisher to keep track of the polarization operator. Via Kubo formula, we find the optical conductivity to be $\sigma(\omega) \sim \frac{\psi}{(\ln \omega)^{\frac{5}{2}}} \omega^{\frac{3}{2}}$ at low frequencies, where $\psi = (1 + \sqrt{5})/4$.

11:51AM Z32.00004 A 1D, $\times 1$D, Heisenberg-Kondo Lattice compound Nb$_2$O$_{29}$\textsuperscript{3}, WARREN PICKETT, University of California Davis, KWAN-WOO LEE, Korea University — Local moments embedded in conducting systems form a rich platform for unusual phases, with phenomena including Kondo, heavy fermion, and non-Fermi liquid physics. Using first principles based methods and the refined crystal structure based on columns of 3×4 planar units of NbO$_6$ octahedra, we determine that mixed valent Nb$_2$O$_{29}$ displays tightly bound local moments forming spin chains along one direction cross-coupled by conducting “nanowires” in the perpendicular direction. Just how local moments – very rare for Nb – emerge and coexist with itinerant electrons, an enigma for decades in this system, is elucidated based on the local structure of the NbO$_6$ octahedra and orbital-$s$ spin ordering. The resulting 1D, $\times 1$D, Heisenberg-Kondo lattice ($s=$spin, $c=$charge) picture will be discussed.

\textsuperscript{3}NRF-2013R1A1A1A0008946 (K.W.L.), DOE DE-FG02-04ER46111 (W.E.P.)

12:03PM Z32.00005 Competition between heavy-fermion and Kondo interaction in isoelectronic A-site ordered perovskites, DEREK MEYERS, S. MIDDEY, University of Arkansas, J.-G. CHENG, Beijing National Laboratory for Condensed Matter Physics, S. MUKHERJEE, Department of Condensed Matter Physics and Materials Science, B.A. GRAY, Y. CAO, University of Arkansas, J.-S. ZHOU, J.B. GOODENOUGH, University of Texas, Y. CHOI, Advanced Photon Source, D. HASKEL, Advanced Photon Source, J.W. FREELAND, Advanced Photon Source, T. SAHA-DASGUPTA, S.N.Bose National Centre for Basic Sciences, J. CHAKHALIAN, University of Arkansas — With current research efforts shifting towards the 4d and 5d transition metal oxides, understanding the evolution of the electronic and magnetic structure as one moves away from 3d materials is of critical importance. Here weX-ray spectroscopy and electronic structure calculations on A-site ordered perovskites with Cu in the site and the B-sites descending along the 9th group of the periodic table to elucidate the emerging properties-orientals change from partially filled 3d, 4d, to 5d. The results show that when descending from Co to Ircharge transfers from the cuprate like Zhang-Rice state on Cu to the t2g orbital of the B site. As the Cuorbital occupation approaches the Cu$^{2+}$ limit, a mixed-valence state in CaCu$_3$RhO$_{4}$O$_{12}$ and heavy fermion CaCu$_3$IrO$_{4}$O$_{12}$ are observed. The investigated d-electron compounds are mapped onto the Doniach phaseof the competing RKKY and Kondo interactions developed for f electron systems.

12:51PM Z32.00007 Stability of the AFM phase in the three-band Hubbard-Holstein model . EDWIN HUANG, Stanford Univ, STEVE JOHNSTON, University of Tennessee, YVONNE KUNG, Stanford Univ, BRIAN MORITZ, SLAC, TOM DEVEREAUX, Stanford Univ / SLAC — The interplay between electron-electron interactions and electron-phonon coupling in cuprates can be explored via the Hubbard-Holstein model. Here, we use determinant quantum Monte Carlo simulations to study the three-band version of the model with electron coupling to c-axis optical oxygen vibrations. The model exhibits competition between an antiferromagnetic phase and a charge density wave phase. The corresponding phase diagram is compared against that from existing single-band Hubbard-Holstein results. Finally we investigate the evolution of the phase diagram due to changes in doping and temperature.

1:03PM Z32.00008 Geometrical Effects in Orbital Magnetism , YANG GAO, UT Austin, SHENGYUAN YANG, SUTD, QIAN NIU, UT Austin — Within the wave-packet semi classical approach, the Bloch electron energy is derived to second order in the magnetic field and classified into gauge-invariant terms with clear physical meaning, yielding a fresh of the complex behavior of orbital magnetism. The Berry curvature and quantum metric of the Bloch states rise to a geometrical magnetic susceptibility, which can be dominant when bands are filled up to a small energy gap.is also an energy polarization term, which can compete with the Peierls-Landau and Pauli magnetism on a Fermi surface. These, and an additional Langevin susceptibility, can be calculated from each single band, leaving the Vn Vleck susceptibility the only term truly from interband coupling.

1:15PM Z32.00009 Effective transient states for nonequilibrium charge density wave systems under ultrafast control pulses . BIN HWANG, JENNI PORTMAN, PHILLIP DUXBURY, Michigan State University — A central challenge for implementing Mott-insulator transition in nonequilibrium time-dependent charge density wave systems is finding an effective pulse to achieve the goal. Effective ultra laser pulses have been found for the transient states in nonequilibrium time-dependent charge density wave systems based on a promising optimal-control method. Intense ultrafast laser pulses allow the preparation of transient states of matter exhibiting strong non-equilibrium between electrons and lattice. By controlling the laser pulse, we are able to change the transient states of these quantum systems. The optical and structural properties as well as the temporal evolution of such states provide insights into the mutual dependence of electronic and atomic structure. We approach the problem by showing examples from charge-density-wave systems. Nonequilibrium techniques can be used to qualitatively describe the common short-time experimental features. Through simulations based on non-equilibrium Green’s function formalism we show how to achieve effective transient states for nonequilibrium systems under ultrafast control pulses.

1:27PM Z32.00010 Interplay of 3d-5d interactions in high-T_c osmium-based double perovskites , A.E. TAYLOR, S. CALDER, Quantum Condensed Matter Division, Oak Ridge National Laboratory, R. MORROW, P.M. WOODWARD, Department of Chemistry, The Ohio State University, J.Q. YAN, Materials Science & Technology Division, Oak Ridge National Laboratory, B. WINN, M.D. LUMSDEN, A.D. CHRISTIANSON, Quantum Condensed Matter Division, Oak Ridge National Laboratory — In 3d-5d systems the strongly magnetic 3d orbitals and extended 5d orbitals with enhanced spin-orbit coupling lead to a range of high T_c magnetic states and novel behavior not present in systems consisting solely of 3d or 5d ions. The two distinct octahedral sites in double perovskites A_2BB'O_6 allow an ordered 3d-5d structure to form, providing a variety of systems to be investigated. Unravelling the interactions controlling these systems, however, is an open challenge. The highest known T_c in such a system, 725K, is found in insulator Sr_2CrOsO_6. This questions the theory for high-T_c systems such as T_c=400K Sr_2FeReO_6 which relies on half-metallic behavior. To unravel the nature of the interactions in 3d-5d systems, we have studied the series of compounds Sr_2XOsO_6. We have utilized elastic and inelastic neutron scattering to probe the spin states in the systems, and therefore test predictions that the magnetic interactions are controlled by a frustrated AFM Heisenberg model [1]. By studying the series, we are able to relate changes in the spin wave spectrum to dramatic changes in the magnetic order from T_N = 95K antiferromagnetism to T_c = 725K ferrimagnetism.


Friday, March 6, 2015 11:15AM - 1:51PM – Session Z34 DMP: Hydrogen Production, Storage, Delivery 210A - Zachary Gabelle, Carnegie Institute for Science

11:15AM Z34.00001 Gettering of Hydrogen and Methane from a Helium Gas Mixture . ROSA E. CARDENAS, Department of Physics, The University of the Incarnate Word, 4301 Broadway, San Antonio, TX 78209, DONALD F. COWGILL, KENNETH D. STEWART, Sandia National Laboratories, Hydrogen and Metallurgical Sciences, 7011 East Avenue, Livermore, CA 94550 — In this study, we developed an approach for accurately quantifying the helium content in a gas mixture also containing hydrogen and methane using commercially available getters. We performed a systematic study to examine how both H2 and CH4 can be removed simultaneously from the mixture using two SAES St 172 getters operating at different temperatures. The remaining He within the gas mixture can then be measured directly using a capacitance manometer. The optimum combination involved operating one getter at 650°C to decompose the methane, and the second at 110°C to remove the hydrogen. This approach eliminated the need to reactivate the getters between measurements, thereby enabling multiple measurements to be made within a short time interval, with accuracy better than 1%. We anticipate that such an approach will be particularly useful for quantifying the He-3 in mixtures that include tritium, tritiated methane, and helium-3. The presence of tritiated methane, generated by tritium activity, often complicates such measurements.

11:27AM Z34.00002 Effects of the Electronic Doping In the Stability of the Metal Hydride NaH1, MONICA-ARACELI OLEA-AMEZCUA, JUAN-FRANCISCO RIVAS-SILVA, OMAR DE LA PEÑA-SEAMAN, Institute of Physics (IFUAP), Benemérita Universidad Autonoma de Puebla (BUAP), ROLF HEID, KLAUS-PETER BOHNEN, Institute of Solid State Physics (IFP), Karlsruher Institute of Technology (KIT) — Despite metal hydrides light weight and high hydrogen volumetric densities, the Hydrogen desorption process requires excessively high temperatures due to their high stability. Attempts for improvement the hydrogenation properties have been focus on the introduction of defects, impurities and doping on the metal hydride. We present a systematic study of the electronic doping effects on the stability of a model system, NaH doped with magnesium, forming the alloying system Na_1-xMg_xH. We use the density functional theory (DFT) and the self-consistent version of the virtual crystal approximation (VCA) to model the doping of NaH with Mg. The evolution of the ground state structural and electronic properties is analyzed as a function of Mg-content. The full-phonon dispersion, calculated by the linear response theory (LRT) and density functional perturbation theory (DFPT), is analyzed for several Mg-concentrations, paying special attention to the crystal stability and the correlations with the electronic structure. Applying the quasiharmonic approximation (QHA), the free energy from zero-point motion is obtained, and its influence on the properties under study is analyzed.

1 This work is partially supported by the VIEP-BUAP (OMPS-EXC14-I) and CONACYT-Mexico (No. 221807) projects
11:39AM Z34.00003 High Efficiency, Surface Stable Photocatalytic H2 evolution on TiO2-passivated GaAs1. JING QIU, GUANGTONG ZENG, University of Southern California, STEPHEN B. CRONIN, STEPHEN B. CRONIN NANO RESEARCH LAB TEAM — III-V compounds, such as GaAs, are used widely for high efficiency photovoltaic solar energy conversion. The electrochemical instabilities of these materials, however, has limited their applicability in photocatalysis. Here, we demonstrate that thin (1-5nm) films of TiO2 deposited by atomic layer deposition on planar GaAs provide electrochemical stability and substantial improvements in the efficiency of photocatalytic water splitting. The TiO2-passivated GaAs shows no photochemical degradation or corrosion after 48 hours, while bare GaAs shows substantial degradation after just 15 minutes. This TiO2 passivation layer produces a 32-fold enhancement over bare GaAs, with an overall photoconversion efficiency of 11%. We find that just 1nm of TiO2 produces the optimum conditions for photocatalysis. This is not thick enough to form a continuous film, and instead produces small regions of non-stoichiometric TiO2, which is rich with Ti3+ surface states that are known to be catalytically active sites. These charged sites stabilize, or lower the energy of, OH- intermediate species in this reaction, thus lowering the reaction barrier height. X-ray photoemission spectroscopy and photoluminescence spectroscopy provide further evidence for these Ti3+ surface states.

1We acknowledge the grant from Florida Energy Systems Consortium and support from Florida Polytechnic University.

11:51AM Z34.00004 Aging Effects on the Hydrogen Storage Characteristics of Li-Mg-B-N-H Complex Hydrides1. SESHA SRINIVASAN, Florida Polytechnic University, College of Innovation and Technology, ERIC VICKERS, JAMES MUL-HARAN, Florida Polytechnic University, College of Engineering, GHAZI DARKAZALLI, Florida Polytechnic University, YOGI GOSWAMI, ELIAS STEFANAKOS, University of South Florida, Clean Energy Research Center. FLPOLY-CERC COLLABORATION — The aging effects on the hydrogen storage characteristics and chemical formulations of the complex hydrides are discussed in this study. The aging effects due to atmospheric events such as oxygen and moisture coverage and self-decomposition are currently under investigation. The candidate material chosen for this study is Lithium/Magnesium based complex hydride LiBH4/LiNH2/MgH2. These materials were prepared using high energy ball milling under Ar/H2 atmosphere with different milling durations. The chemical, structural and microstructural characteristics of the synthesized and aged materials were compared and investigated using TGA/DSC, FTIR, XRD, BET and SEM analytical tools. Hydrogen storage properties such as hydrogen sorption kinetics, cycle life and pressure-composition isotherm (PCI) was examined via high pressure, high temperature Sievert’s type apparatus. This current study will shed light to compare and contrast the above mentioned characteristics for the aged samples practically at the same experimental conditions. Furthermore, we have investigated the relationship between the aging effects with respect to the crystallite sizes of the candidate materials and their nano-dopant variants.

1We acknowledge the grant from Florida Energy Systems Consortium and support from Florida Polytechnic University.

12:03PM Z34.00005 Molecular simulation of hydrogen storage on hydrogen storage in layered graphite oxide: effect of functional group and intercalated ion, JAEHYUN BAE, JISOON IHM, Seoul Natl Univ, SEOUL NATIONAL UNIVERSITY TEAM — The adsorption of molecular hydrogen gas into layered graphite oxide (GO) has been studied using both classical grand-canonical Monte-Carlo simulations and ab initio calculations. Different from graphite, interlayer distance of graphite oxide can be varied by controlling the functional group density or introducing alkali metal ion in the synthesis process, this gives new ways of searching for efficient hydrogen storage in porous materials. Our ab initio calculations show that average hydrogen binding energy in the graphite oxide layers is enhanced due to the dipole interaction and small hybridization between hydrogen and functional groups. Introducing alkali metal inside the graphite oxide layers further increases average binding energy by 0.1eV and interlayer distance and hydrogen storage capacity increases close to 3wt% at 300K and 10MPa, similar to recent experiments. In the grand-canonical Monte-Carlo simulations, we use ab initio fitted H2-GO and H2-H2 interaction potential and simulation results are understood by equilibrium of interacting gases in the quasi 2-dimensional potential landscape inside the GO layers. Our computational results suggest the best way of synthesizing the optimal chemical and atomic structure of GO for hydrogen storage medium.

12:15PM Z34.00006 ABSTRACT WITHDRAWN —

12:27PM Z34.00007 Hydrothermal synthesis and characterization of CuFeO2 Delafossite Crystals1, M. SARABIA, S. ROJAS, Pontificia Universidad Catolica de Chile, Z. LOPEZ-CABANA, Universidad de Talca, Chile, R. VILLALBA, G. GONZALEZ, Instituto Venezolano de Investigaciones Cientificas, Caracas, Venezuela, A.L. CABRERA, Pontificia Universidad Catolica de Chile — In this study we synthesized CuFeO2 compounds using as precursors CuO and FeOOH with fused NaOH. The synthesis takes place in a Teflon vessel lasting 97 (Synthesis I) or 48 hrs (Synthesis II) at 210 °C. The compound obtained were analyzed for crystal structure and morphology with Raman Spectroscopy, X-Ray Diffraction (XRD), X-Ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS). Optical properties were obtained by UV-Vis Spectroscopy and Gas adsorption measured with a Quartz-Crystal Microbalance (QCM). Our results show that this type of hydrothermal synthesis is capable to recreate the Delafossite structure of this copper-iron oxide. This material chemisorbs water and carbon dioxide.

1Funds FONDECyT 1130372

13:39PM Z34.00008 Rapid Facile Microwave-assisted Solvothermal Synthesis of Rod-like CuO/TiO2 for High Efficiency photocatalytic Hydrogen Evolution, YI-HSIEN YU, YING-PIN CHEN, ZHENGDONG CHENG, Texas A&M Univ — Rod-like CuO/TiO2 was prepared by a rapid facile microwave-assisted solvothermal method for high efficiency photocatalytic hydrogen evolution. The structure of obtained CuO/TiO2 samples were characterized by X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), high resolution transmission electron microscopy (HR-TEM), and the amount of produced hydrogen was analyzed by gas chromatography (GC). CuO decorated TiO2 rods exhibited greatly improvement of photocatalytic hydrogen evolution. Utilizing 30 mg of CuO/TiO2 rods sample showed highest hydrogen evolution rate over utilizing 50 mg and 100 mg. Comparing to hydrogen evolution rate of 45.4 µmol h−1 g−1 by using bare Rod-like TiO2, 1 wt% CuO loaded TiO2 rods presented the highest hydrogen evolution rate of 3508.7 µmol h−1 g−1 while hydrogen evolution rate of 0.5 wt%, 5 wt%, and 10 wt% CuO loaded TiO2 rods were 157.1, 2817, and 2595 µmol h−1 g−1, respectively. Such enhancement of photocatalytic activity could be ascribed to that CuO improves not only light harvesting but also enhanced separation of electron-hole carriers.
12:51PM Z34.00009 The Electrical and Structural analysis of degraded Single Junction Amorphous Silicon Solar Modules1. GILBERT OASAYEMWENYE, Fort Hare Institute of Technology, ENERGY EFFICIENCY TEAM — This paper outlines a systematic approach used in evaluating the quality, performance and reliability of single junction amorphous silicon solar modules (a-Si:H).

The analytical techniques include an electrical and structural analysis. These techniques were used to obtain a holistic view of the state of affairs of these readily available PV modules for small stand-alone systems. Specifically, current-voltage (I-V) characterization and scanning electron microscopy (SEM) will be presented as diagnostic tools in this article. The SEM (JEOL, JED-2300) was used to study the surface morphology of the affected regions, results show structural damage in the affected regions. The experiment shows that the energy output of the modules varies a degradation variation of 2.5% to 25.7%, was observed. The detailed results will be presented in the final paper. In conclusion, this research established the degradation which occurs and correlate it to the morphological damage. The module with the worst case scenario has an efficiency of 59% decrease, this could be unacceptable in a device where stability is of priority.

1We sincerely thank GMDRC and Eskom for financing this project.

1:03PM Z34.00010 First-principles quantum-mechanical investigations: The role of water in catalytic conversion of furfural on Pd(111)1, WENHUA XUE, University of Tulsa, MIGUEL GONZALEZ BORJA, DANIEL E. RESASCO, University of Oklahoma. SANWU WANG, University of Tulsa — In the study of catalytic reactions of biomass, furfural conversion over metal catalysts with the presence of water has attracted wide attention. Recent experiments showed that the proportion of alcohol product from catalytic reactions of furfural conversion with palladium in the presence of water is significantly increased, when compared with other solvents including dioxane, decalin, and ethanol. We investigated the microscopic mechanism of the reactions based on first-principles quantum-mechanical calculations. We particularly identified the important role of water and the liquid/solid interface in furfural conversion. Our results provide atomic-scale details for the catalytic reactions.

1Supported by DOE (DE-SC0004600). This research used the supercomputer resources at NERSC, of XSEDE, at TACC, and at the Tandy Supercomputing Center.

1:15PM Z34.00011 Study of effects of transport properties of a biodiesel derived from soybean on the mixture process formation using CFD OpenFOAM1, ADOLOF BENITEZ MOLINA, OSCAR ALEJANDRO DE LA GARZA LEON, SIMON MARTINEZ MARTINEZ, FAUSTO ALEJANDRO SANCHEZ CRUZ, Universidad Autonoma de Nuevo Leon-FIME, LIITE-Laboratory for Research and Innovation in Energy Technology, Mexico — In this work has been studied the effects of the transport properties of biodiesel derived from soybean on the mixing process, using a CFD code OpenFOAM. For this the most relevant properties in this mixing process have been determined: density, viscosity, surface tension and vapor pressure. These fuel properties govern the spray formation however, there are only very limited studies that determined for its subsequent implementation in a CFD code, such as the OpenFOAM code. Such properties were obtained using empirical correlations based on the molecular structure of the fatty acids that compose the biodiesel and applying nonlinear regression are implemented in the programed models used in the OpenFOAM code for a diesel spray simulation. The results achieved in the present study on the one side, have been confirmed how the biodiesel properties affect the mixture process, and on the other side, the obtained coefficients which can be used in the proposed models by the CFD code OpenFOAM for the implementation of this properties as a temperature function without the correlations based on the molecular structure of the fatty acid.

1Also they thank the CONACYT from Mexican Government for granting the Master degree of Adolfo Benitez

1:27PM Z34.00012 Catalytic hydrogenation of cresol: first-principles density-functional calculations and ab initio molecular dynamics simulations1, YAPING LI, Department of Physics and Engineering Physics, University of Tulsa, ZHIMIN LIU, FRIEDERIKER JENTOFT, School of Chemical, Biological and Materials Engineering, University of Oklahoma, SANWU WANG, Department of Physics and Engineering Physics, University of Tulsa — Biomass is an important renewable energy resource. Cresol is one of components in crude bio-oil generated from biomass, and hydrogenation of cresol is often involved in the upgrading process. We studied catalytic hydrogenation of cresol on the Pt(111) surface with and without the presence of water. In particular, we used first-principles density-functional theory and ab initio molecular dynamics simulations to obtain adsorption geometries, binding energies, reaction energies, activation energies, and reaction pathways for hydrogenation of cresol with possible products of 2-methylcyclohexanone and 2-methylcyclohexanol. Our theoretical results are used to explain the available experimental measurements, which show a strong influence of water.

1Supported by DOE (DE-SC0004600). This research used the supercomputer resources at NERSC, of XSEDE, at TACC and at the Tandy Supercomputing Center.

1:39PM Z34.00013 Hybrid functional calculation of Na and K impurities in CuInSe2 and CuIn5Se8 solar cell materials1, JANOS KISS, Max Planck Institute for Chemical Physics of Solids Dresden, ELAHEH GHORBANI, Institute of Inorganic and Analytical Chemistry JGU Mainz, HOSSEIN MIRHOSSEINI, Max Planck Institute for Chemical Physics of Solids Dresden, GUIDO ROMA, Service de Recherches de Metallurgie Physique DMN/DEN CEA-Saclay, CLAUDIA FESLER, Max Planck Institute for Chemical Physics of Solids Dresden — Although it is widely known that the presence of Na and K dopants increase the efficiency of CuIn1−ySey (CIGS) thin film solar cells, the incorporation of these impurities and their effect upon the atomic and electronic structure of the light absorber materials is not yet well understood. Using the HSE06 hybrid functional we studied the structure and energetics of Na and K impurities and also Na-Na, K-K and Na-K dumbbells in different substitutional and interstitial positions in CuInSe2 and CuIn5Se8 solar cell materials. We found that among substitutional positions, occupying Cu position is energetically more favorable compared to In and Se positions. The interstitial position, where the impurity is tetrahedrally coordinated by four Se atoms is the most stable site to form Na or K interstitials in CuInSe2, whereas in CuIn5Se8 the pristine copper vacancy positions are more stable. Our data show that Na-Na, Na-K and K-K dumbbells can form both in CuInSe2 and in CuIn5Se8 as well. Comparing the formation energy of various dumbbell configurations, creating dumbbells in a pristine vacant copper site in CuInSe2 has the highest association energy between the impurities.

1comCIGS I (No. 0327665A) and comCIGS II (No. 0325448C).

Friday, March 6, 2015 11:15AM - 2:15PM –
Session Z36 DAMOP: Focus Session: Non-equilibrium Dynamics in Quantum Systems 211 -
Stefan Natu, University of Maryland, College Park
11:15 AM Z36.00001 Locality in quenched systems with long-range interactions, MICHAEL FOSS-FEIG, Joint Quantum Institute, NIST, and the University of Maryland — For more than a decade, ultracold atomic and molecular systems have been exploited to simulate non-equilibrium models of strongly correlated materials. However, the extremely low (often sub nano-kelvin) temperatures required to realize the most interesting equilibrium states of such models have proven extremely difficult to achieve. When these ultracold systems are driven far from equilibrium, however, very small temperatures get traded in for very long time-scales, which enable the observation of dynamic phenomena that were never even envisioned in the context of real materials. In this talk, I will describe some recent experimental and theoretical explorations of non-equilibrium dynamics in quenched AMO systems, and will discuss some of the interesting questions that arise naturally from their remarkable tunability. In particular, I will describe recent efforts to understand the fate of locality — i.e. constraints on the propagation of information/entanglement — as interactions become increasingly long-ranged.

11:51 AM Z36.00002 Slowest local operators in quantum spin chains, HYUNGWON KIM, Rutgers University, MARI CARMEN BANULS, IGNACIO CIRAC, Max-Planck-Institute for Quantum Optics, MATTHEW HASTINGS, Station Q, Microsoft Research, DAVID HUSE, Princeton University — We numerically construct slowly relaxing local operators in a nonintegrable spin-1/2 chain. Restricting the support of the operator to M consecutive spins along the chain, we exhaustively search for the operator that minimizes the Frobenius norm of the commutator with the Hamiltonian and show that the Frobenius norm bounds the time scale of relaxation of the operator. We find operators with significantly slower relaxation than the slowest slow operator. Using both exhaustive search and tensor network techniques, we find similar slowly relaxing operators for a Floquet spin chain and for quantum circuits on spin chains; these systems are hydrodynamically “trivial,” with no conservation laws restricting their dynamics. We argue that such slow relaxation may be a generic feature following from locality and unitarity.

12:03 PM Z36.00003 Limit cycle phase in driven-dissipative spin systems, CHING-KIT CHAN, TONY LEE, ITAMP, Harvard University, SARANG GOPALAKRISHNAN, Harvard University — Quantum simulator experiments based on trapped ions and atomic ensembles offer an attractive platform to study nonequilibrium many-body phases and phase transitions. We theoretically explore the phase diagram of a driven and dissipative Heisenberg spin system featured by a time-dependent limit cycle phase in which the magnetization oscillates in time. We present a Gaussian-Floquet theory to study the fluctuation of this phase that spontaneously breaks time-translational symmetry. As a time-dependent generalization of the Mermin-Wagner theory, we show how spatial fluctuations destroy the limit cycle ordering for dimension $d \leq 2$. We also demonstrate how the limit-cycle phase leads to new features in the power spectrum measurable in fluorescence experiments.

12:15 PM Z36.00004 ABSTRACT WITHDRAWN —

12:27 PM Z36.00005 Ramping through a topological critical point in two dimensions, MARIN BUkov, PHILLIP WEINBERG, MICHAEL KOLODRUBETZ, Boston University — The recent realization of Floquet Chern insulators has resulted in a prolific study of periodically driven models. In order to probe equilibrium physics, the driving protocol is gently ramped up, in the process of which the system undergoes a dynamical phase transition to a topologically non-trivial state. Since such transitions are controlled by closing and re-opening a band gap, the notion of adiabaticity inevitably breaks down and the system gets excited. In this talk, I shall present recent results based on scaling arguments within Kibble-Zurek theory to study the excitations due to a ramp through a topologically critical point in 2 dimensions. I shall show convincing evidence that the occupation of the chiral edge modes follows similar universal scaling as the bulk as a function of the ramp speed and the system size. Further, I shall apply these results to study the build-up of magnetisation due to the non-adiabatic population of the edge states in Haldane’s model of graphene, which has recently been proposed to detect the topological character of the state of the system. Finally, I shall show that the quantisation of magnetisation is robust against non-adiabaticity due to crossing the critical point.

12:39 PM Z36.00006 The Floquet Adiabatic Theorem revisited, PHILLIP WEINBERG, MARIN BUkov, Boston University, LUCA D’ALESSIO, Boston University, Penn State University, MICHAEL KOLODRUBETZ, SHAINEN DAVIDSON, ANATOLI POLKOVNIKOV, Boston University — The existence of the adiabatic theorem for Floquet systems has been the subject of an active debate with different articles reaching opposite conclusions over the years. In this talk we clarify the situation by deriving a systematic expansion in the time-derivatives of a slow parameter for the occupation probabilities of the Floque states. Our analysis shows that the in a certain limit the transition between Floquet eigenstates are suppressed and it is possible to define an adiabatic theorem for Floquet systems. Crucially we observe however that the conditions for adiabaticity in ordinary and Floquet systems are different and that this difference can become important when the amplitude of the periodic driving is large. We illustrate our results with specific examples of a periodically driven harmonic oscillator and cold atoms in optical lattices which are relevant in current experiments.

12:51 PM Z36.00007 Thermal Steady States in Fermionic Dissipative Floquet Systems, KARTHIK SEETHARAM, CHARLES-EDOUARD BARDYN, California Institute of Technology, MARK RUDNER, University of Copenhagen, NETANEL LINDNER, Technion - Israel Institute of Technology, GIL REFAEL, California Institute of Technology — The possibility to drive quantum systems periodically in time offers unique ways to deeply modify their fundamental properties, as exemplified by Floquet topological insulators. It also opens the door to a variety of non-equilibrium effects. Resonant driving fields, in particular, lead to excitations which can expose the system to heating. Inspired by existing studies of photoexcited semiconductors, we demonstrate that the analog of thermal states can be achieved in a fermionic Floquet system including carrier-carrier interactions, phonon scattering, and spontaneous emission. We show that inelastic “Floquet-Umkopp” processes are responsible for non-thermal heating effects, and identify practical conditions under which they are suppressed. We propose to use suitably engineered external reservoirs of carriers to further stabilize thermal features and control the effective chemical potential of the resulting Floquet distributions.

1:03 PM Z36.00008 Dynamical preparation of Floquet Chern insulators: A no-go theorem and the experiments, LUCA D’ALESSIO, MARCOS RIGOL, Pennsylvania State University — Recently, it has been proposed that time-periodic perturbations can induce topological properties in otherwise non-topological materials, opening the exciting possibility of studying non-equilibrium topological transitions. Here we address what should happen in an experiment when one turns on the periodic driving. On the one hand, for infinite (translationally invariant) systems we prove a no-go theorem. We show that the Chern number is conserved under unitary evolution, i.e., it is impossible to change the possible to define an adiabatic theorem for Floquet systems. Crucially we observe however that the conditions for adiabaticity in ordinary and Floquet systems are different and that this difference can become important when the amplitude of the periodic driving is large. We illustrate our results with specific examples of a periodically driven harmonic oscillator and cold atoms in optical lattices which are relevant in current experiments.

1:15 PM Z36.00009 Universal post-quench prethermalization at a quantum critical point, PETER P. ORTH, PIA GAGEL, JOERG SCHMALIAN, Karlsruhe Institute of Technology (KIT) — We consider an open system near a quantum critical point that is suddenly moved towards the critical point. The bath-dominated diffusive non-equilibrium dynamics after the quench is shown to follow scaling behavior, governed by universal exponents that differ from those for equilibrium and critical exponents. We determine this exponent and show that it describes universal prethermalized coarsening dynamics of the order parameter in an intermediate time regime. Implications of this quantum critical prethermalization are a powerlaw rise of order and correlations after an initial collapse of the equilibrium state and a crossover to thermalization that occurs arbitrarily late for sufficiently shallow quenches. [1] P. Gagel, P. P. Orth, J. Schmalian, Phys.Rev. Lett. (in press) arXiv:1406.6387
The distribution of the times in-between the quantum jumps reveals quantitative information about the population and dynamics of quasiparticles [3]. The amplifier (a Josephson Parametric Converter) we can observe quantum jumps between the 0 and 1 states of the qubit in thermal equilibrium with the environment.

11:15AM Z39.00001 Measurement of recombination and single-vortex trapping of quasiparticles in a superconducting qubit, CHEN WANG, Y.Y. GAO, I.M. POP, U. VOOL, C. AXLINE, T. BRECHT, R.W. HEERES, L. FRUNZIO, Yale Univ, G. CATELANI, Peter Gruberg Institut (PGI-2), M.H. DEVORET, L.I. GLAZMAN, R.J. SCHOELKOPF, Yale Univ — We measure the dynamics of quasiparticle relaxation over multiple orders of magnitude in density in superconducting transmon qubits using a contactless injection technique by microwave pulses. We demonstrate the power-law decay characteristics for quasiparticle recombination and exponential decay for single quasiparticle loss due to trapping effects, and find both mechanisms play a significant role in quasiparticle relaxation depending on device geometry. We observe quantized changes in quasiparticle trapping rate due to individual vortices, and thus quantitatively measure the interaction between non-equilibrium quasiparticles and a single vortex in a superconducting aluminum film. These results are described in Ref. [1]. [1] C. Wang et al. arXiv:1406.7300 [quant-ph]

11:27AM Z39.00002 Suppressing decoherence of superconducting qubits by trapping non-equilibrium quasiparticles, YVONNE GAO, CHEN WANG, I.M. POP, U. VOOL, C. AXLINE, T. BRECHT, R.W. HEERES, L. FRUNZIO, M.H. DEVORET, Yale University, G. CATELANI, Peter Gruberg Institute, L.I. GLAZMAN, R.J. SCHOELKOPF, Yale University — We report a counter-intuitive observation that vortices can improve the coherence of superconducting qubits by suppressing non-equilibrium quasiparticles. This effect is systematically studied by measuring the magnetic-field dependence of qubit coherence times and quasiparticle lifetimes in transmons with different geometries in a 3D cQED architecture. Varying quasiparticle dynamics by vortices allows separation of dissipation mechanisms and measurement of the stray generation rate of quasiparticles in our devices. More details are described in Ref [1]. Our results indicate that quasiparticles contribute significantly to qubit decoherence. Hence suppression of quasiparticle density in the device is essential for further improvement of coherence times of superconducting qubits and we will present recent results aimed at alleviating decoherence due to quasiparticles. [1] C.Wang, Y.Y.Gao et al arXiv:1406.7300

11:39AM Z39.00003 Coherent Suppression of Quasiparticle Dissipation in Superconducting Artificial Atom1, IOAN M. POP, Department of Applied Physics, Yale University — We demonstrate immunity to quasiparticle dissipation in a Josephson junction. At the foundation of this protection rests a prediction by Brian Josephson from fifty years ago: the particle-hole interference of superconducting quasiparticles when tunneling across a Josephson junction [1]. The junction under study is the central element of a fluxonium artificial atom, a Josephson junction. At the foundation of this protection rests a prediction by Brian Josephson from fifty years ago: the particle-hole interference of superconducting quasiparticles when tunneling across a Josephson junction [1]. The junction under study is the central element of a fluxonium artificial atom, a Josephson junction. The junction under study is the central element of a fluxonium artificial atom, a Josephson junction.

1Work supported by: IARPA, ARO, and ONR.
12:15PM Z39.00004 From quantum jumps to quasiparticle population1, . U. VOOL, I.M. POP, K. SLIWA, B. ABDO, C. WANG, Y.Y. GAO, A. KOU, W.C. SMITH, T. BRECHT, S. SHANKAR, M. HATRIDGE, Department of Applied Physics, Yale University, G. CATELANI, Peter Grünberg Institut (PGI-2), Forschungszentrum Jülich, L. FRUNZIO, R.J. SCHOELKOPF, L. GLAZMAN, Department of Applied Physics, Yale University, M. MIRRAHIMI, Department of Applied Physics, Yale University and INRIA Paris Rocquencourt, M.H. DEVORET, Department of Applied Physics, Yale University — Superconducting quasiparticles (QP) play a dominant role in the relaxation of the fluxonium qubit in the vicinity of the half-flux-quantum bias point. Recent experiments integrating the fluxonium with a quantum-limited amplifier have measured quantum jump trajectories between the ground state and the first excited state. These trajectories show a change in the characteristic lifetime of the fluxonium qubit as a function of time, arising from a change in the number of QP’s in the sample [1]. Using a simple model of QP dynamics and their effect on the fluxonium qubit, we can access the QP population with temporal resolution better than a 100 microsecond. Such rapid monitoring of QP dynamics is essential for understanding the sources of QP’s and ultimately suppressing them.

1Work supported by: IARPA, ARO, and ONR.

12:27PM Z39.00005 Simulation and measurement of a fluxonium qubit inductively coupled to a readout resonator1, W.C. SMITH, A. KOU, U. VOOL, I.M. POP, R.J. SCHOELKOPF, M.H. DEVORET, Department of Applied Physics, Yale University — Prototypical circuit QED experiments can be performed using a fluxonium qubit that shares a portion of its superinductance with an on-chip LC oscillator, dubbed an “antenna”, that is used as a readout resonator. However, the complete fluxonium-antenna artificial atom had not been previously understood in all coupling regimes. We have measured Hamiltonian parameters and decay rates by channeling microwave pulses into a rectangular waveguide containing the antenna-qubit system. Accurate modeling of energy spectra, dispersive shifts, and Purcell loss is achieved by diagonalizing the effective circuit Hamiltonian. We will present spectroscopy data, coherence times, and simulation results.

1Work supported by: IARPA, ARO, and ONR.

12:39PM Z39.00006 Quantum and Ionic Transport Across Superconductor-based Heterostructures. OSAMA NAYFEH, SON DINH, BENJAMIN TAYLOR, MARCIO DE ANDRADE, PAUL SWANSON, BRUCE OFFORD, ANNA LEESH ESCOBAR, Spawar Systems Center Pacific, STEPHANIE CLAUSSSEN, Colorado School of Mines, SAM KASSEGNE, San Diego State University — We present analysis of quantum and ionic transport across superconductor/normal metal/normal metal/superconductor heterostructures. Calculations for various ionic configurations demonstrate modification of the quantum transport coherence length and energy profile with moderate ionic transport away from the superconductor-barrier interface. The effect of electric field and cryogenic temperature on the stability of the ionic configurations for quantum information state storage is examined. Characterization and analysis of fabricated normal metal and superconductor-based device structures are presented. Acknowledgements: We acknowledge the support of the SSC Pacific In-house Laboratory Independent Research Science and Technology Program managed by Dr. Dave Rees, the Naval Innovative Science and Engineering Program managed by Mr. Robin Laird, and the ONR Summer Faculty Research Program. Interactions with Dr. Van Vechten (ONR) and Dr. Manheimer (IARPA) are appreciated. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of SPARWAR or the U.S. Government. Approved for Public Release; distribution is unlimited.

12:51PM Z39.00007 Correlations of microwave photons emitted by inelastic Cooper pair tunneling, ALEXANDER GRIMM, SALHA JEBARI, DIBYENDU HAZRA, CEA, INAC-SPSMS, F-38000 Grenoble, France, CARLES ALTIMIRAS, OLIVIER PARLAVECCCHIO, FABIEN PORTIER, CEA, IRAMIS-SPEC, F-91911 Gif-sur-Yvette, France, MAX HOFHEINZ, CEA, INAC-SPSMS, F-38000 Grenoble, France — A simple DC voltage-bias on a small Josephson junction leads to emission of microwave radiation via inelastic Cooper-pair tunneling. In this process a tunneling Cooper pair emits one or several microwave photons with a total energy of 2eV. The observed average photon emission rate is well explained within the so-called P(E) theory, but this theory does not make any predictions about the statistics of the emitted photons. Recent theory indicates that these statistics can be highly nontrivial. Depending on the bias conditions and the impedance of the circuit in which the junction is embedded, correlations can range from strongly bunched to anti-bunched. I will present experiments investigating photon correlations in circuits with specifically engineered environments. This type of devices might offer a new way of generating useful photon states for circuit quantum optics experiments, without the need of carefully calibrated control pulses. Moreover, the frequency of the emitted radiation is only limited by the gap of the superconductor. We are building our devices using NbN-MgO-NbN tunnel junctions which should in principle allow operation up to the THz regime.

1:03PM Z39.00008 Can a strain yield a qubit?1, COLIN BENJAMIN, National Institute of Science education and Research, Bhubaneswar, India — A Josephson qubit is designed via the application of a tensile strain to a topological insulator surface, sandwiched between two s-wave superconductors. The strain applied leads to a shift in Dirac point without changing the conducting states existing on the surface of a topological insulator. This strain applied can be tuned to form a π-junction in such a structure. Combining two such junctions in a ring architecture leads to the ground state of the ring being in a doubly degenerate state—“0” and “1” states of the qubit. A qubit designed this way is easily controlled via the tunable strain. We report on the conditions necessary to design such a qubit. Finally the operating time of a single qubit phase gate is derived.

1This work was supported by funds from Dept. of Science and Technology (Nanomission), Govt. of India, Grant No. SR/NM/NS-1101/2011.

1:15PM Z39.00009 Nonequilibrium noise and current fluctuations at the superconducting phase transition1, DMITRY BAGRETS, University of Cologne, ALEX LEVCHENKO, Michigan State University — We study non-Gaussian out-of-equilibrium current fluctuations in a mesoscopic NSN circuit at the point of a superconducting phase transition. The setup consists of a voltage-biased thin film nanobridge superconductor (S) connected to two normal-metal (N) leads by tunnel junctions. We find that above a critical temperature fluctuations of the superconducting order parameter associated with the preformed Cooper pairs mediate inelastic electron scattering that promotes strong current fluctuations. Though the conductance is suppressed due to the depletion of the quasiparticle density of states, higher cumulants of current fluctuations are parametrically enhanced. We identify experimentally relevant transport regime where excess current noise may reach or even exceed the level of the thermal noise.

1This work was supported by NSF Grant No. ECCS-1407875
1:27PM Z39.00010 Manipulating the Quantum State of a Single Cooper Pair in a One-Atom Contact, CRISTIAN URBINA, CAMILLE JANVIER, LEANDRO TOSI, ÇAĞLAR GIRIT, MICHAEL STERN, PATRICE BERTET, DENIS VION, PHILIPPE JOYEZ, DANIEL ESTEVE, MARCELO COFFMAN, HUGUES POTTHIER, Quantronics Group, CEA-Saclay — Superconducting qubits presently used in quantum information experiments are based on Josephson tunnel junctions. Nevertheless, these circuits exploit only partially the richness of the Josephson effect, as they overlook the existence of an internal, spin-like degree of freedom, inherent to all Josephson structures. Each conduction channel of a weak-link gives rise to a doublet of discrete subgap states (the Andreev bound states), which represents the two possible states of a localized Cooper pair. We spotlight these doublets with experiments on the simplest Josephson weak-link: a one-atom contact between two superconductors. The atomic contact is inserted in a superconducting loop coupled to a microwave resonator. This standard circuit-QED architecture allows performing single shot measurements of the state of a localized Cooper pair, and to manipulate coherently its quantum state, as illustrated by Rabi oscillations, Ramsey fringes and spin echoes.

1:39PM Z39.00011 Flux Solitons Studied for Energy-Conserving Reversible Computing, KEVIN D. OSBORN, WALTRAUT WUSTMANN, Laboratory for Physical Sciences, College Park, MD — On-chip logic is desired for controlling superconducting qubits. Since qubits are very sensitive to photon field noise, it is desirable to develop an energy-conserving reversible logic, i.e. one which can compute without substantial energy dissipation or applied drive fields. With this goal in mind, simulations on discretized long Josephson junctions (DLJJs) have been performed, where the flux soliton is a potential information carrier. Undriven soliton propagation is studied as a function of discreteness, dissipation, and uncertainty in the junction critical current. The perturbing parameters are low in the simulations such that the solitons fit well to an ideal Sine-Gordon soliton. Surprisingly, using realizable parameters a single flux soliton in a DLJJ is found to travel hundreds of Josephson penetration depths without backscattering in the absence of a driving force. In addition, even with a non-ideal launch, solitons are found to propagate predictably such that they show potential for synchronous routing into reversible logic gates.

2:03PM Z39.00013 Long Time Electrical Stability of Plasma Oxidized Aluminum Tunnel Barriers, ZACHARY BARCIKOWSKI, JOSH POMEROY, National Institute of Standards and Technology, Gaithersburg, MD — By measuring resistance-area product values over time, we assess the electrical stability of tunnel junctions with plasma oxidized AlOx tunnel barriers. AlOx is a commonly used material in the superconducting qubit community due to its ease of fabrication, but often has a high density of electrically active defects. We believe that plasma oxidation, as opposed to the standard thermal oxidation, can lead to tunnel barriers with lower defect densities and improved electrical properties. This talk will present measurements taken on tunnel barrier devices taken over a period of months and correlate observed stability/instability with the process conditions used to fabricate them.

2:03PM Z39.00012 Flux Soliton Interactions in Coupled Long Josephson Junctions, WALTRAUT WUSTMANN, KEVIN D. OSBORN, Laboratory for Physical Sciences, College Park, MD — Flux solitons and long Josephson junctions are being studied as structures for energy-conserving reversible computing. The solitons in long Josephson junctions are generally described by the Sine-Gordon equation. Simulations have been performed on discrete long Josephson junctions (DLJJs), where the soliton extends over at least a few unit cells. We will report on the dissipation and mutual interaction of two solitons in separate DLJJs. Single fluxon dissipation in DLJJs is found to arise from junction damping as well as radiation loss created by discreteness and perturbed soliton oscillations. Dissipation of interacting solitons in coupled DLJJs will be compared to the single fluxon case.

2:15PM Z39.00014 Fluctuation-dissipation relations of a tunnel junction driven by a quantum circuit, DANIEL ESTEVE, OLIVIER PARLAVECCHIO, CARLES ALTIMIRAS, Service de Physique de l’Etat Condensé (CNRS URA 2464), IRAMIS, CEA Saclay, 91191 Gif-sur-Yvette, France, JEAN-RENE SOUQUET, PASCAL SIMON, INES SAFI, Laboratoire de Physique des Solides, Université Paris-Sud, 91405 Orsay, France, PHILIPPE JOYEZ, DENIS VION, PATRICE ROCHE, FABIEN PORTIER, Service de Physique de l’Etat Condensé (CNRS URA 2464), IRAMIS, CEA Saclay, 91191 Gif-sur-Yvette, France, NONELECTRONIC-QUANTRONICS GROUPS COLLABORATION, THEORY GROUP TEAM — We derive fluctuation-dissipation relations derived for classical forces hold, provided the effect of the circuit's quantum fluctuations is incorporated into a modified non-linear I(V) curve. We also demonstrate that all quantities measured under a coherent time-dependent bias can be reconstructed from their直流 counterpart with a photo-assisted tunneling relation. We confirm these predictions by implementing the circuit and measuring the dc current through the junction, its high frequency admittance and its current noise at the frequency of the resonator. Results available in arXiv:1409.6696.

Friday, March 6, 2015 11:15AM - 2:15PM –
Session Z41 DPOLY: Focus Session: Biopolymers II: Phase Behavior, Rheology, and Mechanics
11:15AM Z41.00001 Chirality-selected phase behavior in ionic polypeptide complexes, MATTHEW TIRELL, University of Chicago — We demonstrate that chirality determines the phase state of polyelectrolyte complexes formed from mixing dilute solutions of oppositely charged polypeptides. In these systems, the physical state of the resultant complex is determined by the combination of electrostatic and hydrogen bonding interactions. The formation of fluid complexes occurs when at least one of the polypeptides in the mixture is racemic, which disrupts backbone hydrogen bonding networks. Pairs of purely chiral polypeptides, of any form, sense compact, fibrillar solids with a β-sheet structure on mixing. Analogous behavior occurs in micellar cores formed from polypeptide block copolymers with polyethylene oxide, where microphase separation into discrete, self-assembled aggregates with either solid or fluid cores, and eventually into ordered phases at high concentrations, is possible. Chirality is an exploitable tool for manipulating material properties in systems based on polyelectrolyte complexation. Its role in these systems gives insight into polyelectrolyte complex phase behavior more broadly.

1This work was supported by the U.S. Department of Energy Office of Science Program in Basic Energy Sciences, Materials Sciences and Engineering Division.

11:51AM Z41.00002 Biomimetic Coacervate Environments for Protein Analysis, SARAH PERRY, Univ of Mass - Amherst, PATRICK MCCALL, SAMAVAYAN SRIVASTAVA, DAVID KOVAR, MARGARET GARDEL, MATTHEW TIRELL, University of Chicago — Living cells have evolved sophisticated intracellular organization strategies that are challenging to reproduce synthetically. Biomolecular function depends on both the structure of the molecule itself and the properties of the surrounding medium. The ability to simulate the in vivo environment and isolate biological networks for study in an artificial milieu without sacrificing the crowding, structure, and compartmentalization of a cellular environment, represent engineering challenges with tremendous potential to impact both biological studies and biomedical applications. Emerging experience has shown that polypeptide-based networks for study in an artificial milieu without sacrificing the crowding, structure, and compartmentalization of a cellular environment, represent engineering challenges with tremendous potential to impact both biological studies and biomedical applications. Emerging experience has shown that polypeptide-based coacervate-based systems are particularly attractive for use in biochemical assays because the compartmentalization afforded by liquid-liquid phase separation does not necessarily inhibit the transport of molecules across the compartmental barrier.
12:03PM Z41.00003 Molecular Rigidity and Entropy-Enthalpy Compensation in DNA Hybridization , JACK DOUGLAS, FERNANDO VARGAS-LARA, Materials Science and Engineering Division, NIST, Gaithersburg, MD 20899 — Entropy-enthalpy compensation (EEC) is a general and relatively poorly understood pattern in the energetic parameters governing both binding constants and relaxation processes in condensed matter. After defining the basic phenomenology, we focus on how polymer additives, chain confinement, chain length variation affect a well-studied molecular binding process, the hybridization of duplex DNA. Our study is based on a coarse-grained model of DNA that does treat water explicitly. We find that both crowding due to polymer additives and geometrical confinement lead to a change of the effective chain rigidity and that changes in DNA generally lead to a pattern entropy-enthalphy compensation in the DNA association similar to experimental observations. Modulation of the rigidity of binding sites by constraints associated with chain structure or environmental conditions can greatly influence both the location and cooperativity of molecular binding transition and the relative enthalpy and entropy contributions to the free energy of binding. Entropy-enthalpy compensation arises in numerous synthetic and biological molecular binding processes and we suggest that that changes in molecular rigidity might provide a common explanation of this ubiquitous phenomenon.

12:15PM Z41.00004 Spider Silks-Biomimetics Beyond Silk Fibers: Hydrogels, films & Adhesives from Aqueous Recombinant Spider Silk dopes: A Synchrotron X-Ray Nano-Structural Study , SUJATHA SAMPATH, University of Utah, JUSTIN JONES, THOMAS HARRIS, RANDOLPH LEWIS, Utah State University — With a combination of high strength and extensibility, spider silk’s (SS) mechanical properties surpass those of any man made fiber. The superior properties are due to the primary protein composition and the complex hierarchical structural organization from nanoscale to macroscopic length scales. Considerable progress has been made to synthetically mimic the production of fibers based on SS proteins. We present synchrotron x-ray micro diffraction (SXRD) results on new fibers and gels (hydrogels, lyogels) from recombinant SS protein water-soluble dopes. Novelty in these materials is two-fold: water based rather than widely used HFIP acid synthesis, makes them safe in medical applications (replacement for tendons & ligaments). Secondly, hydrogels morphology render them as excellent carriers for targeted drug delivery biomedical applications. SXRD results reveal semi-crystalline structure with ordered beta-sheets and relatively high degree of axial orientation in the fibers, making them the closest yet to natural spider silks. SXRD on the gels elucidate the structural transformations during the self-recovery process through mechanical removal and addition of water. Studies correlating the observed structural changes to mechanical properties are underway.

12:27PM Z41.00005 Seeing believes: Watching entangled sculpted branched DNA in real time , AH-YOUNG JEE1, JUAN GUAN, KEJIA CHEN, STEVE GRANICK, Univ of Illinois - Urbana — The importance of branching in polymer physics is universally accepted but the details are disputed. We have sculpted DNA to various degrees of branching and used single-molecule tracking to image its diffusion in real time when entangled. By ligating three identical or varying length DNA segments, we construct symmetric and asymmetric Y scaffolds. These constructs form gel-like phases of micelles arranged with cubic order at room temperature. A 10 base pair and a 25 base pair DNA ladder were used as samples in gel electrophoresis. The monotonically decreasing mobility with increasing length observed in the agarose separations is not observed in separations in Pluronics®. Rather, a complicated dependence of mobility on DNA length is observed, where mobility vs. length increases for short DNA molecules then decreases for longer molecules. There is also a variation of mobility with length correlated to the micelle diameter. Brownian dynamics simulations of a discrete wormlike chain model were performed to simulate short DNA molecules migrating in free solution and in a face-centered cubic matrix. By incorporating hydrodynamic interactions, the trend of simulated length-dependent mobility qualitatively agrees with experimental measurements.

12:39PM Z41.00006 DNA electrophoresis in tri-block copolymer gels—experiments and Brownian dynamics simulation , LING WEI, DAVID H. VAN WINKLE, Department of Physics, Florida State University — The mobility of double-stranded DNA ladders in Pluronics® P105, P123 and P127, was measured by two-dimensional gel electrophoresis. Pluronics® are triblock copolymers which form gel-like phases of micelles arranged with cubic order at room temperature. A 10 base pair and a 25 base pair DNA ladder were used as samples in gel electrophoresis. The monotonically decreasing mobility with increasing length observed in the agarose separations is not observed in separations in Pluronics®. Rather, a complicated dependence of mobility on DNA length is observed, where mobility vs. length increases for short DNA molecules then decreases for longer molecules. There is also a variation of mobility with length correlated to the micelle diameter. Brownian dynamics simulations of a discrete wormlike chain model were performed to simulate short DNA molecules migrating in free solution and in a face-centered cubic matrix. By incorporating hydrodynamic interactions, the trend of simulated length-dependent mobility qualitatively agrees with experimental measurements.

12:51PM Z41.00007 Injectable Self-Assembling Peptide Hydrogel: Effects of Hydrophobic Drug Encapsulation and Delivery , JESSIE SUN, BRANDON STEWART, ALISA LITAN, University of Delaware, SIGRID LANGHANS, Nemours Alfred I duPont Hospital for Children, JOEL P. SCHNEIDER, National Institute of Health, DARRIN J. POCHAN, University of Delaware — We successfully encapsulated and continuously delivered a hydrophobic drug over the course of a month at effective, significant concentrations in a beta-hairpin chain model were performed to simulate short DNA molecules migrating in free solution and in a face-centered cubic matrix. By incorporating hydrodynamic interactions, the trend of simulated length-dependent mobility qualitatively agrees with experimental measurements.

1:03PM Z41.00008 Anomalous diffusion dynamics of associating artificial proteins in hydrogels , SHENCANG TANG, MUZHOU WANG, BRADLEY OLSEN, Massachusetts Institute of Technology — Associative polymer gels have attracted a great deal of interest as responsive materials and biomaterials; while a great deal is known about their mechanical properties, knowledge about self-diffusion in these materials is still limited. Using coiled-coil proteins as a model associative polymer system where the number of stickers per polymer and molar mass of chains between stickers are exactly defined, we investigate self-diffusion in associative polymeric hydrogels using forced Rayleigh scattering on the length scales ranging from 0.3 to 50 μm. Although the presence of associative groups reduces the rate of diffusion, “superdiffusive” scaling is observed for the first time up to a length scale of 10 μm. Fickian diffusion is recovered at larger length scales. The anomalous diffusion strongly depends on the hydrogel concentration. We propose a simple two state model to capture the interplay between the diffusion of the proteins and the association of the coiled-coil segments. The model is able to both the anomalous regime and the Fickian regime, and provides estimation of the apparent diffusivities and the dissociation rates of the coiled-coil domains.

1:15PM Z41.00009 Physics of soft hyaluronic acid-collagen type II double network gels , SVETLANA MOROZOVA, MURUGAPPAN MUTHUKUMAR, University of Massachusetts — Many biological hydrogels are made up of multiple interpenetrating, charged components. We study the swelling, elastic diffusion, mechanical, and optical behaviors of 100 mol% ionizable hyaluronic acid (HA) and collagen type II fiber networks. Dilute, 0.05-0.5 wt% hyaluronic acid networks are extremely sensitive to solution salt concentration, but are stable at pH above 2. When swelled in 0.1M NaCl, single-network hyaluronic acid gels follow scaling laws relevant to high salt semidilute solutions; the elastic shear modulus $G^*$ and diffusion constant $D$ scale with the volume fraction $\phi$ as $G^* \sim \phi^2$ and $D \sim \phi^{4.1}$, respectively. With the addition of a collagen fiber network, we find that the hyaluronic acid network swells with rigid collagen fibers, providing extra strength to the hydrogel. Results on swelling equilibria, elasticity, and collective diffusion on these double network hydrogels will be presented.
heterogeneously. Stress autocorrelation and elongation results were analyzed as a function of the nano-filler concentration. Globally, as we increase the filler fraction, into fibrous structures. We observe the formation of a percolated nework of these fibrous structures, with ordered local structure but disordered short-range attraction between the nanofillers and polymer chain ends. The structure, dynamics and mechanics of this polymer gel was studied as function was studied by Molecular Dynamics simulation. Nanofillers were modeled as rigid bodies of disk-like shapes and crosslinks were simulated by introducing a...
11:27AM Z42.00002 Polymer Crowding and Depletion-Induced Interactions in Polymer-Nanoparticle Mixtures¹, WEI KANG LIM, ALAN DENTON, Dept. of Physics, North Dakota State University — Macromolecules in crowded environments, such as biopolymers (DNA, RNA, proteins) in biological cells or synthetic polymers in nanocomposite materials, adopt conformations that can differ substantially from those in unconfined spaces. In mixtures of nanoparticles and nonadsorbing (free) polymers, depletion of polymers induces effective interactions between the nanoparticles. Depletion-induced interactions in turn affect the structure and thermodynamic phase behavior of polymer-nanoparticle mixtures. Such interactions can drive bulk demixing and may be involved in compartmentalization of macromolecules in the cell nucleus. Within a coarse-grained model of hard-sphere nanoparticles and ellipsoidal polymer, we perform Monte Carlo simulations to compute polymer shape distributions², depletion-induced pair potentials, and pair distribution functions, and to explore demixing of polymer-nanoparticle mixtures in the protein limit. We compare our results with theoretical predictions and available experimental data.

¹This work was supported by the National Science Foundation under Grant No. DMR-1106331.

11:39AM Z42.00003 Depletion potential between nanoparticles: From small molecule liquids to dense polymer melts, DEBAPRIYA BANERJEE, KENNETH SCHWEIZER, University of Illinois at Urbana Champaign — An entropic depletion attraction generically exists between two hard spheres dissolved in a nonadsorbing fluid. PRISM integral equation theory is used to study this problem over an exceptionally wide range of polymer-particle size ratio and chain length (N) including the monomer limit. To mimic constant atmospheric pressure conditions, the dimensionless melt compressibility is fixed at realistic values and polymer density varied with N accordingly. At constant polymer size, the attractive contact minimum of the particle potential of mean force (PMF) scales roughly as particle radius. At fixed particle size, this contact minimum deepens logarithmically with N before generically saturating beyond a crossover N ≈ 150. The equilibrium aggregation behavior is dominated by this local feature. However, the PMF beyond contact has features (including repulsive barriers) of a spatial range and amplitude that vary non-monotonically with N which are most pronounced when the particle radius is of order the polymer radius of gyration, Rg. At fixed particle size, this implies a value of N exists that maximizes kinetic stabilization. A weak but long range (Rg-scale) component of the PMF is also found when the radius of gyration is smaller than, or comparable to, the particle radius.

11:51AM Z42.00004 Self-assembled chains of polymer-grafted nanorods in homopolymer films, CHRISTINA TING, Sandia Natl Labs, BORIS RASIN, RUSSELL COMPOSTO, University of Pennsylvania, AMALIE FRISCHKNECHT, Sandia Natl Labs — An understanding of the self-assembly of nanoparticles in a polymer matrix is needed to utilize their tunable optical and electrical properties. In particular, for anisotropic nanoparticles, the inter-particle distance and orientation are important variables to consider. Using self-consistent field theory (SCFT), we study the self-assembly of polymer-grafted nanorods in homopolymer melts of the same chemistry. The theoretical calculations are performed over a range of parameters for an experimental system of CdSe/CdS nanorods coated with polystyrene brushes of varying molecular weights. Previously, we have shown that polymer-grafted nanorods were found to transition from dispersed to aligned (side by side) as the matrix chain lengths were increased, depending also on the grafting density and the dimensions of the nanorods. Here, we explore the parameters required for end to end linking, where it has been shown that coupling of localized surface plasmon resonances in a chain of end-linked nanorods can result in a periodic array of enhanced electric fields (hot spots).

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12:03PM Z42.00005 Field-theoretic study on polymer-depletion interaction between colloids in solution, WEI LI, KRIS DELANEY, GLENN FREDRICKSON, Univ of California - Santa Barbara — Using field-theoretic simulations, we study the depletion interaction between colloidal particles in a solution of free block copolymers. Our system consists of two solid non-adsorbing plates and polymer solution in between. A field theory model formulated in the grand canonical ensemble is used for our simulations, and the potential of mean force between two colloids is computed by means of Derjaguin approximation. We begin the investigation with solvent that is neutral to the copolymer blocks. Several effects on the depletion interaction are considered, including surface affinity of the plates to the copolymer, and block copolymer architecture and composition.

12:15PM Z42.00006 Field Theoretic Simulations of Polymer Nanocomposites in the Presence of Adsorbing Block Copolymers¹, JASON KOISKI, ROBERT RIGGLEMAN, University of Pennsylvania — The immersion of nanoparticles in a polymer matrix has given rise to improved mechanical, electrical, and optical properties of polymer-based materials. Understanding the phase behavior and controlling the spatial distribution of nanoparticles in these systems plays a critical role in controlling the resulting material properties. Polymer field theory continues to play an important role in our understanding of polymeric materials, and recently we have extended the field theoretic framework to incorporate nanoparticles with arbitrary shape and surface grafting. In this talk, I will demonstrate some more recent extensions that incorporate local surface attraction either between nanoparticles or between the particles and a strongly adsorbing polymer, which could be important for systems where one block of the polymer has strong preferential interactions with the particle surface. Our approach enables the study of systems where many-body particle effects could become important and systems that can macro- or microphase separate while fully incorporating fluctuation effects.

¹NSF DMR-1410246

12:27PM Z42.00007 Theory and Simulation Studies of Effect of Entropic and Enthalpic Driving Forces on Morphology in Polymer Grafted Particle Filled Nanocomposites, TYLER MARTIN, Chemical and Biological Engineering - University of Colorado at Boulder, Chemical and Biomedical Engineering - University of Delaware, ARTHI JAYARAMAN, Chemical and Biomedical Engineering - University of Delaware, Materials Science and Engineering - University of Delaware — Polymer nanocomposites are a class of materials that consist of a polymer matrix embedded with nanoscale fillers or additives that enhance the inherent properties of the matrix polymer. To engineer polymer nanocomposites for specific applications it is important to have design rules that relate molecular features to morphologies of the composite. Using theory and simulation, we previously studied polymer nanocomposites with homopolymer grafted particles in a homopolymer matrix with chemically identical graft and matrix polymers. Specifically, we found that increasing the polydispersity in grafted chain lengths or decreasing the graft and matrix chain flexibility stabilizes the dispersed phase of polymer nanocomposites, due to increased wetting of the grafted layer by matrix chains. We now explore composites with chemically different graft and matrix polymers, that allow us to tune in enthalpic driving forces in addition to the entropic driving forces for particle dispersion/aggregation. We vary the grafting density, composition of the graft and matrix polymers, and strength of the attractive interactions between the grafts and matrix monomers, to study their impact on the phase behavior and structure of polymer grafted particles in a polymer matrix.
12:39PM Z42.00008 Disentanglement in polymer-star mixtures, HENDRIK MEYER, Institut Charles Sadron, CNRS UPR22, Strasbourg, France — Recent molecular dynamics simulations provide new insights to entangled polymer melts and mixtures with compact stars as a model system of nanocomposites without polymer-particle adsorption. The particle size is in the order of the tube diameter, the particles remain well dispersed over the whole concentration range and the stars are sufficiently compact that the pure system is jammed. For this system, we observe a weak compression of the matrix chains with increasing volume fraction of stars. Short (untangled) matrix chains get slowed down by adding particles to the system. When the matrix chains become significantly longer than the entanglement length, this trend is inverted and the matrix chains become faster because the particles dilute the entanglement network. The center-of-mass (CM) dynamics exhibits regimes of anomalous diffusion in accordance with viscoelastic hydrodynamic interactions (VHI) [1]. At low and intermediate star-particles concentration, the particles themselves vary little in mobility, only at high concentration (above percolation), they become slowed down because of colloidal packing. [1] J. Farago et al. PRL 107, 178301 (2011); PRE 85, 051807 (2012).

This work is supported by NSF Grant DMR-1309892.

1:03PM Z42.00010 Detailed atomistic simulations of functionalized graphene/polymer systems, PETRA BACOVA, ANASTASSIA RISSANOU, Institute of Applied and Computational Mathematics (IACM), Foundation for Research and Technology Hellas (FORTH), GR-70013, Heraklion, Crete, Greece, VAGELIS HARMANDARIS, Department of Mathematics and Applied Mathematics, University of Crete, GR-70013, Heraklion, Crete, Greece — Graphene structures produced by the reduction of the graphene oxide contain some oxygen percentage coming mainly from the carboxyl groups remained on the edges of the graphene. With the increasing importance of the graphene in the material science, here we draw our attention to the effect of these groups on the properties of the graphene-based materials. Molecular simulations can be a valuable tool for the study of such complex materials at the molecular level. We have performed detailed atomistic simulations of hybrid nanostructured polymer/graphene materials for different polymer matrices. We study the behaviour of polymer nanocomposites with three types of dispersed graphene: (a) the pure non-functionalized sheet, (b) graphene with hydrogens grafted on the edges and (c) carboxyl-functionalized graphene. Data concerning the structural and dynamical properties of the polymer chains are presented. In addition, we compute the dynamic properties of the particular graphene sheets and we discuss in detail the importance of the strong electrostatic interactions present in the systems. The information obtained on the molecular scale in our work contributes to the understanding of the miscibility and the mechanical properties of the graphene/polymer nanocomposites.

1:15PM Z42.00011 Surface Tension of Nano-Confined Lattice Polymers, PENGFEI ZHANG, QIANG WANG, Department of Chemical and Biological Engineering, Colorado State University — Surface tension at solid/liquid interface is a key concept in understanding many important surface and interfacial phenomena such as wetting and capillarity. It is, however, not trivial to accurately calculate surface tension in lattice Monte Carlo (LMC) simulations, which are much faster than simulations in continuum. Here we propose a novel, efficient, and accurate method for calculating the surface tension of polymers confined between two parallel and impenetrable surfaces in LMC simulations, and examine how surface tension varies with the degree of confinement (i.e., separation distance between the two surfaces). Direct comparisons between our LMC results and the corresponding lattice self-consistent field (LSCF) calculations also unambiguously and quantitatively reveal the fluctuation/correlation effects on surface tension neglected in LSCF theory. Keywords: Surface tension, lattice polymers, Monte Carlo simulations.

1:27PM Z42.00012 Polymer adsorption transition: Applications of the Wang-Landau and partition function zeros methods, MARK TAYLOR, SAMIP BASNET, Dept. of Physics, Hiram College, JUTTA LUETTMER-STRATHMANN, Dept. of Physics, University of Akron — The Wang-Landau (WL) algorithm is a Monte Carlo simulation technique providing a direct computation of the density of states (and thus the partition function) of a many-body system. The partition function encodes all thermodynamic information about a system, and thus, its construction allows for an efficient determination of phase behavior. Here we describe the application of the WL approach to the adsorption transition for both lattice [1] and continuum chains tethered to an attractive surface. We compute the canonical partition function for chains up to length \( N=1536 \) and analyze the zeros of these functions in the complex inverse-temperature plane. These zeros define a nearly closed circular region, centered on the origin, intersected near the positive real axis by two flaring tails. With increasing chain length the intersection point pinches down towards the positive real axis, dividing the real axis into two distinct regions or phases in accord with Yang-Lee theory. We apply finite size scaling theory for the leading partition function zeros to locate the adsorption transition in the thermodynamic limit and obtain values for the polymer crossover, order parameter, and specific heat exponents. \[1\] M.P. Taylor and J. Luettmerr-Strathmann, J. Chem. Phys., in press, (2014).

1:39PM Z42.00013 Molecular Simulation studies of adsorption of polymers on non-planar surfaces: Influence of surface characteristics, ABISHEK VENKATAKRISHNAN, University of Cincinnati, ANNE SHIM, Ohio State University, AQUIL FROST, Central State University, JOHN LEWNARD, VIKRAM KUPPA, University of Cincinnati — Molecular simulations are employed to investigate the adsorption of freely rotating polymer chains adsorbing on to non-planar surfaces. Adsorption studies on planar surfaces have been studied extensively and fairly well understood. However, in reality, surfaces are non-planar and cannot be represented using smooth surface models. We investigate the effect of surface characteristics on adsorption via molecular dynamics and Monte Carlo molecular simulations in the NVT ensemble. Both regular (uniform) and irregular (self-affine) roughness parameters are studied. The adsorbed polymer chains are characterized by density and orientation profiles, adsorbed fraction and chain topologies. Our results elucidate the extent to which surface roughness influences adsorption, in competition with other factors such as chain length and monomer-surface interaction. We also demonstrate how both adsorption and desorption can be controlled solely by tuning surface inhomogeneities.
streaming and the generation of higher harmonic oscillations. Both steady and time-harmonic flows are considered.

The entrance length is estimated from the exponential spatial decay of the lowest components, and/or velocity gradients are specified at the entrance boundary. The entrance length is estimated from the exponential spatial decay of the lowest

gradients, excess entry pressure, and vorticity. Various types of appropriate entrance conditions are identified in which combinations of pressure, velocity components, and/or velocity gradients are specified at the entrance boundary. The entrance length is estimated from the exponential spatial decay of the lowest normal-mode solution; the estimated entrance length is one-tube-radius for axisymmetric flow and two-tube-radii for non-axisymmetric flow. As a special case, the backbone methylene groups have a broad angular distribution and on average tilt along the surface plane, independent of tactility and temperature. We have compared the SFG results with theoretical spectra calculated using MD simulations and ab initio calculations.

2:03PM Z42.00015 Molecular-dynamics study of the Case-II diffusion of methanol in PMMA

11:15AM Z43.00001 Capillary Leveling of a Free-Standing Film

2:17PM Z43.00002 Visualization of the Flow Field induced by an Oscillating Post in a 2D Fluid Membrane

11:39AM Z43.00003 Time-harmonic Stokes Flow of a Newtonian Fluid in the Entrance Region of a Semi-infinite Circular Tube: Insights Involving the Estimation of Entrance Length and the Selection of Appropriate Entrance Boundary Conditions

Work supported by the Petroleum Research Fund of the American Chemical Society
11:51 AM Z43.00004 Effect of surface elasticity on the rheology of nanometric and micrometric liquids. ELISABETH CHARLAIX, Université Joseph Fourier Grenoble France — The rheological properties of liquids confined to nanometer scales are important in many situations, yet are still a widely debated topic. The change in bulk viscosity and apparition of visco-elasticity under confinement is a particularly controversial question. In this talk, we use a new approach for this problem by addressing the effect of the long-range elastic deformations of the confining surfaces on the liquid flow. This effect could help reconciling some discrepancies within the literature concerning the intrinsic mechanical behavior of nanometric liquids. In the case of a squeeze-flow geometry, we show that below a critical distance Dc, the liquid is clamped by its viscosity and its intrinsic properties cannot be disentangled from the global system response. The theoretical approach [1] is confirmed by nanorheology experiments [2, 3] on various simple liquids, using both very soft (PDMS) and very rigid (Pyrex) confining surfaces. In every case we demonstrate that the elastic deflections of the confining surfaces, even if they are of very small amplitude, can dominate the overall mechanical response of nanometric liquids confined between solid walls.


12:27PM Z43.00005 The Effect of Compression Frequency on the Collapse Dynamics of Langmuir Monolayers. JEREMY EATON, MICHAEL DENNIN, Univ of California - Irvine — We investigate the effects of compression speed and particle size on the collapse dynamics of an SDS-DODAB monolayer uniformly interspersed with fluorescent polystyrene nanoparticles ranging from 40 to 1000 nm in diameter. Folding and buckling are induced in the monolayer-particle system by compressing and expanding it between Teflon barriers which move at areal speeds ranging from 5 to 90 cm²/min. Video capture and fluorescence microscopy were used to image the monolayer over five compression-expansion cycles. Image processing is used to measure the surface particle density and is further used to characterize the number, structure and reversibility of the folds over time. These details provide insight on dynamics of monolayer collapse and will serve useful in determining the role folding plays in particle transport both within and across the monolayer interface.

We gladly acknowledge the support of NSF grant DMR-1309402.

12:39PM Z43.00006 Plateau-Rayleigh Instability and Capillary Droplet Propulsion on a Fiber. SABRINA HAEFNER, Saarland University, Experimental Physics, D-66041 Saarbruecken, Germany, MICHAEL BENZAQUEN, PCT Lab, UMR CNRS 7083 Gulliver, ESPCI ParisTech, PSL Research University, Paris, France, OLIVER BAEUMCHEN, Max-Planck Institute for Dynamics & Self-Organization (MPIDS), 37077 Goettingen, Germany, THOMAS SALEZ, PCT Lab, UMR CNRS 7083 Gulliver, ESPCI ParisTech, PSL Research University, Paris, France, ROBERT PETERS, McMaster University, Dept. of Physics & Astronomy, Hamilton, ON, Canada, JOSHUA D. MCGRAW, KARIN JACOBS, Saarland University, Experimental Physics, D-66041 Saarbruecken, Germany, ELIE RAPHAEL, PCT Lab, UMR CNRS 7083 Gulliver, ESPCI ParisTech, PSL Research University, Paris, France, KARI DALNOKI-VERESS, McMaster University, Dept. of Physics & Astronomy, Hamilton, ON, Canada — The Plateau-Rayleigh instability (PRI) of a liquid column underlies a variety of hydrodynamic phenomena. Compared to the classical case of a free liquid column, the description of a liquid layer on a fiber requires the consideration of the solid-liquid interface in addition to the free surface. We revisit the PRI of a liquid layer on a solid fiber by varying the hydrodynamic boundary condition at the fiber-liquid interface from no-slip to slip. We find that the growth rate depends on the system geometry and the boundary condition, which is in agreement with theory. In the late stages of liquid column breakup on slip-fibers, a three-phase contact line can be formed on one side of the droplet. The resulting capillary imbalance leads to droplet propulsion, which is studied as a function of temperature and molecular weight.

1 Graduate school GRK 1276, NSERC of Canada, German Research Foundation (DFG) under grant numbers BA3406/2 and SFB 1027.

12:51PM Z43.00007 Parametric study of Newtonian droplet entering smaller confinement— a numerical study. ZHIFENG ZHANG, Washington State Univ, JIE XU, University of Illinois at Chicago, XIAOLIN CHEN, Washington State Univ, COMPUTER AIDED ENGINEERING LAB TEAM, XU GROUP: MICROFLUIDICS LAB COLLABORATION — Model of droplet entering a micro-confinement has wide applications in either design of microfilter or understanding of biological process such as Circulating Tumor Cell metastasis/ capillary blockage et al. In present numerical study, we explore the transient behavior of soft matter being squeezed through a micro-confinement by Newtonian droplet model. Parameter study quantify the relation between squeezing pressure under different channel/droplet size, channel geometry influence (circular, square, triangular) and flow velocity variance.

1:03PM Z43.00008 Line tension and entropy in a liquid crystal Langmuir film. ELIZABETH MANN, PRITAM NANDAR, JOSEPH YARZEBINSKI, NABIN THAPA, Department of Physics, Kent State University, J. ADIN MANN, Department of Chemical Engineering, Case Western Reserve University — Often two or more phases coexist within a monolayer or bilayer: the connection between these and possible dynamic or static microdomains within cell membranes is still debated. The line tension associated with the boundary between two phases within a monolayer or bilayer controls the size distribution, shape, and dynamics of domains. Theoretical models for this energy remain relatively untested. This work considers a model fluid system, trilayer/monolayer coexistence within a Langmuir film. The line tension associated with the boundary between these phases is measured as a function of temperature over a large range (12-37°C). Compact, isolated trilayer domains are stretched from their equilibrium circular shape, and the free relaxation is analyzed with a hydrodynamic model previously tested by Wintersmith et al. [1] Line tension decreased with rising temperature. A careful treatment of the thermodynamics of the line boundary allow us to estimate the line entropy associated with the trilayer, and test possible models for the boundary.


1 CBET-0730475
2 Mechanical Engineering, KAUST, Thuwal, Saudi Arabia

1:15PM Z43.00009 Active nemato-hydrodynamics in toroidal microchannels. RICHARD GREEN, Instituut-Lorentz, Leiden University, JOHN TONER, Department of Physics and Institute of Theoretical Science, University of Oregon, VINCENZO VITELLI, Instituut-Lorentz, Leiden University — We investigate flow driven by activity in nematic and polar fluids confined in a toroidal geometry. Using a perturbative expansion in the activity strength, we obtain closed form analytic solutions for the activity-driven flow. A distinguishing feature of this system is that there is no critical threshold which the activity needs to overcome in order to initiate the flow; rather, the flow is a consequence of the combination of activity and curved geometry at any non-zero activity, however small.
1:27PM Z43.00010 Can a hard-sphere fluid feel the topology of a confining pore? 1 GERD SCHROEDERTURK, JOHANNES KNAUF, Friedrich-Alexander University Erlangen-Nuremberg, ROLAND ROTH, University Tuebingen, KLAUS MECKE, Friedrich-Alexander University Erlangen-Nuremberg — The confinement of simple fluids to narrow pore spaces changes the phase behaviour. A central question is the dependence of thermodynamic properties on the pore shape \( K \). The morphometric approach for simple fluids is derived by assuming that the grand potential \( \omega(K,\mu,T) \) on a functional of \( K \). Hadwiger's theorem states that \( \omega(K,\mu,T) \) only depends on \( K \) as a linear combination of the Minkowski functional, \( \Omega = -p(\mu,T)V(K) + q(\mu,T)A(K) + \kappa(\mu,T)C(K) + \gamma(\mu,T)K(K) \) where \( V \) and \( A \) are the volume and interface and \( C(K) \) the integrated mean curvature. \( X(K) \) is the Euler number that characterises the pore topology. We use density functional theory to demonstrate that this theory is consistent, for the case of triply-periodic network-like pore geometries. For these, the formula \( \langle X \rangle(K,\mu,T) = -\partial\Omega/\partial\mu \) can be inverted to give an estimate of \( X \) deduced from the simulated densities – the Euler number 'felt' by the fluid. We show that for the Primitive, Gyroid and Diamond minimal surfaces the obtained values are close to \( X \). Counter-intuitively, this result suggests that hard sphere fluids can feel topological properties of a confining space, in addition to geometric ones.

1:39PM Z43.00011 Controllable Coexistence of Multiple Instabilities on a Single Liquid Filament 1, MICHAEL HEIN, JEAN-BAPTISTE FLEURY, RALF SEEMANN, Saarland University — Droplet based microfluidics exploits the decay of a liquid filament or cylinder into droplets of micrometric size. While the physics of droplet breakup on small scales remains a field of vivid interest, droplet based microfluidics has become widely used both in fundamental science and application such as (bio-)analytics or micro-chemistry. We present experimental research on the formation of droplets by breakup of a squeezed liquid filament surrounded by an immiscible phase that flows over a topographic step. This non-equilibrium process arises from the interplay between flow properties and interfacial instabilities when the filament is suddenly released from confinement at the step. In contrast to previous studies, a rich variety of different droplet breakup regimes was observed for the used geometry which are characterized by the coexistence of multiple liquid instabilities on a single filament. Surprisingly, these instabilities can be of different type while the filament is exposed to a symmetric flow-field. This spontaneous symmetry breaking is a nontrivial consequence of volume throughput constraints of each individual instability and allows for the specific production of heterogeneous droplet families from one single filament under constant flow rates. (Submitted 2014)

1 Authors gratefully acknowledge the DFG-GRK1276 for financial support.

1:51PM Z43.00012 Ginzburg-Landau and Weakly Nonlinear Analysis of 3D Pillar Growth in NanoBenard Instability 1, CHENGZHE ZHOU, SANDRA TROIAN, California Institute of Technology, MC 128-95, Pasadena, CA — We examine the nonlinear response of a molten nanofilm subject to strong interface deformation and patterned growth by destabilizing thermocapillary forces and stabilizing capillary forces. The equation for the moving boundary describes 3D growth induced by large thermocapillary stresses in the long wavelength approximation. A bifurcation analysis via the method of multiple scales elucidates the influence of initial conditions, system geometry and material properties on the regimes describing stable and unstable flow. Investigation of the corresponding Ginzburg-Landau amplitude equation by finite element simulations reveals the existence of rich spatio-temporal phenomena. We will discuss how tightly ordered symmetric growth can arise from resonance effects induced by spatially periodic external forcing in analogy to behavior recently reported for the spatially forced version of the Swift-Hohenberg equation in 1- and 2- dimensions.


2:03PM Z43.00013 Influence of Film Thickness and Substrate Geometry on the Growth of Taylor Cones in Perfectly Conducting Films 1, THEODORE ALBERTSON, SANDRA TROIAN, California Institute of Technology, MC 128-95, Pasadena, CA — Liquid metal ion and droplet sources are finding application in many different fields ranging from high resolution focused ion beam imaging and lithography to space micropropulsion to nanofabrication and nanomanufacturing. These applications require ever improved understanding of the process by which Maxwell forces deform a smooth molten metal film into a liquid cusp known as a Taylor cone. While recent computational studies have elucidated how the cone-jet transition controls the mass and charge flux, less attention has been paid to the regime involving very thin coating films and how frictional effects influence the shape and timescale of the evolving conical elongations. We describe recent efforts in our group using moving mesh techniques to quantify the influence of substrate geometry and film thickness on the shape and formation of transient Taylor cones in perfectly conducting films. Our results appear to confirm self-similar exponents predicted theoretically upon onset of cone formation. Under certain conditions, we find not only Taylor cone formation at the tip of a sharp axisymmetric emitter but also Taylor coronal rings away the sharpest point. Such secondary formations can ultimately enhance mass and charge flux.

1 TGA acknowledges support from a NASA Space Technology Research Fellowship.

Friday, March 6, 2015 11:15AM - 1:03PM – Session Z44 GSNP GSÖFT: Focus Session: Jamming in Granular Media III 214D - Justin Burton, Emory University

11:15AM Z44.00001 Short time intermittency and long time plastic correlations in jammed systems 1, ARKA ROY, CMU, CRAIG MALONEY, NEU — Using numerical simulations of model amorphous, frictionless, soft discs, we study the effect of strain rates (\( \dot{\gamma} \)) and volume fractions (\( \phi \)) on the microscopic dynamics and plastic activity near, but above, the jamming point (\( \phi_j \)). Well above \( \phi_j \), at slow shear rate, the system responds in a highly intermittent way, reminiscent of other dynamically critical systems with a power law distribution of energy dissipation rates. With increasing \( \dot{\gamma} \) at fixed \( \phi \) or letting \( \phi \rightarrow \phi_j \) from above at a fixed rate, the intermittent behavior vanishes. All displacement distributions show non-Fickian behavior at short time crossing to Fickian behavior at longer times. Very surprisingly, the characteristic strain for that crossover is independent of \( \phi \). We also find that, despite the dramatic differences in the short time dynamics, the long time plastic rearrangements are essentially identical. Long-range spatial correlations in strain are cut off only by the size of the simulation cell.
11:27AM Z44.00002 Local origin of global contact numbers in frictional ellipsoid packings, FABIAN SCHALLER, University Erlangen-Nürnberg, Erlangen, Germany, MAX NEUDECKER, Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany, MOHAMMAD SAADATFAR, Applied Maths, RPPhysSE, ANU, Australia, GARY DELANEY, CSIRO, Clayton South, Victoria, Australia, GERD SCHRODER-TURK, University Erlangen-Nürnberg, Erlangen, Germany, MATTHIAS SCHROTER, Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — In particulate soft matter systems the average number of contacts $Z$ of a particle is an important predictor of the mechanical properties of the system. Using X-ray tomography, we analyze packings of frictional, oblate ellipsoids of various aspect ratios $\alpha$, prepared at different global volume fractions $\phi_l$. We find that $Z$ is a monotonically increasing function of $\phi_l$ for all $\alpha$. We demonstrate that this functional dependency can be explained by a local analysis where each particle is described by its local volume fraction $\phi_l$ computed from a Voronoi tessellation. $Z$ can be expressed as an integral over all values of $\phi_l$: $Z(\phi_l, \alpha, X) = Z_l(\phi_l, \alpha, X) \Phi(\phi_l) \Phi_l$. The local contact number function $Z_l(\phi_l, \alpha, X)$ describes the relevant physics in term of locally defined variables only, including possible higher order terms $X$. The conditional probability $\Phi(\phi_l)\Phi_l$ to find a specific value of $\phi_l$ given a global packing fraction $\phi_g$ is found to be independent of $\alpha$ and $X$. Our results demonstrate that for frictional particles a local approach is not only a theoretical requirement but also feasible.

11:39AM Z44.00003 Mechanical Response in Particulate Media, NIRANJAN WARNAKULASOROY, LEO SILBERT, Department of Physics, Southern Illinois University Carbondale, 62901, USA — We study the mechanical behavior of granular particle system in two dimensions in response to a dynamical intrusive or perturber simulations. We created mechanically stable granular packings of bidisperse discs with various coefficients of friction spanning several orders of magnitude and packing fractions in the vicinity above the critical packing fraction $\phi_c$. For each packing, we find the critical force $F_c$, the minimum force required to induce motion of a probe particle that we are trying to drag through the packing. Below the critical force the probe particle does not sustain continued motion. Just at the critical force, the probe particle moves through the system strongly intermittently. When the force is slightly larger than the $F_c$, the probe moves with well-defined average velocity. We find how the critical force and the average probe velocity depend on the packing pressure and particle fractions.

11:51AM Z44.00004 Rigidity percolation in generic and regular isostatic lattices, LEYOU ZHANG, D. ZEB ROCKLIN, Univ of Michigan - Ann Arbor, BRYAN CHEN, Institutus-Lorentz, Leiden University, XIAOMING MAO, Univ of Michigan - Ann Arbor — Rigidity percolation, the emergence of rigidity as bonds are randomly added to a structure, has been studied using various models, yielding a rich variety of behaviors including continuous/discontinuous transitions as well as mean field/analomalous scalings. Here we present our study of rigidity percolation in isostatic lattices, which are at the verge of mechanical instability and thus adding a vanishing fraction of next-nearest-neighbor bonds ("braces") can rigidify the lattice. However, we find that how the lattice rigidifies as braces are added depends on the lattice architecture in interesting ways. We study this problem in both regular (periodic lattices) and generic (sites are randomly moved, keeping only the topology of the connectivity) versions of isostatic square and kagome lattices via simulation. We discover that (1) rigidity percolation in generic isostatic lattices is discontinuous, with a sudden emergence of a rigid bulk, before which no stress can appear, sharing intriguing similarities with jamming, and (2) regular isostatic lattices, in contrast, show mixed features of continuous and discontinuous transitions. We propose analytic theories to explain our observations.

12:03PM Z44.00005 Experimental avalanches in a two-dimensional rotating drum: Universal- ity or a first-order phase transition?1, ALINE HUBARD, CUNY Graduate Center and Levich Institute and Physics Department of City College of New York, COREY O’HERN, Department of Mechanical Engineering & Materials Science, Department of Applied Physics, and Department of Physics, Yale University, MARK SHATTUCK, CUNY Graduate Center and Levich Institute and Physics Department of City College of New York — We study experimentally the dynamics of steel spheres in a quasi-two dimensional rotating drum to investigate whether avalanches occur as continuous or first-order transitions. In our experiments, monodisperse steel spheres are confined within a cylindrical region between the glass walls of the drum, and the drum rotation axis is perpendicular to the direction of gravity. The drum and spheres first rotate as a solid body, and the slope of the sphere packing increases until the packing becomes unstable. The avalanche proceeds until the system finds another stable packing. Using high-speed video, we track the particle displacements during each avalanche to quantify the statistics of the avalanche sizes and durations as a function of the rotation rate and particle size distribution. We find that the avalanche size and duration distributions display power-law scaling over several decades, which suggests universal behavior in this system.

12:15PM Z44.00006 Mean-field approach for random close packings of non-spherical and adhe- sive particles, ADRIAN BAULE, School of Mathematical Sciences, Queen Mary University of London, ROMAIN MARI, Levich Institute, City College of New York, LIN BO, LOUIS PORTAL, Levich Institute and Physics Department, City College of New York, WENWEI LIU, SHUIQING LI, Department of Thermal Engineering, Tsinghua University, HERNAN MAKSE, Levich Institute and Physics Department, City College of New York — Random packings of objects of a particular shape are ubiquitous in science and engineering. However, such jammed matter states have eluded any systematic theoretical treatment due to the strong positional and orientational correlations involved. Here, a mean field theory based on a statistical treatment of the Voronoi volume is presented, which allows for the calculation of the random close packing of spherical as well as non-spherical hard particles. The extension of the framework to packings of adhesive particles is discussed. A phase diagram is presented that describes non-spherical and adhesive particles in terms of analytic continuations from the spherical random close packing.

12:27PM Z44.00007 Jamming aids jumping in granular media, JEFFREY AGUILAR, Georgia Tech School of Mechanical Engineering, ANDRAS KARSAI, DANIEL L. GOLDMAN, Georgia Tech School of Physics — Little is known about the impulsive force and flow fields generated during jumping on granular media. We use a simple robot jumping on poppy seeds to explore maneuvers that induce jammed (non-yielding) states, and find sensitive dependence of jumping performance to movement strategy. On loose packings (volume fraction $\phi \approx 0.57$), a preliminary hop followed by a delay ("delayed stumper jump") improves the height of a push-off maneuver ("single jump"). Constant speed intruration force measurements suggest that reentry of the foot during the preliminary hop reintroduces surface resistance. An optimal delay time ($t \approx 5$ ms) leads to maximal jump heights, while a short delay time ($t \approx 0$ ms) produces the lowest jumps. Velocimetry of grain flow reveals that non-delay stutters induce fluid-like granular states into which the robot sinks before jamming occurs, lowering jump heights. While simulations of single and delayed stumper jumps are well described using a frictional (depth dependent) plus drag (velocity dependent) penetration resistance, this model does not capture stumper jump performance at low $\phi$. However, addition of an added mass term improves agreement, signaling the need for a more complex reactive force theory in impulsively forced granular media.

12:39PM Z44.00008 Exploring the Bernoulli effect on airfoils in a granular flow, YASIN KARIM, ERIC CORWIN, University of Oregon — The Bernoulli effect describes the decrease in pressure that results from a fluid accelerating over an airfoil. While granular materials lack many of the features of fluids (i.e. they are compressible, do not have a well-defined viscosity, and are non-cohesive) they nonetheless can be made to flow. We report experiments carried out on cylindrical Bernoulli lift in granular flows as a function of flow speed, density, airfoil shape. Using velocimetry and force sensors we probe the existence of a Bernoulli lift on an airfoil as glass beads flow around it in a quasi-two dimensional system.
Non-crystalline states in a 2D dusty plasma. Juan-Jose Liетor-Santos, Caо Cong, Justin Burton, Emory University — When suspended in a plasma, colloidal particles become negatively charged due to a preponderance of collisions with free electrons. If the plasma is weakly-ionized, the resulting repulsive electrostatic forces cause the particles to self-organize into a single 2D layer in the plasma sheath near a surface. At high concentrations and particle charging, a hexagonal crystalline lattice is formed which supports the propagation of underdamped, phonon-like waves. This "dusty plasma" is an ideal model system to study low-temperature dynamics in solids, where the individual particle motions can be visualized and tracked [1]. We have reported the creation of non-crystalline states in a dusty plasma by combining two particle species of different size and material density. By finely-tuning these variables, we show that both particle populations lie in the same plane, leading to a 2D amorphous structure which can be used to study the dynamics of glassy and jammed systems at low temperatures and frequencies.


Friday, March 6, 2015 11:15AM - 2:03PM –
Session Z45 DPOLY: Porous Media, Fibers, and Flow 216AB - Jonathan Brown, Ohio State University

11:15AM Z44.00009 Non-crystalline states in a 2D dusty plasma. Juan-Jose Liетor-Santos, Caо Cong, Justin Burton, Emory University — When suspended in a plasma, colloidal particles become negatively charged due to a preponderance of collisions with free electrons. If the plasma is weakly-ionized, the resulting repulsive electrostatic forces cause the particles to self-organize into a single 2D layer in the plasma sheath near a surface. At high concentrations and particle charging, a hexagonal crystalline lattice is formed which supports the propagation of underdamped, phonon-like waves. This "dusty plasma" is an ideal model system to study low-temperature dynamics in solids, where the individual particle motions can be visualized and tracked [1]. We have reported the creation of non-crystalline states in a dusty plasma by combining two particle species of different size and material density. By finely-tuning these variables, we show that both particle populations lie in the same plane, leading to a 2D amorphous structure which can be used to study the dynamics of glassy and jammed systems at low temperatures and frequencies.


11:27AM Z45.00002 Enhanced Methanol Diffusion in Homogeneous Isotropic and Anisotropic Silica Aerogels1. Jongseop A. Lee, YiZhou Xin, A.M. Zimmerman, Northwestern University, Evanston, IL 60208, Yang Shen, Tongji University, Shanghai, China, 200092, William Halperin, Northwestern University, Evanston, IL 60208 — It has recently been shown that the ballistic mean free path of silica aerogels can be directly measured by measuring diffusion of adsorbed fluids that are in fast exchange with vapor state using nuclear magnetic resonance [1-2]. With this technique we have studied the effect of compression on the mean free path of radially shrunken and isotropic silica aerogels with 98% porosity. We have found unusual behaviors of pore geometry as a function of compression. Our preliminary findings suggest that the average pore geometry and the corresponding anisotropy thereof do not follow classical stress-strain relations suggesting more complex mechanism is at play.

1This work was supported by the DOE BES under grants No. DE-FG02-05ER46248.
11:39AM Z45.00003 Diffusive and Rotational Dynamics of Condensed n-H2 Confined in MCM-411. Paul Sokol, Matthew Bryan, Indiana University, Timothy Prisk, Oak Ridge National Laboratory — We report neutron scattering studies of the condensed phases of normal-hydrogen confined within MCM-41. This is a high surface area, mesoporous silica glass with a narrow pore size distribution. The neutron scattering data suggests a picture of condensed normal-hydrogen within small mesopores in which the adsorbed hydrogen may be conceptually divided into an interfacial layer and the inner core volume. Preferential adsorption of ortho-hydrogen makes the interfacial layer rich in ortho-hydrogen, while the inner core volume consists of a depleted mixture of ortho- and para-hydrogen. In the liquid state, the hydrogen molecules making up the interfacial layer are immobile and tightly bound to adsorption sites, unable to diffuse on picosecond time scales. Molecules within the inner core volume undergo liquid-like jump diffusion, but with residence times much longer than the bulk liquid. In the solid state, only the hydrogen molecules occupying the inner core volume show the free quantum rotor behavior characteristic of the bulk crystal. The ortho-hydrogen molecules bound to the pore walls experience an orientational hindering potential which perturbs their rotational energy levels. Comparison with Vycor suggests the pore walls of MCM-41 are smoother on the atomic-scale.

1This report was prepared under award 70NANB10H255 from the National Institute of Standards and Technology (NIST), U.S. Department of Commerce. The statements, findings, conclusions, and recommendations are those of the authors and do not necessarily reflect the views of the NIST or the U.S. Department of Commerce.

11:51AM Z45.00004 Moleculely thin metal organic framework (MOF) film at air-water interface: Fabrication and buckling under compression1. Pritim Mandal, Sahraoui Chaieb, King Abdullah University of Science and Technology (KAUST), Thuwal, KSA — A metal organic framework (MOF) - a hybrid of inorganic (metal) nodes and organic linkers - is an emerging class of highly crystalline porous materials that provide an extremely high surface area/volume ratio making them very suitable candidates in selective separation, filtration and storage of gases. Though MOFs are usually produced as powders, for many applications such as selective gas separation and filtration, MOFs as flat membrane is the most appropriate candidate. To our knowledge no large-scale fabrication of 2D MOFs has been reported. In this work, we prepared large area MOF film at an air/water interface and employed Brewster angle microscopy (BAM) to directly image the film-formation (surface pressure during and after the film-formation was tracked, although this measurement for a solid film is not accurate due to the elasticity of the film). Metal-ligand coordination was confirmed through FTIR results. Surface morphology as seen via scanning electron microscopy (SEM) shows the film was smooth over several hundred microns. Finally, we discuss the buckling/fracture of the MOF film due to compression by two symmetrically movable barriers, which hinted to the existence of a solid molecular thin film.

1King Abdullah University of Science and Technology (KAUST), Thuwal, KSA

12:03PM Z45.00005 Mechanism of breakup of electrospun jet at the nozzle. Kostya Kornev, Vladislav Vekselman, Gilles Mohl, Clemson University. Department of Materials Science & Engineering Team — In the electrostatic formation of nanofibers, a high voltage is applied to a polymer solution to withdraw it through the nozzle as a jet. We report on an interesting instability leading to the jet breakup right at the supporting meniscus making the generation of sequential jets sporadic and inconsistent. The conventional electrospinning setup was modified to provide visualization of the meniscus inside the nozzle. A glass capillary was used as a nozzle. A wire connecting a high-voltage power supply was inserted into a tube and secured inside the glass capillary. The end of the wire was positioned far away from the free end of the glass capillary where meniscus was formed. In this method, the body of polymer solution was held at the same potential. Using fluorescence microscopy it was observed that meniscus is very sensitive to the applied voltage and is able to move inside the nozzle as the voltage increases. As meniscus moves inside the nozzle, it forms a liquid film leaning to the inner wall of the nozzle. This film connects meniscus and the jet. The jet breakup is caused by the thinning and rupturing of this film. A simple scaling model showing interplay between the capillary pressure and Maxwell stress is proposed and used to explain the jet instability.
12:15PM Z45.00006 Atomic scale images of polyvinylidene fluoride nanofibers by electron microscopy1. DARRELL RENEKER, University of Akron, CHRISTIAN KISIELOWSKI, Lawrence Berkeley National Laboratory, GEORGE CHASE, DINESH LOLLA, JOE CORSE, University of Akron — Atomic scale electron micrographs of polyvinylidene fluoride (PVDF) molecules in thin (∼ 3 nm) nanofibers revealed twist around the axes of molecular chains, small relative motions of adjacent molecular chains and many other structural and dynamical phenomena. The positions and relative motions of CF2 groups, spaced 0.25 nm apart, on (PVDF) molecules, were followed along polymer segments. Atomic scale, aberration corrected electron microscopy is presently at its best when the sample is less than about 3 nanometers thick. Conformations of segments of polymer molecules, and the relations between more ordered and less ordered segments are displayed in this thickness range. The TEAM 0.5 aberration corrected microscope at the Lawrence Berkeley Laboratory “Molecular Foundry,” was used to create hundreds of high magnification images of PVDF molecules in nanofibers, at electron doses much smaller than the doses that produce extensive chain scission or other such chemical changes in the molecules. A commonly held view, that useful high magnification electron micrographs of polymer molecules cannot be obtained without causing overwhelming changes to the molecule, is misleading.

1Support from Coalescence Filtration Nanofiber Consortium.

12:27PM Z45.00007 Flow in wavy walled microchannels, RAGHAVI RAO, PUSHPAVANAM S, IIT Madras — Improving the efficiency of mass transfer processes in microchannels is of significance in many applications. Here the flow is primarily laminar and mass transfer occurs by diffusion. Making the surface of the channel rough allows us to induce convection in transverse directions to the flow. In this work, we will study the effect of periodically varying surface of a channel wall using a perturbation solution. The modification in the velocity profile and its effect on improving mass transfer will be analyzed. The analysis will be illustrated for the case of extraction of a solute from one liquid phase to another. The effect of various parameters like surface tension, density ratio and viscosity ratio of the fluids will be studied and the regions in parameter space where a significant improvement in performance is expected will be determined. The results of the perturbation series solution will be compared with numerical results. Two cases, that of a constant and a deformed interface between the liquid phases, will be analyzed.

12:39PM Z45.00008 Micropillar sequence design for inertial fluid flow sculpting1, DANIEL STOECKLEIN, BASKAR GANAPATHYSUBRAMANIAN, Iowa State University, CHUEH-YU WU, DINO DI CARLO, University of California at Los Angeles — New methods for controlling fluid flow in microchannels make use of inertial fluid flow deformation around pillar structures spanning the height of the channel. A small set of micropillar sizes and locations has been shown to produce a rich phase space with a wide variety of flow transformations, demonstrating the untapped wealth of possibilities in this fluid flow manipulation scheme. Previous work has successfully demonstrated the potential, with experimental validation, for manual hierarchical design where sequences of pillars are stacked to create flow sculpting. But such a method is not ideal for seeking out complex sculpted flows where the search space quickly becomes too large for efficient manual construction. This is further complicated by the non-uniqueness of pathways to a desired fluid transformation, and the effect of diffusion as the number of micropillars increases. We formulate the inertial fluid flow transformation as a set of state transition matrix operations. This allows rapid simulation of different design configurations, enabling efficient optimization over a large search space. We show how this framework can be used for novel fluid sculpting targets with application in microelectronics and medical diagnostics, and also show validation via confocal imaging.

1This research is supported in part by the National Science Foundation through XSEDE resources provided by TACC under grant number TG-CTS110007 and supported in part by NSF-1306866, NSF-1307550, and NSF-1149365.

12:51PM Z45.00009 Three-dimensional microstreaming flows1, BHARGAV RALLABANDI, Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, ALVARO GOMEZ-MARIN, MASSIMILIANO ROSSI, Institute of Fluid Mechanics und Aerodynamics, Bundeswehr University Munich, CHENG WANG, Mechanical and Aerospace Engineering, Missouri University of Science and Technology, CHRISTIAN KAEHLER, Institute of Fluid Mechanics und Aerodynamics, Bundeswehr University Munich, SASCHA HILGENFELDT, Mechanical Science and Engineering, University of Illinois at Urbana-Champaign — Streaming due to acoustically excited bubbles has been used successfully for applications such as size-sorting, trapping and focusing of particles, as well as fluid mixing. Many of these applications involve the precise control of particle trajectories, typically achieved using cylindrical bubbles, which establish planar flows. Using astigmatic particle tracking velocimetry (APTV), we show that, while this two-dimensional picture is a useful description of the flow over short times, a systematic three-dimensional flow structure is evident over long time scales. We demonstrate that this long-time three-dimensional fluid motion can be understood through asymptotic theory, superimposing secondary axial flows (induced by boundary conditions at the device walls) onto the two-dimensional description. Beyond microbubble streaming, this leads to a general framework that describes three-dimensional flows in confined microstreaming systems, guiding the design of applications that profit from minimizing or maximizing these effects.

1We acknowledge support by the National Science Foundation for this work under grant number CBET-1236141.

1:03PM Z45.00010 Retarded desorption from porous media caused by wetting/dewetting of the external surface, THOMAS LEE, BENOIT COASNE, ROLAND J.-M. PELLENOQ, FRANZ-JOSEF ULM, Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA, LYDÉRIC BOCUET, Laboratoire de Physique Statistique, École Normale Supérieure, Paris, France, MULTISCALE MATERIAL SCIENCE FOR ENERGY AND ENVIRONMENT COLLABORATION1 — Despite the increasing attention devoted to nanofluidics, the role of external surfaces on transport in nanopores has not been fully investigated. Here, we report molecular dynamics simulations showing that methane recovery from a hydrophobic nanoporous membrane is retarded by the presence of liquid water at the external surface. Despite the pressure gradient used to trigger methane desorption and the hydrophobicity of the membrane, methane remains trapped for long times until water desorbs from the external surface. Using umbrella sampling calculations, we show that this retardation effect is induced by the free energy cost of dewetting the external surface as water is replaced by an adsorbed methane film. To account for this effect, we propose a simple thermodynamic model which describes the increase in free energy during extraction (dominated by the large methane-water surface tension). We also extend our approach to hybrid external surfaces made up of hydrophilic/hydrophobic regions, and consider fluids other than water (CO2), as these are relevant to practical applications such as gas/oil recovery from shale. Such retarded processes also have implications for transport in nanofluidic systems and adsorption/transport in solid catalysts, chromatographic devices, etc.

1CNRS/MIT, UMI 3466, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge
The sorting process is passive and relies on large forces induced by the streaming flow that lead to particle migration across streamlines. While a thresholded size sorting can be understood from simple arguments about the uniaxial stretching, we show that more sophisticated size separation is achievable through a better understanding of the flow at short time scales. We present experimental data (high-speed videography) and theoretical analysis (asymptotic description of the flow fields) that show how particles undergo significant migration and separation on time scales ranging from milliseconds to microseconds, and on length scales of about 10 μm. The highly tunable experimental set-up and the accurate analytical description of the flow field make this system an extremely fast and versatile device for applications ranging from flow cytometry to lab-on-a-chip micromanipulation.

We acknowledge support by the National Science Foundation for this work under grant number CBET-1236141.

**1:15PM Z45.00011 Particle Migration and Sorting in Microbubble Streaming Flow*** SASCHA HILGENFELDT, RAQEEB THAMEEM, BHARGAV RALLABANDI, RUI YANG, Mechanical Science and Engineering, University of Illinois at Urbana-Champaign — Ultrasonic driving of sessile semicylindrical bubbles results in powerful steady streaming flows that are robust over a wide range of driving frequencies. In a microchannel, this flow field pattern can be fine-tuned to achieve size-sensitive sorting and trapping of particles at scales much smaller than the bubble itself. The sorting process is passive and relies on large forces induced by the streaming flow that lead to particle migration across streamlines. While a thresholded size sorting can be understood from simple arguments about the uniaxial stretching, we show that more sophisticated size separation is achievable through a better understanding of the flow at short time scales. We present experimental data (high-speed videography) and theoretical analysis (asymptotic description of the flow fields) that show how particles undergo significant migration and separation on time scales ranging from milliseconds to microseconds, and on length scales of about 10 μm. The highly tunable experimental set-up and the accurate analytical description of the flow field make this system an extremely fast and versatile device for applications ranging from flow cytometry to lab-on-a-chip micromanipulation.

**1:27PM Z45.00012 ABSTRACT WITHDRAWN —**

**1:39PM Z45.00013 Effects of the uniaxial elongation of a polymer/CNT fiber on its electrical properties**, HYUN WOO CHO, BONG JUNE SONG, Department of chemistry, Sogang University, Seoul 139-701, Republic of Korea — We elucidate the effects of the uniaxial elongation of a polymer/CNT fiber on its electrical properties. Polymer fibers containing conductive nanofillers (such as carbon nanotubes (CNTs), and silver nanoparticles) have been utilized extensively for fabricating various forms of stretchable electronics including artificial muscles or electric conductive fabric. The electric conductivity of the polymer fiber usually decreases when it is stretched along the fiber axis, which would limit the scope of application. In addition, the reason and mechanism of decrease in the electrical conductivity remain elusive. In this work, we employ a coarse-grained model for the polymer/CNT fiber, and obtain the configurations of the fiber with respect to the strain via dynamic Monte Carlo (MC) simulations. Using global tunneling network (GTN) model, we calculate the electric conductivity as a function of strain. We find that the electric conductivity decreases during the elongation of the polymer/CNT fiber as was in experiments. We also find from tunneling network diagrams and critical path approximation (CPA) that the topological structure of the electrical network of the CNTs changes collectively during the elongation, which is responsible for the reduction of the electrical conductivity.

**1:51PM Z45.00014 High thermal conductivity polymers**, MORTAZA SAEIDIJAVASH, Graduate Student at University Of Oklahoma, Department of Aerospace and Mechanical Engineering, JIVTESH GARG, University of Oklahoma — In this work we investigate the effect of mechanical stretching on polymer thermal conductivity. Polymer materials are used as electrical insulators, but their poor thermal conductivity also makes them thermal insulators making removal of heat generated in such electronic systems challenging. Enhancement of polymer thermal conductivity can allow for better thermal management including design of low cost heat sinks and compliant thermal interface materials. Stretching is known to induce alignment of molecular chains in a polymer system increasing thermal conductivity. In this work we explore this idea by mechanically stretching ultra-high molecular weight (UHMW) polyethylene bars using a tensile load cell. The in-plane thermal conductivity of stretched polymer is measured using laser-flash method. We have measured thermal conductivity enhancement of almost 100% for stretch ratios of 6 to 10. These results are consistent with previous studies of thermal conductivity enhancement through such stretching. Ways to chemically achieve this molecular alignment are being explored using techniques of spin coating and electrospinning.

Friday, March 6, 2015 11:15AM - 2:15PM
Session Z46 DBIO: Invited Session: Mechanical Interactions and Pattern Formation in Multi-cellular Systems 217A - Ingmar Riedel-Kruse, Stanford University

**11:15AM Z46.00001 Tissue mechanics and dynamics during development**, FRANK JULICHER, Max Planck Institute for the Physics of Complex Systems — The fly wing is an important model system for the study of tissue dynamics during development. During pupal stages, the early fly wing undergoes a spectacular dynamic reorganization that involves cell flows, cell divisions and cell shape changes. In this dynamic process, the final shape of the wing is generated. We characterize tissue remodelling by the contributions of specific cellular processes such as cell shape changes and cell neighbour exchanges to macroscopic shear at different times. We discuss the dynamics and the mechanics of this dynamic tissue using an active medium theory that captures the essential physics of tissue remodelling. Our work suggests that local tissue contraction together with anisotropic active processes drive tissue remodelling in the fly wing. This process is guided by external stresses mediated via elastic attachments of the tissue to an external scaffold. We test our model by experiments in which perturbations are imposed by laser ablation or by mutant conditions.

**11:51AM Z46.00002 Spatiotemporal control of the forces that drive cell rearrangements within multicellular tissues**, KAREN KASZA, Sloan Kettering Institute — The local rearrangements of cells within multicellular tissues are actively driven by forces generated in the actin-myosin cytoskeleton. During development, these forces are patterned to bias or orient cell rearrangements, resulting in changes in tissue shape and structure that build functional tissues and organs. We use the fruit fly embryo as a model system, where polarized patterns of myosin activity are required for oriented cell rearrangements that drive rapid tissue elongation along the head-to-tail axis. To uncover mechanisms of how active, myosin-generated forces drive cell rearrangement, we quantify how perturbations to myosin activity influence the number, speed, and orientation of rearrangements. First, to investigate microscopic mechanisms by which myosin drives contraction of cell edges to initiate rearrangement, we generated myosin variants predicted to alter the speed at which myosin translocates actin filaments. These myosin variants display slowed turnover dynamics at cell edges and result in decreased numbers of cell rearrangements, indicating a role for myosin-driven actin sliding during rearrangement. Next, to study how myosin activity levels influence cell rearrangements, we generated myosin variants that mimic the active, phosphorylated state of myosin. These variants accelerate rearrangements but, surprisingly, also alter the spatial pattern of forces in the tissue and result in reduced tissue elongation. These myosin variants increase the rate of cell edge contraction but cause defects in the formation of new contacts between cells. Finally, we discuss how higher-order, collective cell rearrangements called rosettes are influenced by these perturbations to myosin activity. This work is in collaboration with D. Farrell and J. Zallen at the Sloan Kettering Institute.
12:27PM Z46.00003 Cell mechanics and non-genetic developmental defects. M. SHANE HUTSON, Vanderbilt University — Genetic mutations are not the only, nor necessarily the most prevalent route to misregulation of morphogenesis. In fact, remarkably specific developmental defects can be caused by non-specific environmental stress — e.g., heat shock, anoxia or chemical exposure. I will discuss one example from Drosophila embryos in which the funneling from broad-spectrum insult to specific developmental defects can be traced to cell and tissue mechanics. In particular, I will discuss heat shocks applied to Drosophila embryos at the onset of gastrulation. These lead to common developmental defects in head involution and germ band retraction — the latter phenocopying U-shaped mutants. Although these heat shocks induce a wide range of transient effects — on protein synthesis, cytoskeletal structures, and the cell cycle — morphogenetic movements resume after heat shock and proceed nearly normally for several hours. Then, four to ten hours after heat shock, dramatic holes open between cells in the amnioserosa, disrupting the integrity of this monolayer epithelium. The presence of holes in the amnioserosa at this stage (germband extension) is highly correlated with later defects in retraction of the germ band — a tissue adjacent to the amnioserosa. This observation begs two questions: (1) how does heat-shock of the entire embryo lead to mechanical disruption of this specific tissue; and (2) how does this mechanical disruption lead to morphogenetic defects in adjacent tissues? Using a combination of quantitative live imaging, laser-micsurgery, FRAP and computational models, we find answers to both questions in the underlying cell- and tissue-level mechanics.

1:03PM Z46.00004 Surface cell expansion drives radial cell intercalations in zebrafish gastrulation. CARL-PHILIPP HEISENBERG, IST Austria — Radial cell intercalations are commonly associated with tissue spreading in many developmental and disease-related processes. Yet, how radial cell intercalations are controlled and function in tissue spreading remains unknown. Here, we use a combination of experiments and theory to analyze radial cell intercalations during doming, the initial spreading of the blastoderm over the yolk cell at early zebrafish gastrulation. Strikingly, we found that radial cell intercalations do not drive doming, but rather determine the viscous relaxation behavior of the blastoderm in response to tissue surface tension (TST)-driven deformation. We further show that radial cell intercalations and, consequently, doming are triggered by surface epithelial cells expanding their surface area and thus reducing TST. Thus, radial cell intercalations are required for translating changes in tissue-scale forces into tissue deformation.

1:39PM Z46.00005 Glass transition originating from a rigidity transition in confluent biological tissues. DAPENG BI, Syracuse University — Cells must move through tissues in many important biological processes, including embryonic development, cancer metastasis, and wound healing. Often these tissues are dense and a cell’s motion is strongly constrained by its neighbors, leading to glassy dynamics. Although there is a density-driven glass transition in self-propelled particle (SPP) models for active matter, these cannot explain liquid-to-solid transitions in confluent tissues, where there are no gaps between cells and the packing fraction remains fixed and equal to unity. We have recently described a different type of rigidity transition that occurs in confluent tissue monolayers in the limit of vanishing cell motility, where the onset of rigidity is governed by changes to single-cell properties such as cell-cell adhesion and cortical tension. Here we alter the model to include cell motility using an equation for polarization similar to those in SPP models. We identify a glass transition line that originates at the critical point of the rigidity transition, and compare the results to an analytic trap model. The model provides a novel signature for mechanical behavior in confluent tissues, which has been successfully tested in experimental systems. I will also demonstrate that this model provides a framework for studying the Epithelial-to-Mesenchymal transition in cancer invasion and cell sorting during embryonic development.

Friday, March 6, 2015 11:15AM - 2:15PM — Session Z47 DBIO: Physics of Genome Organization 217B - Alexandre Morozov, Rutgers University

11:15AM Z47.00001 The Stochastic Signature of Mixed Promoter States. LEONARDO SEPULVEDA, Department of Biochemistry and Molecular Biology, Baylor College of Medicine and Center for Theoretical Biological Physics, Rice University, IDO GOLDING, Department of Physics and Center for the Physics of Living Cells, University of Illinois at Urbana-Champaign — Gene promoters typically contain multiple binding sites for transcription factors. This allows for distinct transcription-factor binding configurations, each characterized by a different transcriptional activity of the regulated gene. However, at a given transcription-factor concentration, the promoter is not expected to exhibit a single configuration, but, instead, a “mixed state” with fractional probabilities for the different configurations. What is the nature of these mixed promoter states at the single-cell level? We investigate this question by measuring simultaneously, in individual cells, the concentration of the CI transcription factor and the transcriptional output of the regulated promoter, P_{RM}, in E. coli. We use the mRNA copy-number statistics to reconstruct the stochastic kinetics of the different promoter configurations and calculate their probabilities at each CI concentration. We find that the mRNA distribution for cells in a mixed state can be described as a convolution of the pure-state distributions, indicating rapid switching between the pure promoter states. Thus, mixed promoter states do not result in different cell populations but instead appear as a new, well-defined promoter activity.

11:27AM Z47.00002 Direct Quantification of Transcriptional Regulation at an Endogenous Gene Locus. HENG XU, Department of Biochemistry and Molecular Biology, Baylor College of Medicine; Center for Theoretical Biological Physics, Rice University, ANNA SOKAC, Department of Biochemistry and Molecular Biology, Baylor College of Medicine, IDO GOLDING, Department of Physics and Center for the Physics of Living Cells, University of Illinois at Urbana-Champaign — The stochastic kinetics of gene activity in individual cells has been well characterized, but how this kinetics is modulated by the transcription factors that regulate expression remains largely unknown. We address this question using the Bicoid (Bcd) transcription factor and hunchback (hb) gene in early Drosophila embryos. We measure, simultaneously, the number of nascent hb mRNAs, nuclear Bcd concentration, and number of bound Bcd proteins, at individual gene loci. Using stochastic theoretical analysis, we find that Bcd modulates the probability of hb switching to an active transcriptional state, while not affecting the probabilities of transcription initiation or gene inactivation. Gene activation is achieved through the cooperative binding of 6 Bcd copies. Our data also reveals additional Bcd binding states of unknown function. In contrast to Bcd, binding of the Hunchback transcription factor represses hb transcription. Our approach can be used to elucidate the combinatorial activity of multiple transcription factors without the need for genetic perturbation.
11:39AM Z47.00003 Fast Chromatin Assembly facilitated by Nucleosome Breathing and Replication-Guided Packing . JOHANNES NUEBLER, BRENDAN OSBERG, Theory of Complex Biosystems, Physik-Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany, PHILIPP KORBER, Adolf-Butenandt-Institut, University of Munich, Schillerstrasse 44, 80336 Munich, Germany, ULRICH GERLAND, Theory of Complex Biosystems, Physik-Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — The condensation of eukaryotic DNA into chromatin entails the formation of nucleosome arrays with high density at species-dependent nucleosome spacing. These arrays are frequently destroyed by transcription and replication, such that reassembly is required. Due to a well-known jamming effect in the random adsorption of mutually exclusive objects (aka the "car parking problem"), the question was raised how in vivo nucleosome densities, and patterns, can be reached in the biologically relevant timescale of minutes [1]. We show that the "softness" of nucleosomes alleviates the kinetic challenge [2]. Nucleosome softness arises due to transient DNA unwrapping (breathing) and stepwise nucleosome assembly. From a physics perspective, the "soft car parking problem" differs fundamentally from its hard counterpart by exhibiting non-monotonic density and rapid equilibration. We also discuss scenarios how the progression of the replication fork can promote rapid reassembly in its wake. For example, tight packing arises naturally if the fork progresses slowly compared to the reassembly rate.


11:51AM Z47.00004 Topology, structure and energy landscape of human chromosomes , BIN ZHANG, PETER WOLYNES, Rice University — The genomes' three-dimensional (3D) organization is crucial in regulating many biological processes, including gene regulation, DNA replication, and cell differentiation. We develop a statistically rigorous approach based on maximin entropy principle to determine a least-biased potential energy landscape that reproduces experimentally determined Hi-C contact frequency between genome pairs. The resulting energy landscape supports a knotless chromosome conformation, which has been highly anticipated since complex knotted conformations prohibit the access of gene information for transcription and hinder DNA replication. We further show that the topologically associating domain signal alone also enforces a chromosome structure free of knots. Our results highlight the importance of local interactions in determining the global topology of the chromosome structure. Finally, the derived landscapes for multiple chromosomes support the formation of territories that have long been observed in microscopy experiments. Together with Hi-C experiments, our approach provides a coherent picture of the 3D architecture of the genomes that is consistent with many the available experimental data.

12:03PM Z47.00005 Expediting the Sequencing Process: Using Soft Lithography to Fragment Aligned DNA Molecules1 . MEENA JAGADEESAN, Phillips Exeter Academy, Exeter NH 03833, ADINA SINGER, Stella K. Abraham High School for Girls, Hewlett Bay Park NY 11557, NAHYUN CHO, KE ZHU, JULIA BUDASSI, JONATHAN SOKOLOV, Stony Brook University — Current sequencing technologies output short read lengths on the order of 10 kb, requiring DNA to be fragmented into small pieces, analyzed separately and recombined to obtain the full sequence. The accuracy and cost efficiency of sequencing has been limited by the computer algorithms required to assemble the random subsequences. The fragmentation method in this study can significantly simplify the assembly process with a novel lithographic cutting procedure that retains the position and order of DNA fragments. DNA was stretched linearly on a polymer coated silicon wafer. A polydimethylsiloxane (PDMS) lithographic stamp was coated in DNase I (DNA cutting enzyme) solution. The stamp was placed in contact with the surface aligned DNA, producing 3.5 micron (10 kbp) DNA fragments. Fluorescence imaging of dye labeled DNA was used to monitor the cutting effectiveness. The improved enzyme application procedure presented in this study enabled uniform, ordered cutting of the surface aligned DNA over approximately 80% of the 2 cm x 3 cm samples. Means to extract the cut DNA from the polymer surface were also explored. The effectiveness of solution methods, electric field desorption, and microfluidics will be discussed.

1 NSF funding (DMR-0606387) is gratefully acknowledged.

12:15PM Z47.00006 New insights into nucleosome positioning , RAZVAN CHEREJI, JOSEFINA OCAMPO, TARA BURKE, DAVID CLARK, Natl Inst of Health - NIH — A human body contains enough DNA to circle the Earth's Equator more than 2.5 million times. Nevertheless, the entire genetic material is packed inside the tiny nuclei of our cells. The basic units of DNA packaging are called nucleosomes. Their locations on the chromosomes play an essential role in gene regulation. We study nucleosome positioning in yeast, fly and mouse, both in vivo and in vitro, and build biophysical models in order to explain the genome-wide nucleosome organization. We show that DNA sequence is not the major cause of the phased arrays of nucleosomes observed in vivo near the transcription start sites. We discuss simple models which can account for the formation of nucleosome depleted regions and nucleosome phasing at the gene promoters. We analyze the effects of different factors which influence the chromatin organization in living cells: existence of potential barriers and wells, sequence-dependent nucleosome affinity, nucleosome unwrapping, competition between different DNA-binding proteins, action of ATP-dependent remodelers, among others.

12:27PM Z47.00007 Statistical mechanics of nucleosome assembly and chromatin packaging , ALEXANDRE MOROZOV, Rutgers University, Department of Physics and Astronomy — Eukaryotic genomes are organized into arrays of nucleosomes. Each fully wrapped nucleosome consists of 147 base pairs of genomic DNA bent around a histone octamer core. The resulting complex of DNA with histones forms a multi-scale structure called chromatin. At the most fundamental level of chromatin organization, arrays of nucleosomes form 10-nm fibers which resemble beads on a string; these in turn fold into higher-order structures. Depending on the organism and cell type, 75-90% of genomic DNA is packaged into nucleosomes. The question of how cellular functions are carried out on this chromatin template is one of the outstanding puzzles in biology. Nucleosomal DNA may transiently peel off the histone octamer surface due to thermal fluctuations or interactions with chromatin remodelers. Thus neighboring nucleosomes can invade each other’s territories through DNA unwrapping and translocation, or through initial assembly in partially wrapped states. A recent high-resolution map of distances between neighboring nucleosomes in baker’s yeast [1] has revealed that at least 25% of all nucleosomes overlap with DNA territories of their neighbors. To explain this observation, we have developed a statistical mechanics model of nucleosome assembly and unwrapping [2]. Our model is in agreement with genome-wide nucleosome positioning data and in vitro measurements of accessibility of nucleosome-covered target sites. Furthermore, it explains nucleosome-induced cooperativity between DNA-binding factors. The observed extent of nucleosome crowding in the yeast genome strongly suggests that its treatment should be included in all future models of chromatin structure and energetics.


1:03PM Z47.00008 Exploring telomeric DNA-protein-DNA interactions under nanofabrication . MAEDEH ROUSHAN, PARMINDER KAUR, JIANGUO LIN, HONG WANG, ROBERT RIEHN, North Carolina State University, RIEHN LAB TEAM, WANG LAB COLLABORATION — Genomes are organized through DNA binding proteins. In particular, telomeres are organized into ~ 10 kbp loops by a multi-protein complex. For understanding how proteins interact with DNA we have investigated the effect of different DNA-binding proteins on DNA configuration by injecting different proteins inside a nanofabricated channel system. DNA molecules stretch in nanochannels with a channel cross-section roughly about 100x100 nm2, so allowing analysis by observation of a fluorescent dye. The length and configuration of DNA can be directly observed, as well as the binding location of proteins. Here we show the binding patterns and molecular action of a set of telomere-associated proteins, namely TRF1, TRF2,RAP1, SA1, as well the model protein T4 DNA ligase. In particular, we demonstrate formation of stable loops, sliding, and general DNA condensation.
1:15PM Z47.00009 Computational modeling of autocatalytic heteropolymer replication, HEMACHANDER SUBRAMANIAN, ROBERT GATENBY, Moffitt Cancer Center — We computationally study replication of a hypothetical autocatalytic heteropolymer using Kinetic Monte Carlo. When cooperativity is included in the model, we observe better replication characteristics and higher fitness in strands with certain symmetries broken. We correlate this symmetry-breaking with the observed broken mirror symmetry of extant heteropolymers.

1:27PM Z47.00010 A unified description of biological effects caused by radiation exposure: Whack-a-mole (WAM) model, TAKAHIRO WADA, Department of Pure and Applied Physics, Kansai University, YUCHIRO MANABE, Graduate School of Engineering, Osaka University, ISSEI NAKAMURA, State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, MASAKI BANDO, Research Center for Nuclear Physics (RCNP), Osaka University — We present our novel rate equations to study DNA mutation in cells caused by artificial radiation exposure, accounting for the DNA damage and repair simultaneously. In our theory, the dependence of mutation frequencies on the dose rate is critically important to predict both the time course and the stationary effect of the DNA mutation in cell cycles. Experimentally, irradiation at high dose rates causes linear increases in the mutation frequency with total dose, whereas the saturation of the mutation frequency is observed at low dose rates. We demonstrate that this fact arises from counteracting effects among the DNA damage and mutation, the DNA repair, and the proliferation and apoptosis of cells. Our theory thus captures observed quantities at both high and low dose rates, marking a substantial difference from conventional theories based only on the total dose. Importantly, we have derived a scaling function from our rate equations that predicts a universal feature in the mutation frequency of living organisms. In this study, we have analyzed the experimental data of five species; mouse, drosophila, chrysanthemum, maize, and tradescantia. Despite the difference between animal and plant, all these data reasonably fall on a single line for our scaling function.

1:39PM Z47.00011 Extracting free energies of interaction from chromosome conformation capture data, ELDON EMBERLY, Physics, Simon Fraser University, Burnaby, BC — A variety of DNA binding proteins are involved in regulating and shaping the packing of chromatin. They aid the formation of loops in the DNA that function to isolate different structural domains. A recent experimental technique, Hi-C, provides a method for determining the frequency of such looping between all distant parts of the genome. Given that the binding locations of many chromatin associated proteins have also been measured, it is possible to make estimates for their influence on the long-range interactions as measured by Hi-C. However, a challenge in this analysis is the predominance of non-specific contacts that has made making quantitative estimates for the strengths of interactions between chromatin factors difficult. In this talk I will show that transforming the Hi-C contact frequencies into free energies of interaction gives a natural method for separating out the distance dependent non-specific interactions. In particular, using Principal Component Analysis (PCA) on the transformed free energy matrix can identify the dominant modes of interaction within the genome. Some of these modes correspond to systematic biases that can then be subtracted out. I will then show that a pairwise interaction model can be fit to the corrected free energies to determine the couplings between known bound chromatin factors. By correcting for the systematic effects identified by PCA, a consistent set of predictions for the couplings among the various chromatin factors can be made. Many of the known interactions within the network of chromatin factors are found along with several novel predictions. Finally, I will present efforts to predict the local 3D structure of chromatin using the fitted interaction model and the locations of bound factors.

Friday, March 6, 2015 11:15AM - 1:51PM — Session Z49 GSOF: Focus Session: Self-Phoretic Colloids and Active Emulsions II 217D - Michelle Driscoll, New York University

11:15AM Z49.00001 Building a dynamic cell from the bottom up, VIVA R. HOROWITZ, THOMAS G. DIMIDUK, Department of Physics, Harvard University, IREP GOZEN, School of Engineering and Applied Sciences, Harvard University, YUE N. REN, Harvard University, VINOTHAN N. MANOHARAN, School of Engineering and Applied Sciences, Harvard University — We aim to understand cellular processes, particularly intracellular transport, at a physical level by building simple, well-controlled systems that mimic the functions of a cell. We have created a simple artificial cell using a bilayer phospholipid vesicle containing Janus swimmers as microscale motors. These Janus swimmers are propelled by the catalytic breakdown of hydrogen peroxide on their platinum hemispheres. We encapsulate these Janus swimmers in the interior of the artificial cell. We investigate the superdiffusive motion using multimodal imaging tools, including digital holography and fluorescence, to shed light on how the dynamics of Janus swimmers depends on the confinement. These dynamics and transport processes may prove necessary to sustain gene expression, growth, and reproduction in future artificial cells.

11:27AM Z49.00002 Internally driven solids, ANANYO MAITRA, SUROPRIYA SAHA, Indian Inst of Science, RAMIN GOLESTANIAN, Rudolf Peierls Center for Theoretical Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, United Kingdom, SRIRAM RAMASWAMY, TCIS, TIFR — What is the long-wavelength, long-time dynamics of an elastic solid composed of motile orientable particles? Can different types of interactions between the motile particles lead to different varieties of active solid? What is the dynamics if the motile particles orient along a spontaneously chosen axis? Is it different from a passive solid which is driven externally? What if the inter-particle interactions instead favour aster-like configurations? I will present an answer to these questions and point out the differences and similarities between internally driven and externally driven solids.

11:39AM Z49.00003 Controlling Compartmentalization Through Active Confinement, MATTHEW SPELLINGS, MICHAEL ENGEL, DAPHNE KLOTHSA, Univ of Michigan - Ann Arbor, KYLE BISHOP, The Pennsylvania State University, SHARON GLOTZER, Univ of Michigan - Ann Arbor — Active matter is an exciting area of study that displays promising new behaviors previously unobtainable in equilibrium systems and could help bridge the gap between equilibrium colloidal- and nanoscale particles and living cells. In this talk, we will discuss novel, emergent behavior observed simulations of confined "cells" comprised of active particles. We show how the results of a microscopic model are reproduced in a continuum model.

11:51AM Z49.00004 Self Propelled nanorods at an interface, JEREMIE PALACCI, Department of Physics, UCSD/ Courant Institute NYU, TAKUJI ADACHI, NYU Chemistry, JUN ZHANG, NYU Physics/ Courant Institute NYU, LEIF RISTROPH, Mike SHELLEY, Courant Institute NYU — Self-propelled colloids are micron-scale particles which can harvest the energy from the surrounding medium and convert it into propulsion and work. Here we study the impact of the interface —solid, fluid, slipping, non-slipping— on the dynamics of the self-propulsion for a suspension of active nanorods.
12:03PM Z49.00005 Velocity distributions in self-assembled phases of active magnetic colloids\textsuperscript{1}, ALEXEY SNEZHKO, Argonne National Laboratory — Colloids of strongly interacting particles driven out-of-equilibrium by an external periodic forcing often develop nontrivial collective dynamics and dynamically assembled structures. We use ferromagnetic colloidal micro-particles suspended over a water-air interface. The system is energized by a single-axis alternating magnetic field applied in-plane of the interface. Experiments revealed a rich variety of self-assembled phases (in particular, “wires,” “rotators”) emerging in such systems in a certain range of excitation parameters. Velocity distributions of particles in driven magnetic colloids in “rotators” phase were carefully examined. The studies revealed strongly non-Maxwellian nature of velocity statistics for both subsystems: single particles and self-assembled rotators. The high energy tails of velocity distributions are stretched exponential. Dissipations due to inelastic collisions and viscous damping contribute to the form of the high energy tails. When viscous damping dominates over collisional dissipation the distribution is nearly exponential (such behavior is observed for the gas of rotators) while in the opposite case (single particles driven by field) the core of the distribution is Gaussian and only high energy tails are close to exponential.

\textsuperscript{1}The research was supported by the U.S. DOE, Office of Basic Energy Sciences, Division of Materials Science and Engineering, under the Contract No. DE AC02-06CH11357

12:15PM Z49.00006 Strongly confined active brownian particles, YAOQUEN FILY, APARNA BASKARAN, MICHAEL HAGAN, Brandeis University — We explore the effect of boundaries on active suspensions by considering non-aligning self-propelled particles confined by hard frictionless walls. In small boxes, the density and pressure are sensitively controlled by the shape of the box. We show those quantities can be predicted for arbitrary box shapes, and discuss the role of concavity and dimensionalities. This in turn provides a tool to design and understand such confining boxes.

12:27PM Z49.00007 Using light patterns to manipulate self-propelled particles, MELISSA FERRARI, MICHELLE DRISCOLL, Department of Physics, New York University, JEREMIE PALACCI, Department of Physics, University of California, San Diego, STEFANO SACANNA, Department of Chemistry, New York University, DAVID PINE, PAUL CHAIKIN, Department of Physics, New York University — Soft active matter systems, characterized by their ability to extract energy from their environment to perform mechanical work, exhibit phenomena far from equilibrium. We study a class of synthetic light activated colloidal swimmers which self-propel osmotically on a surface. Here we propose a method to manipulate the migration of the light activated colloids by carefully tuning their macroscopic environment. Through integration of a modified commercial projector with an optical microscope, we are able to shine static and dynamic light patterns onto the sample plane where the light activated swimmers live. We can use specific light patterns to set up swimmer density gradients in our sample.

12:39PM Z49.00008 Active droplets as biomimetic model swimmers\textsuperscript{1}, CORINNA MAASS, Max Planck Institute for Dynamics and Self-Organization, Göttingen — Large ensembles of biological swimmers form one of the biggest ecosystems on earth: marine phytoplankton. Investigating the dynamics of such a system is of prime ecological importance, however, as any modelling would need to include the interplay of turbulence, long-range hydrodynamics, buoyancy, as well as the self-propelled motion of the swimmers, this proves a daunting task both analytically and numerically. A scalable system of artificial swimmers with well understood and tunable interactions should help with decoupling some of these effects and studying them separately. Active emulsions of self-propelled droplets present a suitable experimental model system for the collective behaviour of biological swimmers, as they exhibit both autonomous motion and chemotaxis, move freely in three dimensions, can be produced and stored in large, monodisperse quantities and are stable over time scales comparable to biological systems. We demonstrate some of these features on a system of liquid crystal droplets driven by solubilisation into a micellar aqueous surfactant solution.

\textsuperscript{1}Supported by the DFG SPP 1726 “Microswimmers.”

1:15PM Z49.00009 Active Brownian and Run-and-Tumble particles: A comparison of the large scale dynamics, BENJAMIN HANCOCK, APARNA BASKARAN, Brandeis Univ — Active Brownian particles, such as self phoretic colloids, are a class of self propelled particles which swim at fixed speed with orientation that gradually changes through rotational diffusion. Some bacteria obey Run-and-Tumble dynamics, in which particles swim along a fixed orientation until a tumble event occurs that randomly selects a new orientation. At long time and length scales the diffusive-drift limit of the above dynamics appear to be identical. In this large scale limit, we study the effects of external fields on the dynamical properties of these two classes of self propellled particles.

1:27PM Z49.00010 The role of hydrodynamics and confinement on the collective behavior of active emulsions, SHASHI THUTUPALLI, DELPHINE GEYER, HOWARD STONE, Princeton Univ — Active droplets i.e. emulsion droplets which exhibit self-propelled motion are of tremendous interest in understanding the collective dynamics of systems far from thermal equilibrium. A particularly appealing feature of these active droplet systems is that the coupling between the individuals is well-controlled and mediated by purely physical effects such as steric interactions and hydrodynamics. We create such active droplet systems using liquid crystalline emulsions in aqueous phases stabilized by surfactants. The propulsion of the individual droplets is fully 3 dimensional and occurs via a spontaneously broken symmetry (unlike colloidal swimmers which are often asymmetric by design) which is sustained via dissipation of chemical energy. Here, we show that hydrodynamics and geometry play a crucial role in the emergent self-organization of the active droplets. In particular, we describe the pair-correlations emerging in a population of active droplets confined in Hele-Shaw geometry. We further demonstrate that these interactions result in the formation of stable travelling bands in reduced confinement and self-organize into crystalline vortices at a single interface.

1:39PM Z49.00011 Glassy dynamics of self-propelled particles: computer simulations and a mode-coupling-like theory\textsuperscript{1}, GRZEGORZ SZAMEL, ELIJAH FLENNER, Department of Chemistry, Colorado State University, LUDOVIC BERTHIER, Laboratoire Charles Coulomb, Universite Montpellier II — We use a combination of computer simulations and theory to elucidate glassy dynamics of self-propelled particles. We compare the relationship between the steady state structure of the self-propelled system and its long-time dynamics with that of an equilibrium Brownian system. We find that an athermal self-propelled system can have a more pronounced local structure but faster relaxation than a similar equilibrium system. Interestingly, the dependence of the dynamics on the persistence time of the self-propulsion can be non-monotonic, with the dynamics speeding up and then slowing down with increasing persistence time. We show that these effects are captured by a mode-coupling-like theory.

\textsuperscript{1}Supported by NSF and ERC

Friday, March 6, 2015 11:15AM - 2:15PM – Session Z50 GSOFT: Membranes, Micelles and Vesicles 218 - Haskell Taub, University of Missouri, Columbia
11:15 AM Z50.00001 Dynamic Heterogeneity in Lipid Structures. CHRISTINA OTHON1, Wesleyan Univ, NEDA DADASHVAND, Wesleyan University — We have characterized the temperature and pressure dependent scaling of dynamic heterogeneity in a homogenous liquid phase of a lipid monolayer using time-resolved fluorescence anisotropy (TRFA) microscopy. Rotational diffusion is far more sensitive to highly correlated motions than translational diffusion due to the enhanced influence of nearest neighbor interactions. Highly correlated motion results in regions of high-density, low mobility lipids, and low-density, high mobility lipids; and are observed as the bimodal distribution of rotational correlation times. For biological lipid membranes the presence of highly correlated motion will greatly influence the rates of protein sorting and self-assembly, as particles suspended in the fluid can become kinetically trapped. Rotational diffusion timescales (~ ns) are far shorter than the lifetime of dynamic clusters and lipid raft-like structures (~ 10 µs), and thus the distribution of rotational correlation times can provide critical insight into the presence of these structures. We have characterized rotational dynamic distributions for a variety of phosphocholine moieties, and found dynamics consistent with highly correlated motion. Using the proximity to the phase transition, and the scaling of the temperature dependence of the heterogeneity we apply theoretical models developed for other condensed matter systems help us define limits on the size and lifetime of dynamic clusters in lipid structures.

1 corresponding author

11:27 AM Z50.00002 Interplay between group function of kinesin based transport and lipid bilayer mobility. JOSEPH LOPES, LINDA HIRST, JING XU, University of California, Merced — Motor proteins, discovered in recent decades, are important building blocks to life. These molecular machines transport cargo and although indispensable to cell function, are not well understood at present. Single kinesin transport properties have been documented, but their group function remains unknown. In this project, the properties of kinesin-based transport by multiple motors are investigated in-vitro to establish a link between travel distance and lipid diffusion in the vesicle membrane. In the experiments, silica beads coated in a supported lipid membrane and giant vesicles are transported along a microtubule by embedded kinesin motors. In an alternate geometry, this system can be inverted, whereby motors are bound to a surface of a lipid bilayer and microtubules are deposited. We have characterized motor function with respect to the fluidity of the membrane. To measure the diffusion properties of different membranes, planar lipid bilayers are prepared on silica slides and supported by bovine serum albumin protein. To establish a diffusion constant at room temperature for the lipid membrane we use the FRAP technique (fluorescence recovery after photobleaching). Using this method we can investigate if there is any interplay between group travel function and membrane fluidity.

11:39 AM Z50.00003 Nanoscopic Dynamics of Phospholipid Based Unilamellar Vesicles: Effect of Phase Transition and Addition of Melittin Peptide and Cholesterol. V. K. SHARMA, Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, E. MAMONTOV, Chemical and Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, D. B. ANUNCIADO, H. O’NEILL, V. URBAN, Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — Dynamics of DMPC phospholipid in unilamellar vesicles (ULV) has been investigated using quasielastic neutron scattering (QENS) techniques and reported here. Effect of addition of melittin and cholesterol on the dynamics of the lipid molecules in the ULV is also investigated. For DMPC ULV, a sharp fall in the elastic scan intensity is observed at 296 K, which is an indication of a solid gel to fluid phase transition. The addition of cholesterol or melittin inhibits this steep fall indicating that these molecules do have an influence on the main phase transition of DMPC ULV. QENS experiments have been carried out on DMPC ULV solution in the presence and absence of these additives at 280 K, in the solid gel phase, and at 310K, where lipids are in the fluid phase. The nanomolar concentration shows the presence of two distinct motions: lateral and internal motions of the DMPC monomer. Both lateral and internal motions are found to be affected by the main phase transition. The addition of cholesterol or melittin influences the dynamics significantly in a different way, depending on the phase of lipid bilayers and the nature of additives. Effect of phase transition and additives on the dynamics of lipid in ULV will be discussed in details.

11:51 AM Z50.00004 A Molecular Understanding of the Toxic Interactions of Ionic Liquids Towards a Lipid Biomembrane1, BRIAN YOO, EDWARD MAGINN, YINGXI ZHU, Univ of Notre Dame — There is a growing urgency to understand the toxicity of ionic liquids (ILs) due to their potential leakage into aquatic environment via aqueous waste streams in many large-scale commercial applications. Better understanding in the molecular interactions of ILs, primarily those in the popular imidazolium-class, with biological systems can serve as a physical foundation for their future design into ecologically benign ones. Here we investigate the toxic interaction of IL aqueous solutions with a supported lipid bilayer as a model cell membrane, using a combined experimental (fluorescence microscopic measurements) and multiscale simulation-based analysis. Both experimental and computer simulation studies have shown that the interactions of ILs with a supported lipid bilayer can lead to the insertion of ILs into the lipid bilayer, causing biomembrane morphological changes into multilayers, fibers, and/or vesicles with a strong dependence on the alkyl side chain length of IL cations. Using atomistic and coarse grained simulations, we have examined the potential of mean force of IL upon approaching a lipid bilayer and resulting changes in the mechanical compliance of lipid bilayer induced by IL interactions. We find that the resulting IL-lipid bilayer complexes can be strongly dependent on the ILs’ ability to form cationic micelles.

1National Science Foundation (CBET-1134238)

12:03 PM Z50.00005 ABSTRACT WITHDRAWN —

12:15 PM Z50.00006 Curvature coupling influences lipid phases and morphologies on substrates. JUKKA MÄÄTTÄ, SAMPSA VIERROS, MARIA SAMMALKORPI, Aalto Univ — The shape of a lipid aggregate contributes to many crucial biological processes like motility, fusion, fission and trafficking. At a molecular scale, the shapes lipids self-assemble in aqueous solution are coupled to molecular spontaneous curvature. At interfaces, the interface imposes an additional external constraint, which influences the assembled morphology. In this study, we examine the coupling between molecular spontaneous curvature and imposed external curvature in self-assembling lipid systems via molecular simulations. We map the adsorption morphologies for lipids of varying curvature as a function of substrate characteristics; the external curvature imposed by the substrate acts as a control factor in determining the morphology. In two-component systems external curvature introduced by the substrate can result in phase separation. We compare and connect our findings with experimental findings on lipid adhesion and adsorption morphologies.

12:27 PM Z50.00007 Interaction measurement of particles bound to a lipid membrane. RAPHAEL SARFATI, ERIC DUFRESNE, Yale University — The local shape and dynamics of the plasma membrane play important roles in many cellular processes. Local membrane deformations are often mediated by the adsorption of proteins (notably from the BAR family), and their subsequent self-assembly. The emerging hypothesis is that self-assembly arises from long-range interactions of individual proteins through the membrane’s deformation field. We study these interactions in a model system of micron-sized colloidal particles adsorbed onto a lipid bilayer. We use fluorescent microscopy, optical tweezers and particle tracking to measure dissipative and conservative forces as a function of the separation between the particles. We find that particles are driven together with forces of order 100 fN and remain bound in a potential well with a stiffness of order 100 fN/micron.
12:39PM Z50.00008 Effects of water models and simulation system size on dynamic heterogeneity of single component lipid membranes, YOUNGHOON OH, JEONGMIN KIM, BONG JUNE SUNG, Department of Chemistry, Sogang University, Seoul 121-742, Republic of Korea — Biological membranes are composed of various different types of molecules and their composition is usually spatially heterogeneous. Recently it has been reported that the dynamics of lipids could also become spatially heterogeneous, where fast and slow regions of lipids could coexist. A recent simulation study showed that the diffusion of lipids even in single component lipid membranes could be spatially heterogeneous in liquid-ordered phase at sufficiently low temperature. [1] On the other hand, in the liquid-disordered phase at relatively high temperature, the dynamics of lipids was homogeneous in membranes. In this work, we systematically investigated the diffusion of lipids in single component DPPC lipid bilayers by employing three different water models (Big Multipole Water, Polarizable MARTINI and LJ MARTINI) and three different simulation cell sizes (L = 5nm, 10nm and 20nm). We find that even though the liquid-disordered to liquid-ordered phase transition occurs at different temperatures for different water models, the diffusion of lipids become spatially heterogeneous in liquid-ordered phases for all three different force fields. Reference [1] F. W. Starr, B. Hartmann, J. F. Douglas, Soft Matter, 10, 3036 (2014).

12:51PM Z50.00009 Modulation of MscL activity in droplet interface bilayers through tailored interfacial mechanical properties, JOSEPH NAJEM, Virginia Tech, ERIC FREEMAN, University of Georgia, SERGEI SUKHAREV, University of Maryland, DONALD LEO, University of Georgia — MscL, a large-conductance mechanosensitive channel, is an osmolyte release valve that aids bacteria in surviving hypo-osmotic shocks. The large scale of its tension-driven opening transition makes it a strong candidate to serve as a transducer in stimuli-responsive biomolecular materials. In the previous work, a V23T mutant of MscL produced a reliable activation in a droplet interface bilayer (DIB) with applied axial droplet compression. Near the maximal compression, the aqueous droplets deform and the resulting increase in surface area leads to an increase in tension in the water-lipid-oil interface. This increase in tension is the product of the relative change in the droplet surface area and the elastic modulus of the DPhPC monolayer (120 nN/m). Here, we study the interfacial properties of the droplets as a way for modulating the activity of the embedded MscL channels. This is accomplished through varying mixtures of diphantanol phospholipids. The results show that gating probability of MscL in DIBs increases when lipids with a higher elastic modulus are used or when cholesterol is added to the monolayer. Moreover, an intrinsic electrical bias inside the lipid membrane is created when having DPhPC lipids with higher dipole in one droplet and DOPhPC characterized with lower dipole, in the other.

1 We would like to acknowledge the financial support provided by the Air Force Office of Scientific Research Basic Research Initiative Grant FA9550-12-1-0464.

1:03PM Z50.00010 Structural dynamics of surfactant solutions in planar extensional flow, BINBIN LUO, WESLEY BURGHARDT, Northwestern University — We report in situ x-ray scattering investigation of the structure of aqueous surfactant solutions in planar extensional flow. Samples were studied in a cross-slot stagnation flow cell fed by a syringe pump using a highly collimated synchrotron x-ray beam that provides for spatially resolved measurements of fluid structure in the stagnation region of the flow. Prior attempts to use planar stagnation flows for either x-ray or neutron scattering employed low-aspect ratio flow geometries in which the kinematics are dominated by parasitic velocity gradients along the incident beam direction. In contrast, our cross-slot flow cell employs an aspect ratio of 5:1, providing a much more ideal two-dimensional extensional flow field in the stagnation region. This device has been used to study two different surfactant systems, one a wormlike micelle solution at high salt concentration which exhibits rheology similar to that of entangled polymers. Here the focus is on the degree of micelle orientation produced as a function of extension rate. We have also studied a system that forms lamellar ordering. In addition to induced alignment of the mesophase structure, it is also possible to interrogate flow-induced changes in lamellar d-spacing in this material.

1:15PM Z50.00011 Toward a unified view of the structure and dynamics of water associated with single-supported zwitterionic and anionic membranes, ZACHARY BUCK, Univ of Missouri, ANDREW MISKOWIEC, Oak Ridge National Lab, HELMUT KAISER, Univ of Missouri Research Reactor, GAVIN KING, HASKELL TAUB, Univ of Missouri, FLEMMING HANSEN, Technical Univ of Denmark, MADHUSUDAN TYAGI, NIST Center for Neutron Research, SOULEYMANE DIALLO, EUGENE MAMONTOV, KEN-NETH HERWIG, Oak Ridge National Lab — High-resolution quasielastic neutron scattering was used to investigate the diffusive motion of water associated with single-supported bilayers of the zwitterionic lipid DMPC [1] and the anionic lipid DMPG [2]. The temperature dependence of the elastically-scattered neutron intensity from these samples indicates a series of freezing and melting transitions of the hydration water which differ greatly depending on the charge state of the lipid [2]. We interpret these distinct transitions as evidence of different types of water common to the two membranes: bulk-like water probably located above the membrane and two types of confined water in closer proximity to the lipid head groups. The temperature dependence of the diffusion coefficient of the hydration water determined for both membranes supports the interpretation of distinct water types each with its characteristic translational diffusion rate. Although sharing water types, the two membranes differ greatly in the temperature range over which their water freezing and melting transitions occur. [1] M. Bai et al., Europhys. Lett. 98, 48006 (2012). [2] A. Miskowiec et al., Europhys. Lett. 107, 28008 (2014).

1 Supported by NSF Grant Nos. DMR-0944772 and DGE-1069091.

1:27PM Z50.00012 ABSTRACT WITHDRAWN —

1:39PM Z50.00013 Observation of Iron Specific Interaction with a Charge Neutral Phospholipid, WENJIE WANG, HONGHU ZHANG, SHUREN FENG, JOSUE SAN EMETIERO, Ames Laboratory, Iowa State University, IVAN KUZMENKO, Argonne National Laboratory, MARIT NILSEN-HAMILTON, SURYA MALLAPRAGADA, DAVID VAKNIN, Ames Laboratory, Iowa State University — Using surface sensitive X-ray scattering and spectroscopic techniques we show that phosphatidyl choline (PC) head groups attract positively charged iron ions and complexes even at pH values that are lower than 3. DPPC (1,2-dipalmitoyl-sn-glycero-3-phosphocholine) is a zwitterionic lipid typically used as a model system for cell membranes. Within a large pH range (3-11), it carries a negative charge on the phosphate group and a positive charge on the quaternary ammonium cation, thus appears charge neutral. Further lowering the pH, i.e. adding a proton to the phosphate group, results in a positively charged headgroup. Surprisingly, we detect significant enrichment of iron at the interface of the DPPC monolayer and the aqueous subphase with the pH maintained at 3 or even lower. With a supposedly charge neutral or even positive surface, the observation of surface bound, charge positive iron ions or iron hydroxides is counter-intuitive and suggests iron-specific interaction with the phospholipid headgroup, which is not governed by electrostatic interaction. The effect of the integration of Mms6, a membrane protein that promotes the formation of magnetic nanocrystals, into the DPPC monolayer will also be discussed.

1 Research supported by the U.S. Department of Energy under Contract No.DE-AC02-07CH11358 and DE-AC02-06CH11357.
superconductivity and the pairing symmetry puzzle of iron-based superconductors, and also provide clues for further enhancing Tc.

In this talk, I will show our recent angle-resolved photoemission studies on various FeSe-based heterostructures grown by molecular beam epitaxy. We systematically studied the electronic structures and superconducting properties of FeSe with varied strain, different interfacial oxide materials and different Fermi pockets, with minima at the crossings of the two pockets. Our results provide important experimental foundations for understanding the interfacial superconductivity and the pairing symmetry puzzle of iron-based superconductors, and also provide clues for further enhancing Tc.

**Friday, March 6, 2015 11:15AM - 2:15PM**

**Session Z51 DCMP: Invited Session: FeSe/Oxide Interface Superconductivity** Grand Ballroom C1 - Qimiao Si, Rice University

11:15AM Z51.00001 Significant Tc enhancement in FeSe films on SrTiO3 due to interfacial mode coupling , ROBERT MOORE, SLAC National Accelerator Laboratory — The enhanced superconductivity in monolayer FeSe films grown on SrTiO3 (STO) substrates has generated a lot of attention. Several previous studies have shown a dramatic difference between the superconducting monolayer and non-superconducting bilayer films suggesting the substrate or interface plays a critical role in the enhancement of superconductivity. Utilizing Molecular Beam Epitaxy (MBE) and in situ Angle Resolved Photoemission Spectroscopy (ARPES), we explore the role of the substrate on the electronic structure of superconducting monolayer FeSe films. The electronic structure at the Fermi surface of the monolayer film consists of two electron pockets at the M point of the Brillouin zone, in contrast to bilayer and thicker films that show an electronic structure similar to bulk FeSe. The orbital character of the two pockets has been resolved which shows two distinct gaps and places strict constraints on the possible pairing symmetry. Surprisingly, we observe exact replicas of the FeSe bands which are attributed quantum shakeoffs arising from strong electron phonon coupling. Shakeoff bands have never been resolved with such clarity in a solid before and are only observed in the monolayer films. The coupling is between a high energy oxygen phonon in the STO substrate and electrons in the FeSe monolayer. Oxide MBE has been used to grow STO with oxygen 18 to explore the isotope effect on the electron phonon coupled shakeoff bands and will be discussed. Theoretical investigations show how these distinct features result from strong forward scattering which enhances superconductivity. This enhancement does not depend on the origins of superconductivity as it exists in all channels and is responsible for the increase in Tc. These results suggest a possible avenue for engineering superconductors with higher Tc.

11:51AM Z51.00002 Interface-induced high-temperature superconductivity in FeSe/TiO2(001) heterostructure , HAO DING, Tsinghua University — The recently discovered high transition temperature (Tc) superconductivity at the interface of single unit-cell (UC) FeSe films on SrTiO3(001) has generated considerable excitement [1,2], which may eventually lead to the discovery of a new family of high-Tc superconductors at many different interfaces. In this talk, we will present our recent work on a new interfacial system with high-Tc superconductivity, 1 UC FeSe films on anatase TiO2(001). Using molecular beam epitaxy (MBE) techniques, we have successfully prepared high-quality 1 UC FeSe films on anatase TiO2(001) formed onSrTiO3. In situ scanning tunneling spectroscopy (STS) reveals large superconducting gap (Δ) ranging from 17 meV to 22 meV, which is nearly one order of magnitude larger than Δ = 2.2 meV of bulk FeSe with Tc = 9.4 K, indicating the signature of high-Tc superconductivity. The superconductivity of this heterostructure system is further verified by imaging vortex lattice under external magnetic field. By examining the distinct properties of anatase TiO2 films from SrTiO3, as well as their influences on superconductivity, we will discuss about the possible pairing mechanism of this system. Together with our previous work of 1 UC FeSe/SrTiO3 [1,2], this work demonstrates that interface engineering is a powerful way to fabricate new high-Tc superconductors and investigate the mechanism of high-Tc superconductivity.

**References**


12:27PM Z51.00003 Tuning the superconductivity in single-layer FeSe/oxides by interface engineering , RUI PENG, State Key Laboratory of Surface Physics, Department of Physics, Fudan University — The discovery of high Tc in single-layer FeSe films has enormous implications for both searching new high Tc superconductors and exploring the important factors for high temperature superconductivity. In this talk, I will present our recent angle-resolved photoemission studies on various FeSe-based heterostructures grown by molecular beam epitaxy. We systematically studied the electronic structures and superconducting properties of FeSe with varied strain, different interfacial oxide materials and different thicknesses, and uncovered that electronic correlations and superconducting gap-closing temperatures are tuned by interfacial effects. We exclude the direct relation between superconductivity and tensile strain, or the energy of an interfacial phonon mode, and demonstrate the crucial and non-trivial role of FeSe/oxide interface on the high pairing temperature. By tuning the interface, superconducting pairing temperature reaches up to 75K in FeSe/Nb:BaTiO3/KTaO3 with the in-plane lattice of 3.99 Å, which sets a new superconducting-gap-closing temperature record for iron-based superconductors, and may paves the way to more cost-effective applications of ultra-thin superconductors. Besides, in extremely tensile-strained single-layer FeSe films, we found that the Fermi surfaces consist of two elliptical electron pockets at the zone corner, without detectable hybridization. The lifting of degeneracy is clearly observed for the first time for the iron-based superconductors with only electron Fermi surfaces. Intriguingly, the superconducting gap distribution is anisotropic but nodeless around the electron pockets with minima at the crossings of the two pockets. Our results provide important experimental foundations for understanding the interfacial superconductivity and the pairing symmetry puzzle of iron-based superconductors, and also provide clues for further enhancing Tc through interface engineering.
1:03PM Z51.00004 First-principles study of the electron/spin-phonon interaction in compressed FeSe crystal and FeSe/STO system, ZHONG-YI LU, Department of Physics, Renmin University of China — By using the first-principles calculations with van der Waals corrections, we have studied the electronic structures, lattice dynamics, and magnetic properties of crystal FeSe under hydrostatic pressure [1] and FeSe/STO system [2,3]. For bulk FeSe, the frequency of all optical phonon modes increase with pressure. In a range between 5 and 6 GPa, the frequency of the A_1g mode, which related to the Se height from the Fe-Fe plane, shows a sudden jump. This is also the pressure range within which the highest superconducting transition temperature Tc of FeSe is reached in experiments. In comparison with the other phonon modes, the zero-point atomic displacement of the A_1g mode also induces the strongest variation of local magnetic moment on Fe, which reaches the maximum around 5 GPa. These results suggest that the effect of phonon via spin-phonon coupling could not be omitted. For monolayer FeSe epitaxial film on SrTiO_3, the combined effect of electron doping and phonon readily leads to magnetic frustration between the collinear antiferromagnetic state and checkerboard antiferromagnetic Neel state. For bilayer FeSe epitaxial film on SrTiO_3, such a magnetic frustration is much easier induced by electron doping in its bottom layer than its top layer. The underlying physics is that the doped electrons are accumulated at the interface between the FeSe layers and the substrate. These results are consistent with the existing experimental studies. [1] Q.-Q. Ye, K. Liu, and Z.-Y. Lu, Influence of spin-phonon coupling on antiferromagnetic spin fluctuations in FeSe under pressure. First-principles calculations with van der Waals corrections. Phys. Rev. B 88, 205130 (2013). [2] K. Liu, Z.-Y. Lu, and T. Xiang, Atomic and electronic structures of FeSe monolayer and bilayer thin films on SrTiO_3 (001): First-principles study. Phys. Rev. B 85, 235123 (2012). [3] K. Liu, B.-J. Zhang, and Z.-Y. Lu, First-principles study of magnetic frustration in FeSe epitaxial films on SrTiO_3. Submitted.

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1:39PM Z51.00005 Density Functional Plus Dynamical Mean Field Theory of Correlated Oxides, ANDREW MILLIS, Columbia University — The density functional plus dynamical mean field method is outlined and a few recent successes including applications to spin crossover molecules, oxide superlattices and metal-insulator transitions in bulk transition metals are outlined. Insights from the method into the essential role played by lattice distortion (both rotations and bond length changes) in determining the phase diagrams of correlated materials are presented. The key theoretical issue of the double counting correction is outlined, different approaches are compared, and a connection to the energy level differences between strongly and weakly correlated orbitals is presented. Charge transfer across oxide interfaces shown to depend crucially on the double counting correction, suggesting that experiments on oxide superlattices may provide insights into this important problem. Future directions are discussed. This work is performed in collaboration with Jia Chen, Hung Dang, Hyowon Park and Chris Marianetti.

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Friday, March 6, 2015 11:15AM - 2:15PM — Session Z53 DCOMP: Invited Session: Thermal Transport: Modelling and Ab Initio Calculations Grand Ballroom C3 - Matthias Scheffler, Fritz-Haber, Berlin, Germany

11:15AM Z53.00001 Interfacial Heat Conduction in Modern Semiconductor Nanostructures, KENNETH GOODSON, Stanford University — Heat conduction through interfaces in electronic nanostructures grows more important with the dimensional scaling trends throughout the semiconductor industry. The complexity of interfacial transport has increased owing to frequent examples of severe lattice mismatch and strain, boundaries with nanoscale planar-features and, in some cases, the critical role of electron-phonon interactions. This talk will describe measurements and modeling of phonon heat conduction through interfaces in some of the latest semiconductor nanotechnologies and feature a range of material combinations. Examples include GaN-diamond and silicon-diamond composites, chalcogenide-metal multilayers, metal-semiconductor nanolayer stacks, and nonplanar interfaces in modern nanotransistors and interconnect structures. Applications range from conventional CMOS electronics and phase change memory to quantum cascade lasers and RF amplifiers for satellites.

11:51AM Z53.00002 Phonon hydrodynamics in two-dimensional materials, NICOLA MARZARI, Ecole Polytechnique Federale de Lausanne (EPFL) — The conduction of heat in two dimensions displays a wealth of fascinating phenomena of key relevance to the scientific and technological applications of novel layered materials. Here, we use third order density-functional perturbation theory and an exact, variational solution of the Boltzmann transport equation to study fully from first-principles phonon transport and heat conductivity in graphene and related materials (boron nitride, functionalized derivatives, transition-metal dichalcogenides...). Very good agreement is obtained with experimental data, where available, together with a microscopic understanding of the collective character of heat-carrying excitations, and the unusual length scales involved. Last, and at variance with typical three-dimensional solids, normal processes dominate over Umklapp scattering well above cryogenic conditions, extending to room temperature and more. As a result, novel hydrodynamics regimes, hitherto typically confined to ultra-low temperatures, become readily apparent.

Work done in collaboration with Andrea Cepellotti, Giorgia Fugallo, Lorenzo Paulatto, Michele Lazzieri, and Francesco Mauri.

12:27PM Z53.00003 Accurate Thermal Conductivities from First Principles, CHRISTIAN CARBONO, Fritz-Haber-Institut der MPG — In spite of significant research efforts, a first-principles determination of the thermal conductivity at high temperatures has remained elusive. On the one hand, Boltzmann transport technique include anharmonic effects in the nuclear dynamics only perturbatively become inaccurate or inapplicable under such conditions. On the other hand, non-equilibrium molecular dynamics (MD) methods suffer from enormous finite-size artifacts in the computationally feasible supercells, which prevent an accurate extrapolation to the bulk limit of the thermal conductivity. In this work, we overcome this limitation by performing ab initio MD simulations in thermodynamic equilibrium that account for all orders of anharmonicity. The thermal conductivity is then assessed from the auto-correlation function of the heat flux using the Green-Kubo formalism. Foremost, we discuss the fundamental theory underlying a first-principles definition of the heat flux using the virial theorem. We validate our approach and in particular the techniques developed to overcome finite time and size effects, e.g., by inspecting silicon, the thermal conductivity of which is particularly challenging to converge. Furthermore, we use this framework to quantify the degree of anharmonicity expectation on the heat resistance mechanism active in this material, which eventually allows us to discuss how the thermal conductivity can be controlled by doping and co-doping.

This work has been performed in collaboration with R. Ramprasad (University of Connecticut), C. G. Levi and C. G. Van de Walle (University of California Santa Barbara).

1Work supported by National Natural Science Foundation of China (Grants No. 11004243 and No. 11190024), National Program for Basic Research of MOST of China (Grant No. 2011CBAA00112).

1:03PM Z53.00004 Modeling and Ab initio Calculations of Thermal Transport in Si-Based Clathrates and Solar Perovskites\(^1\), YUPING HE, University of California, Davis — We present calculations of the thermal transport coefficients of Si-based clathrates [1,2] and solar perovskites [3], as obtained from ab initio calculations and models, where all input parameters derived from first principles. We elucidated the physical mechanisms responsible for the measured low thermal conductivity in Si-based clathrates [1] and predicted their electronic properties and mobilities, which were later confirmed experimentally [2]. We also predicted that by appropriately tuning the carrier concentration, the thermoelectric figure of merit of Sn and Pb based perovskites may reach values ranging between 1 and 2, which could possibly be further increased by optimizing the lattice thermal conductivity through engineering perovskite superlattices.

\(^1\)Work done in collaboration with Prof. G. Galli, and supported by DOE/BES grant No. DE-FG0206ER46262


1:39PM Z53.00005 The Importance of Complex Electronic Structures in Thermoelectric Materials\(^1\), DAVID SINGH, Oak Ridge National Laboratory — Thermoelectric performance as characterized by the figure of merit, ZT, is a counter-indicated property of matter, meaning that high ZT depends on a combination of transport properties that do not generally occur together. A particularly important conundrum in thermoelectrics is the requirements for simultaneously having high electrical conductivity and high thermopower. I will argue that the resolution of this conundrum is through complex band structures and discuss how these arise in various known and predicted high performance thermoelectric materials.

\(^1\)This work was done in collaboration with David Parker, Mao-Hua Du, Xin Chen and Hongliang Shi. We are grateful for support from the Department of Energy, through the Office of Basic Energy Sciences, S3TEC Energy Frontier Research Center and the Materials